



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 12:35 PM JST

PDB ID : 9JE3 / pdb_00009je3
Title : Structure of #2-911 Fab in complex with MEDI8852 Fab
Authors : Itou, H.; Sano, K.; Ainai, A.; Suzuki, T.
Deposited on : 2024-09-02
Resolution : 2.37 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:

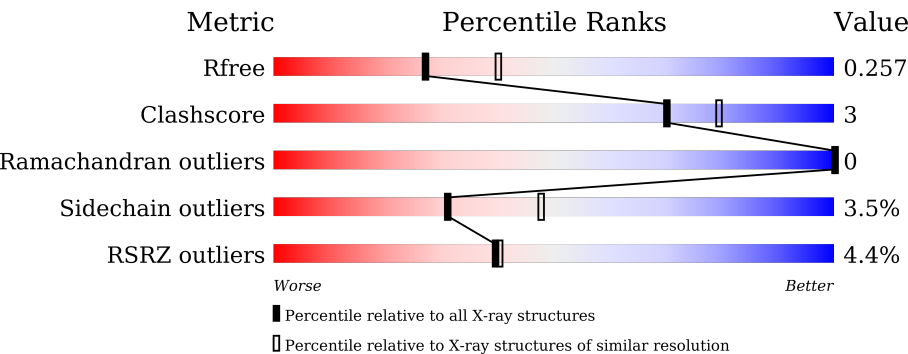
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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	217	<div><div>4%</div><div>88%</div><div>11%</div><div>.</div></div>
1	E	217	<div><div>9%</div><div>82%</div><div>17%</div><div>.</div></div>
2	B	215	<div><div>2%</div><div>90%</div><div>10%</div><div>.</div></div>
2	F	215	<div><div>9%</div><div>89%</div><div>9%</div><div>.</div></div>
3	C	228	<div><div>5%</div><div>86%</div><div>14%</div><div>.</div></div>
3	G	228	<div><div>4%</div><div>92%</div><div>7%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
4	D	210	 93% 7%
4	H	210	 90% 9% 2%
5	I	2	 50% 50%
5	J	2	 100%
5	X	2	 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13553 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 #2-911 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	217	Total	C	N	O	S	0	0	0
			1639	1044	259	328	8			
1	A	217	Total	C	N	O	S	0	0	0
			1639	1044	259	328	8			

- Molecule 2 is a protein called #2-911 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	214	Total	C	N	O	S	0	0	0
			1618	1010	273	328	7			
2	B	215	Total	C	N	O	S	0	0	0
			1624	1013	274	330	7			

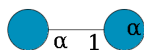
- Molecule 3 is a protein called MEDI8852 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	228	Total	C	N	O	S	0	0	0
			1722	1084	290	342	6			
3	C	228	Total	C	N	O	S	0	0	0
			1722	1084	290	342	6			

- Molecule 4 is a protein called MEDI8852 Fab light chain.

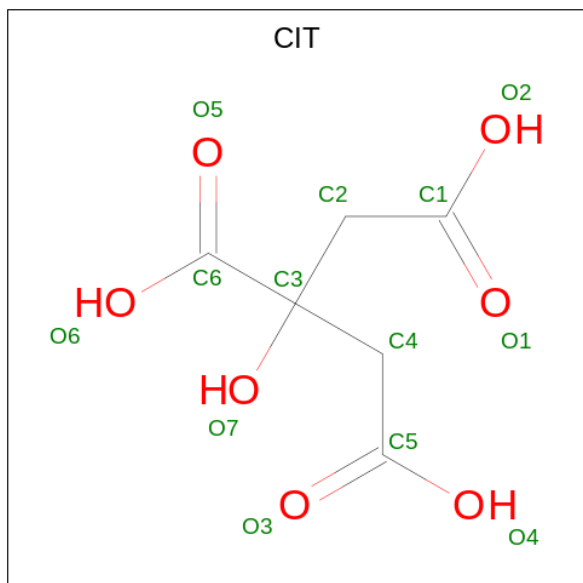
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	210	Total	C	N	O	S	0	0	0
			1608	998	275	329	6			
4	D	210	Total	C	N	O	S	0	0	0
			1608	998	275	329	6			

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	X	2	Total	C	O	0	0	0
			23	12	11			
5	I	2	Total	C	O	0	0	0
			23	12	11			
5	J	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			13	6	7		
6	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	31	Total	O	0	0
			31	31		
7	F	36	Total	O	0	0
			36	36		

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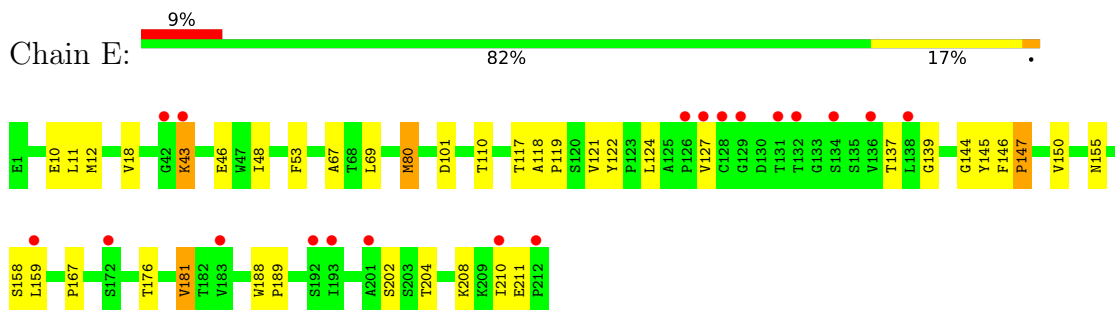
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	33	Total 33	O 33	0	0
7	H	37	Total 37	O 37	0	0
7	A	33	Total 33	O 33	0	0
7	B	46	Total 46	O 46	0	0
7	C	35	Total 35	O 35	0	0
7	D	27	Total 27	O 27	0	0

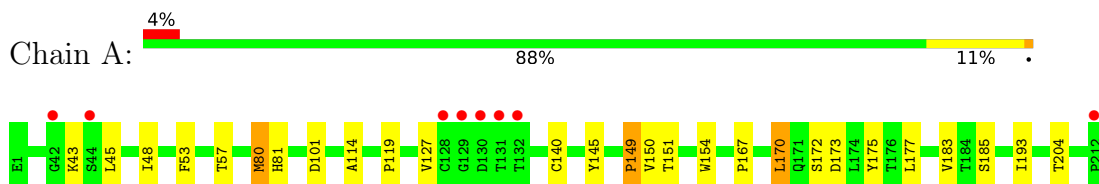
3 Residue-property plots

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.

