



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:36 PM BST

PDB ID : 3ZE2
Title : Integrin alphaIIB beta3 headpiece and RGD peptide complex
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on : 2012-12-03
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