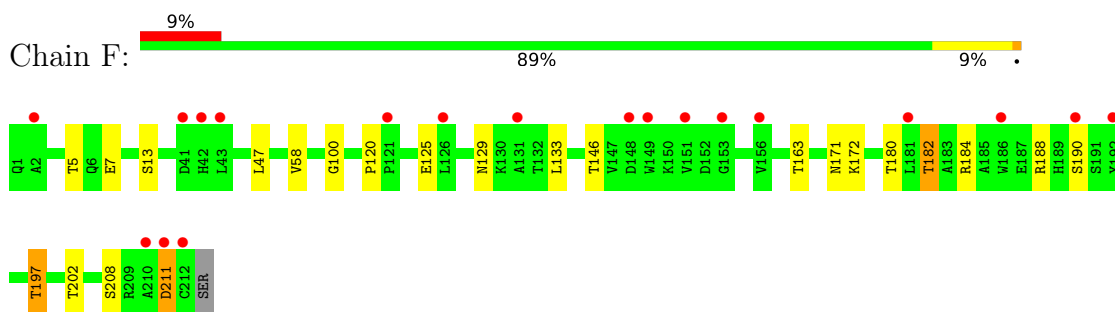
- Molecule 1: #2-911 Fab heavy chain



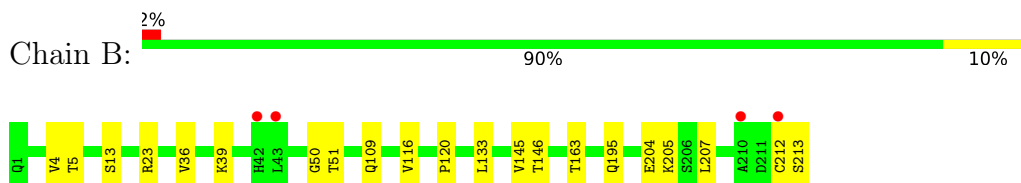
- Molecule 1: #2-911 Fab heavy chain



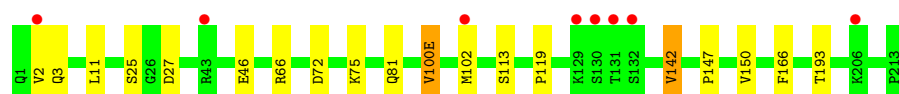
- Molecule 2: #2-911 Fab light chain



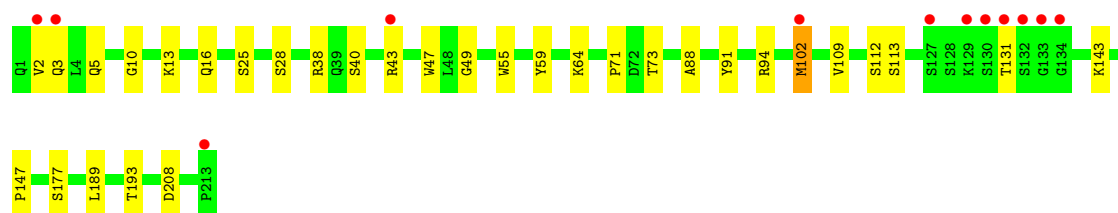
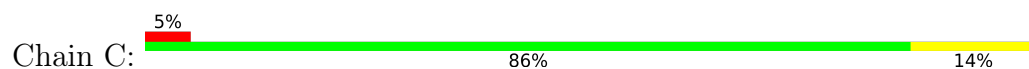
- Molecule 2: #2-911 Fab light chain



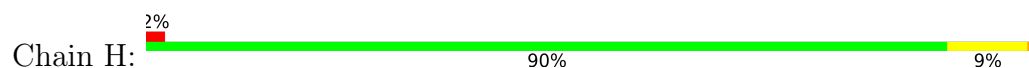
- Molecule 3: MEDI8852 Fab heavy chain



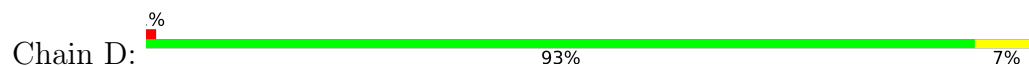
- Molecule 3: MEDI8852 Fab heavy chain



- Molecule 4: MEDI8852 Fab light chain



- Molecule 4: MEDI8852 Fab light chain



- Molecule 5: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



- Molecule 5: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



- Molecule 5: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.28Å 151.11Å 176.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.37 48.43 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.43-2.37) 99.9 (48.43-2.37)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.37Å)	Xtrriage
Refinement program	REFMAC v5.8.0425	Depositor
R, R_{free}	0.200 , 0.254 0.204 , 0.257	Depositor DCC
R_{free} test set	4705 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13553	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6423e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CIT, GLC

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	0.60	0/1686	0.99	6/2305 (0.3%)
1	E	0.62	0/1686	0.98	4/2305 (0.2%)
2	B	0.64	0/1662	1.06	2/2272 (0.1%)
2	F	0.62	0/1656	1.03	2/2264 (0.1%)
3	C	0.63	0/1766	1.02	1/2415 (0.0%)
3	G	0.63	0/1766	1.04	3/2415 (0.1%)
4	D	0.64	0/1641	1.05	2/2224 (0.1%)
4	H	0.65	0/1641	1.11	3/2224 (0.1%)
All	All	0.63	0/13504	1.04	23/18424 (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
3	G	0	1
4	D	0	1
4	H	0	2
All	All	0	4

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	100(E)	VAL	N-CA-CB	-8.86	100.65	112.16
2	F	182	THR	CA-CB-OG1	-6.97	99.14	109.60
1	A	53	PHE	CA-CB-CG	-6.95	106.85	113.80
4	H	20	THR	CA-CB-OG1	-6.30	100.14	109.60
1	E	101	ASP	CA-CB-CG	6.22	118.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	17	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	101	ASP	CA-CB-CG	5.89	118.49	112.60
3	C	208	ASP	CA-CB-CG	5.82	118.42	112.60
4	H	161	GLU	N-CA-CB	-5.76	101.52	111.55
4	D	85	THR	CA-CB-OG1	-5.75	100.97	109.60
3	G	27	ASP	CA-CB-CG	5.68	118.28	112.60
2	B	5	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	57	THR	CA-CB-OG1	-5.56	101.26	109.60
1	A	80	MET	CG-SD-CE	-5.46	88.89	100.90
1	E	46	GLU	N-CA-CB	-5.45	101.66	110.81
2	F	211	ASP	CA-CB-CG	5.41	118.01	112.60
3	G	46	GLU	N-CA-CB	-5.33	102.74	110.84
4	D	27	GLN	CB-CA-C	-5.20	98.87	109.94
1	A	177	LEU	N-CA-CB	-5.13	102.62	111.55
1	E	80	MET	CG-SD-CE	-5.12	89.63	100.90
1	E	53	PHE	CA-CB-CG	-5.09	108.71	113.80
2	B	109	GLN	CB-CA-C	5.08	116.92	110.22
1	A	149	PRO	N-CA-CB	-5.07	97.02	102.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	54	ARG	Sidechain
3	G	66	ARG	Sidechain
4	H	211	ARG	Sidechain
4	H	54	ARG	Sidechain

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	1639	0	1587	11	0
1	E	1639	0	1587	24	0
2	B	1624	0	1564	9	0
2	F	1618	0	1559	12	0
3	C	1722	0	1675	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1722	0	1675	9	0
4	D	1608	0	1562	6	0
4	H	1608	0	1562	11	0
5	I	23	0	21	0	0
5	J	23	0	21	3	0
5	X	23	0	21	0	0
6	A	13	0	5	0	0
6	H	13	0	5	0	0
7	A	33	0	0	1	0
7	B	46	0	0	0	0
7	C	35	0	0	0	0
7	D	27	0	0	0	0
7	E	31	0	0	0	0
7	F	36	0	0	0	0
7	G	33	0	0	0	0
7	H	37	0	0	1	0
All	All	13553	0	12844	86	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 (86) 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:D:149:LYS:NZ	4:D:195:GLU:OE2	2.18	0.77
2:B:212:CYS:O	2:B:213:SER:C	2.42	0.61
3:C:59:TYR:HB2	3:C:64:LYS:HG3	1.82	0.60
1:E:127:VAL:CG2	2:F:211:ASP:HB3	2.31	0.59
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.85	0.58
1:A:81:HIS:HD2	7:A:409:HOH:O	1.88	0.57
4:H:190:LYS:NZ	4:H:210:ASN:HB3	2.20	0.56
3:C:143:LYS:HA	3:C:177:SER:HB2	1.87	0.56
3:C:2:VAL:HG21	3:C:94:ARG:HH12	1.70	0.56
3:C:10:GLY:O	3:C:109:VAL:HA	2.06	0.56
1:E:144:GLY:H	1:E:176:THR:HG22	1.70	0.56
4:H:186:TYR:O	4:H:192:TYR:OH	2.23	0.56
2:F:146:THR:HB	2:F:197:THR:OG1	2.06	0.55
1:E:167:PRO:HG2	2:F:163:THR:HB	1.88	0.55
1:E:118:ALA:HB1	1:E:204:THR:HG21	1.89	0.54
3:C:3:GLN:HE21	3:C:5:GLN:HB2	1.72	0.54
1:E:69:LEU:HD21	1:E:80:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:HG21	1:A:80:MET:HE1	1.91	0.53
4:D:182:SER:HB3	5:J:2:GLC:H62	1.90	0.53
1:E:155:ASN:O	1:E:158:SER:OG	2.24	0.52
2:B:120:PRO:HA	2:B:133:LEU:HD23	1.91	0.51
2:B:116:VAL:O	2:B:205:LYS:HE2	2.11	0.51
2:F:184:ARG:O	2:F:188:ARG:HG2	2.11	0.50
1:E:11:LEU:HD12	1:E:110:THR:HB	1.93	0.50
4:D:175:LEU:C	4:D:175:LEU:HD23	2.36	0.50
2:B:195:GLN:HE21	2:B:204:GLU:CD	2.20	0.50
1:E:121:VAL:HG12	1:E:208:LYS:HD2	1.94	0.50
1:E:124:LEU:HB2	1:E:139:GLY:C	2.37	0.50
3:C:102:MET:HA	3:C:102:MET:HE3	1.94	0.50
1:E:159:LEU:HD21	1:E:181:VAL:HG11	1.93	0.49
1:E:137:THR:HA	1:E:181:VAL:O	2.12	0.49
1:A:183:VAL:HG11	1:A:193:ILE:HD11	1.95	0.49
3:C:2:VAL:HG21	3:C:94:ARG:NH1	2.27	0.49
4:H:89:GLN:HG2	4:H:90:GLN:N	2.28	0.49
1:E:202:SER:OG	1:E:204:THR:HG22	2.14	0.48
1:E:127:VAL:HG21	2:F:211:ASP:HB3	1.95	0.47
4:H:12:SER:HA	4:H:105:GLU:O	2.14	0.47
1:E:127:VAL:HG22	2:F:211:ASP:HB3	1.95	0.47
2:F:129:ASN:O	2:F:129:ASN:CG	2.58	0.46
2:B:120:PRO:HB3	2:B:207:LEU:HD21	1.98	0.46
3:C:91:TYR:CE1	4:D:43:ALA:HB2	2.51	0.46
1:A:48:ILE:HG21	1:A:80:MET:CE	2.46	0.45
3:G:2:VAL:HA	3:G:25:SER:O	2.17	0.45
3:C:13:LYS:HB2	3:C:16:GLN:NE2	2.32	0.45
5:J:1:GLC:O2	5:J:2:GLC:H1	2.16	0.45
3:C:131:THR:HA	3:C:189:LEU:HD12	1.99	0.45
4:H:25:THR:O	4:H:69:THR:HB	2.17	0.45
1:A:140:CYS:HB2	1:A:154:TRP:CH2	2.52	0.45
1:E:118:ALA:CB	1:E:204:THR:HG21	2.47	0.44
3:G:119:PRO:HB2	3:G:142:VAL:HG12	1.98	0.44
2:F:47:LEU:HA	2:F:58:VAL:HG21	1.99	0.44
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.98	0.44
3:C:55:TRP:CE3	3:C:71:PRO:HG3	2.53	0.44
1:E:10:GLU:HG2	1:E:18:VAL:CG2	2.48	0.43
1:E:12:MET:HE2	1:E:18:VAL:HB	2.00	0.43
2:F:197:THR:HG22	2:F:202:THR:OG1	2.17	0.43
1:A:167:PRO:HG2	2:B:163:THR:HB	1.99	0.43
3:C:38:ARG:NH2	3:C:43:ARG:NH1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:SER:H	5:J:2:GLC:C6	2.31	0.43
3:G:72:ASP:OD2	3:G:75:LYS:HD2	2.18	0.43
3:C:47:TRP:CH2	3:C:49:GLY:HA2	2.54	0.43
3:G:3:GLN:CD	3:C:3:GLN:HB2	2.44	0.43
3:G:119:PRO:CB	3:G:142:VAL:HG12	2.49	0.43
2:B:50:GLY:O	2:B:51:THR:HB	2.19	0.43
1:E:48:ILE:HG21	1:E:80:MET:HE1	2.00	0.43
3:G:102:MET:HE3	3:G:102:MET:HA	2.01	0.43
1:A:114:ALA:HB2	1:A:173:ASP:HB3	2.00	0.43
1:E:67:ALA:HB1	1:E:80:MET:HE2	2.01	0.42
4:H:190:LYS:HZ1	4:H:210:ASN:HB3	1.82	0.42
3:C:40:SER:HB3	3:C:88:ALA:HB2	2.01	0.42
1:A:172:SER:O	1:A:173:ASP:HB2	2.18	0.42
2:B:4:VAL:HA	2:B:23:ARG:O	2.19	0.42
1:A:127:VAL:HG11	2:B:207:LEU:HD11	2.00	0.42
1:A:170:LEU:HD23	1:A:175:TYR:CE1	2.55	0.42
3:G:166:PHE:CE1	4:H:164:THR:HG23	2.55	0.41
1:E:146:PHE:HA	1:E:147:PRO:HA	1.81	0.41
1:E:188:TRP:CG	1:E:189:PRO:HA	2.56	0.41
3:G:11:LEU:HB2	3:G:147:PRO:HG3	2.02	0.41
1:E:122:TYR:CE2	2:F:125:GLU:HG3	2.55	0.41
4:H:142:ARG:HD2	4:H:173:TYR:CE1	2.55	0.41
1:E:43:LYS:HD3	2:F:100:GLY:O	2.21	0.40
2:F:120:PRO:HA	2:F:133:LEU:HD23	2.02	0.40
4:D:47:LEU:HD21	4:D:62:PHE:CD2	2.56	0.40
4:H:105:GLU:HB3	7:H:426:HOH:O	2.22	0.40
3:G:100(E):VAL:HG13	4:H:34:HIS:CE1	2.56	0.40
4:H:54:ARG:HD2	4:H:58:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
1	E	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
2	B	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	F	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
3	C	226/228 (99%)	218 (96%)	8 (4%)	0	100	100
3	G	226/228 (99%)	218 (96%)	8 (4%)	0	100	100
4	D	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
4	H	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
All	All	1723/1740 (99%)	1662 (96%)	61 (4%)	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	188/188 (100%)	180 (96%)	8 (4%)	25	39
1	E	188/188 (100%)	181 (96%)	7 (4%)	29	45
2	B	182/182 (100%)	177 (97%)	5 (3%)	40	58
2	F	181/182 (100%)	171 (94%)	10 (6%)	18	28
3	C	198/198 (100%)	190 (96%)	8 (4%)	27	42
3	G	198/198 (100%)	193 (98%)	5 (2%)	42	61
4	D	185/185 (100%)	180 (97%)	5 (3%)	40	58
4	H	185/185 (100%)	181 (98%)	4 (2%)	47	65
All	All	1505/1506 (100%)	1453 (96%)	52 (4%)	31	48

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	43	LYS
1	E	117	THR

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Mol	Chain	Res	Type
1	E	147	PRO
1	E	150	VAL
1	E	181	VAL
1	E	210	ILE
1	E	211	GLU
2	F	5	THR
2	F	7	GLU
2	F	13	SER
2	F	171	ASN
2	F	172	LYS
2	F	180	THR
2	F	182	THR
2	F	190	SER
2	F	197	THR
2	F	208	SER
3	G	81	GLN
3	G	113	SER
3	G	142	VAL
3	G	150	VAL
3	G	193	THR
4	H	20	THR
4	H	145	LYS
4	H	168	SER
4	H	211	ARG
1	A	43	LYS
1	A	45	LEU
1	A	149	PRO
1	A	150	VAL
1	A	151	THR
1	A	170	LEU
1	A	185	SER
1	A	204	THR
2	B	13	SER
2	B	36	VAL
2	B	39	LYS
2	B	145	VAL
2	B	146	THR
3	C	25	SER
3	C	28	SER
3	C	73	THR
3	C	102	MET
3	C	112	SER

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Mol	Chain	Res	Type
3	C	113	SER
3	C	147	PRO
3	C	193	THR
4	D	48	ILE
4	D	103	LYS
4	D	114	SER
4	D	154	LEU
4	D	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	GLN
1	E	164	HIS
2	F	37	GLN
2	F	79	GLN
4	H	90	GLN
4	H	210	ASN
1	A	41	HIS
2	B	53	ASN
3	C	3	GLN
3	C	5	GLN
3	C	39	GLN
3	C	57	ASN
3	C	70	ASN
4	D	38	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	$\# Z > 2$
5	GLC	I	1	5	11,11,12	0.28	0	15,15,17	1.08	0
5	GLC	I	2	5	12,12,12	0.31	0	17,17,17	1.13	1 (5%)
5	GLC	J	1	5	11,11,12	0.26	0	15,15,17	1.09	1 (6%)
5	GLC	J	2	5	12,12,12	0.27	0	17,17,17	1.94	6 (35%)
5	GLC	X	1	5	11,11,12	0.31	0	15,15,17	0.57	0
5	GLC	X	2	5	12,12,12	0.25	0	17,17,17	1.06	1 (5%)

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	GLC	I	1	5	-	0/2/19/22	0/1/1/1
5	GLC	I	2	5	-	0/2/22/22	0/1/1/1
5	GLC	J	1	5	-	0/2/19/22	0/1/1/1
5	GLC	J	2	5	-	2/2/22/22	0/1/1/1
5	GLC	X	1	5	-	0/2/19/22	0/1/1/1
5	GLC	X	2	5	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2	GLC	O1-C1-C2	4.08	120.52	109.03
5	J	2	GLC	C3-C4-C5	-3.31	104.33	110.24
5	J	2	GLC	O4-C4-C3	2.97	117.21	110.35
5	X	2	GLC	O2-C2-C3	-2.50	104.57	110.35
5	J	2	GLC	O2-C2-C3	-2.39	104.82	110.35
5	J	2	GLC	O2-C2-C1	2.32	114.53	109.16
5	I	2	GLC	C3-C4-C5	-2.22	106.29	110.24
5	J	2	GLC	O5-C1-C2	-2.16	106.43	110.28
5	J	1	GLC	C1-C2-C3	2.13	112.28	109.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

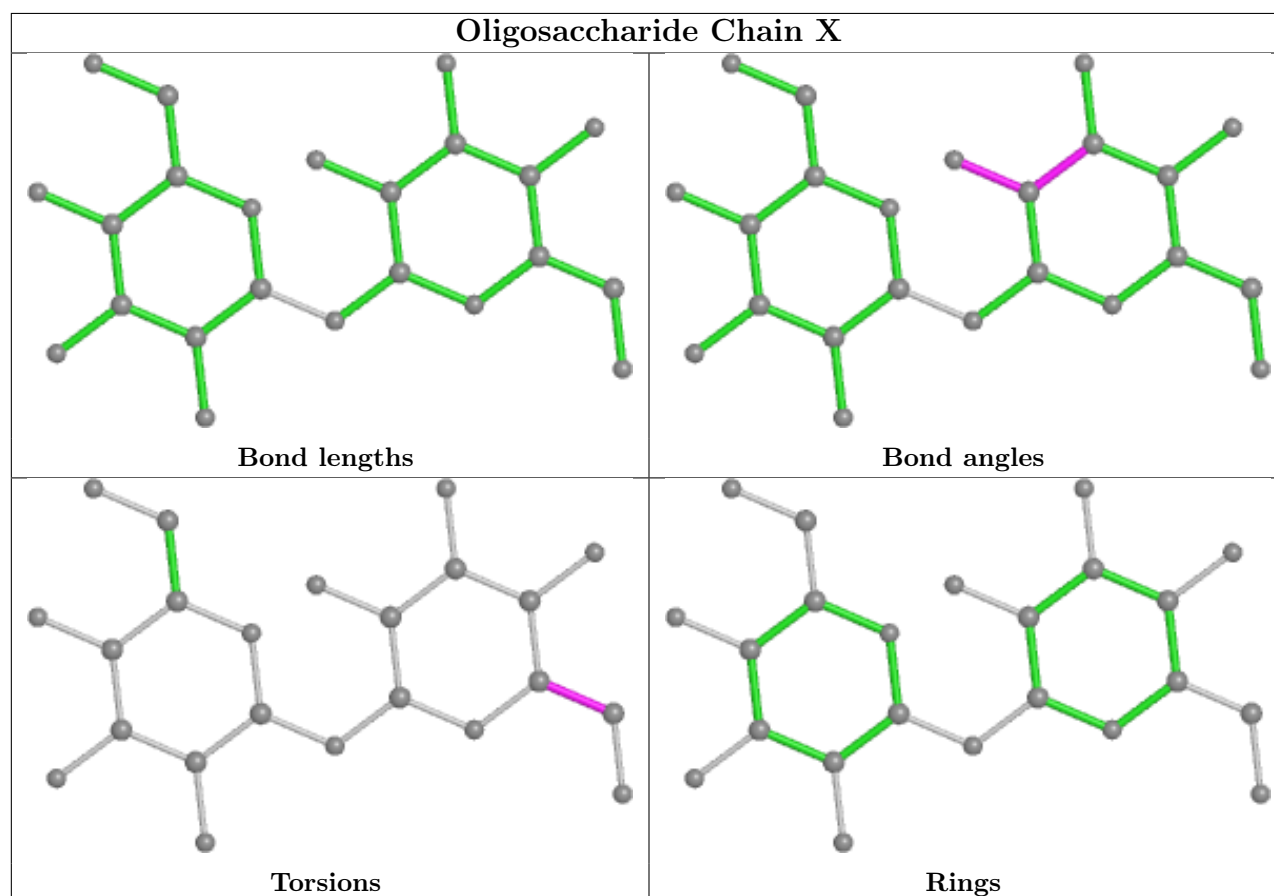
Mol	Chain	Res	Type	Atoms
5	J	2	GLC	O5-C5-C6-O6
5	X	2	GLC	O5-C5-C6-O6
5	J	2	GLC	C4-C5-C6-O6
5	X	2	GLC	C4-C5-C6-O6

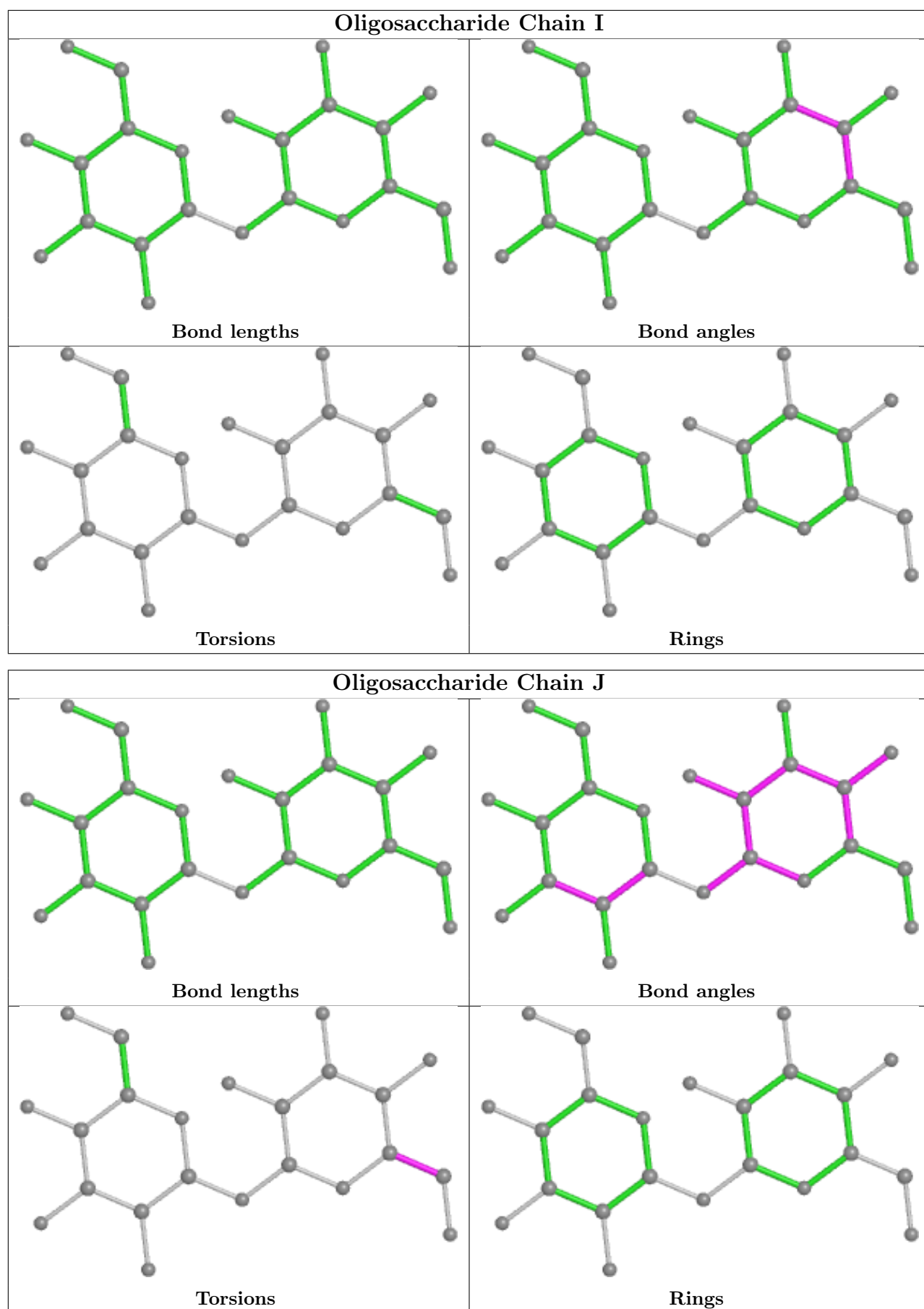
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2	GLC	3	0
5	J	1	GLC	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

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
6	CIT	A	301	-	12,12,12	1.28	1 (8%)	17,17,17	1.44	2 (11%)
6	CIT	H	301	-	12,12,12	1.44	1 (8%)	17,17,17	1.53	2 (11%)

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	CIT	A	301	-	-	12/16/16/16	-
6	CIT	H	301	-	-	5/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	301	CIT	C3-C6	3.81	1.57	1.53
6	A	301	CIT	C3-C6	2.70	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	CIT	O5-C6-C3	-3.64	117.09	122.25
6	H	301	CIT	O6-C6-C3	3.34	118.84	113.05
6	H	301	CIT	O5-C6-C3	-3.24	117.67	122.25
6	A	301	CIT	O6-C6-C3	2.94	118.16	113.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	301	CIT	O7-C3-C6-O5
6	H	301	CIT	O7-C3-C6-O6
6	H	301	CIT	C4-C3-C6-O5
6	H	301	CIT	C4-C3-C6-O6
6	A	301	CIT	C1-C2-C3-O7
6	A	301	CIT	C1-C2-C3-C4
6	A	301	CIT	C1-C2-C3-C6
6	A	301	CIT	O7-C3-C6-O5
6	A	301	CIT	O7-C3-C6-O6
6	A	301	CIT	C4-C3-C6-O6
6	A	301	CIT	C4-C3-C6-O5
6	H	301	CIT	O7-C3-C4-C5
6	A	301	CIT	C2-C3-C6-O6
6	A	301	CIT	C6-C3-C4-C5
6	A	301	CIT	O7-C3-C4-C5
6	A	301	CIT	C2-C3-C4-C5
6	A	301	CIT	C2-C3-C6-O5

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

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	217/217 (100%)	0.13	8 (3%) 45 46	30, 52, 93, 155	0
1	E	217/217 (100%)	0.56	19 (8%) 17 17	28, 62, 119, 158	0
2	B	215/215 (100%)	-0.12	4 (1%) 66 65	28, 44, 73, 116	0
2	F	214/215 (99%)	0.34	19 (8%) 17 17	30, 48, 99, 126	0
3	C	228/228 (100%)	0.14	12 (5%) 33 33	33, 50, 89, 172	0
3	G	228/228 (100%)	0.11	8 (3%) 47 48	32, 49, 83, 169	0
4	D	210/210 (100%)	-0.12	3 (1%) 73 72	30, 44, 67, 124	0
4	H	210/210 (100%)	-0.03	4 (1%) 66 65	29, 46, 72, 125	0
All	All	1739/1740 (99%)	0.13	77 (4%) 39 40	28, 48, 99, 172	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	130	SER	7.2
4	H	214	CYS	6.9
3	G	131	THR	5.8
1	E	212	PRO	5.7
3	C	131	THR	4.8
4	H	1	ASP	4.5
3	G	129	LYS	4.1
3	C	133	GLY	4.0
4	D	2	ILE	3.7
3	C	132	SER	3.7
1	E	172	SER	3.6
3	G	2	VAL	3.6
1	A	44	SER	3.6
1	A	128	CYS	3.6
1	E	210	ILE	3.5
1	A	42	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	186	TRP	3.3
3	C	129	LYS	3.3
2	B	212	CYS	3.2
1	A	130	ASP	3.1
1	A	131	THR	3.1
1	A	132	THR	3.1
1	E	132	THR	3.0
1	E	42	GLY	3.0
1	E	193	ILE	3.0
4	D	214	CYS	3.0
4	D	1	ASP	2.9
1	E	128	CYS	2.9
1	E	127	VAL	2.9
1	E	131	THR	2.8
2	B	43	LEU	2.8
3	G	132	SER	2.8
1	A	129	GLY	2.8
2	F	211	ASP	2.7
3	C	2	VAL	2.7
3	C	213	PRO	2.7
1	E	126	PRO	2.6
2	F	121	PRO	2.6
2	F	181	LEU	2.6
2	B	42	HIS	2.6
3	C	134	GLY	2.5
1	E	138	LEU	2.5
1	E	129	GLY	2.5
4	H	2	ILE	2.5
3	C	127	SER	2.5
3	G	102	MET	2.5
2	F	148	ASP	2.4
1	E	183	VAL	2.4
3	C	43	ARG	2.4
1	A	212	PRO	2.4
2	F	212	CYS	2.4
1	E	43	LYS	2.4
2	F	210	ALA	2.3
2	F	41	ASP	2.3
2	B	210	ALA	2.3
2	F	2	ALA	2.2
3	G	43	ARG	2.2
1	E	136	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	159	LEU	2.2
2	F	151	VAL	2.2
3	C	3	GLN	2.2
2	F	190	SER	2.2
2	F	153	GLY	2.2
3	C	102	MET	2.2
2	F	42	HIS	2.1
1	E	192	SER	2.1
2	F	126	LEU	2.1
1	E	134	SER	2.1
3	G	130	SER	2.1
2	F	43	LEU	2.1
4	H	213	GLU	2.1
3	G	206	LYS	2.1
1	E	201	ALA	2.1
2	F	131	ALA	2.1
2	F	192	TYR	2.0
2	F	149	TRP	2.0
2	F	156	VAL	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](#)

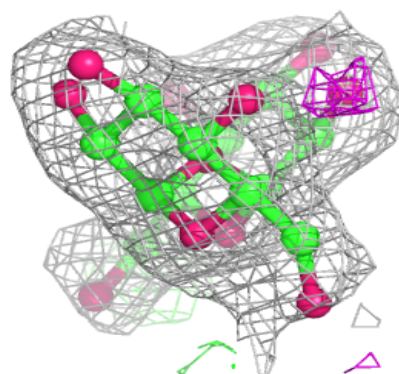
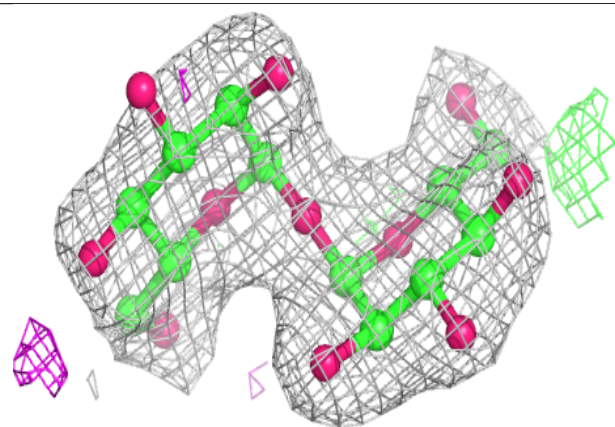
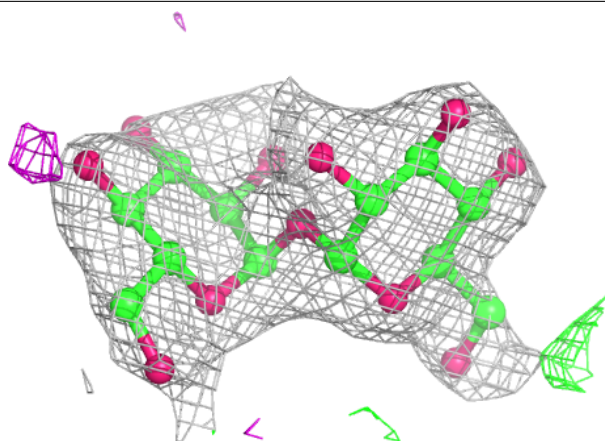
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GLC	X	1	11/12	-	-	56,72,85,88	0
5	GLC	X	2	12/12	-	-	63,78,88,89	0
5	GLC	I	1	11/12	0.87	0.10	59,64,70,76	0
5	GLC	I	2	12/12	0.87	0.11	45,66,78,78	0
5	GLC	J	1	11/12	0.91	0.09	60,63,71,75	0
5	GLC	J	2	12/12	0.91	0.09	66,78,83,88	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.

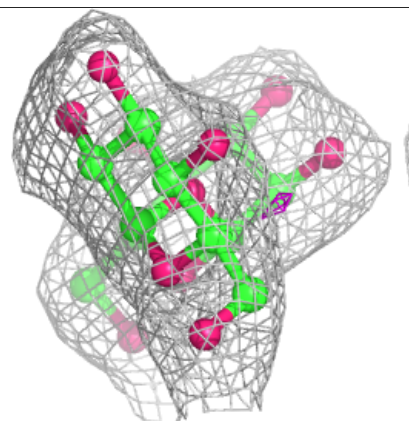
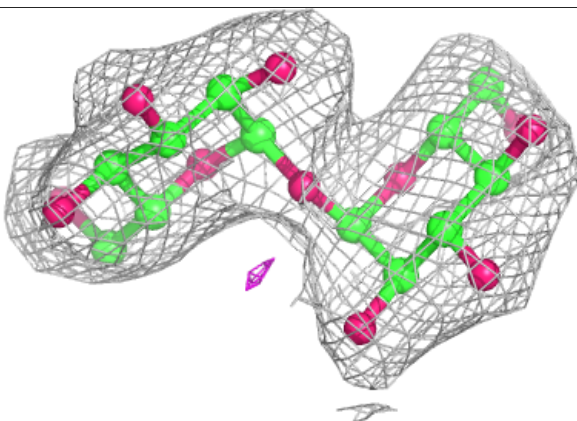
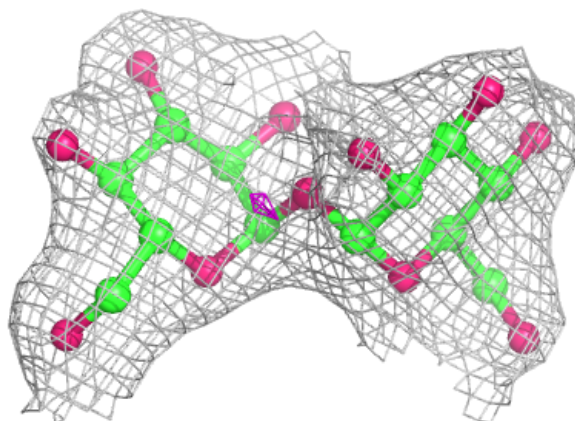
Electron density around Chain X:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

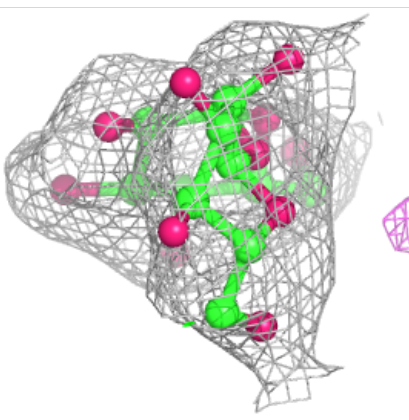
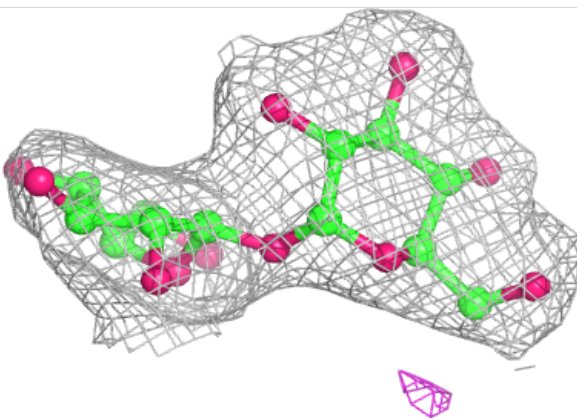
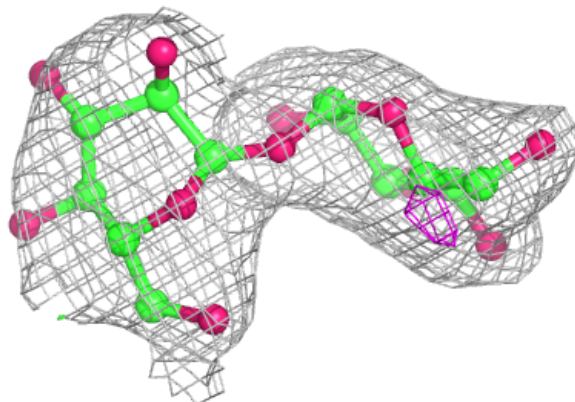


Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain J:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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	CIT	A	301	13/13	0.79	0.15	53,83,106,135	0
6	CIT	H	301	13/13	0.84	0.15	63,77,105,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.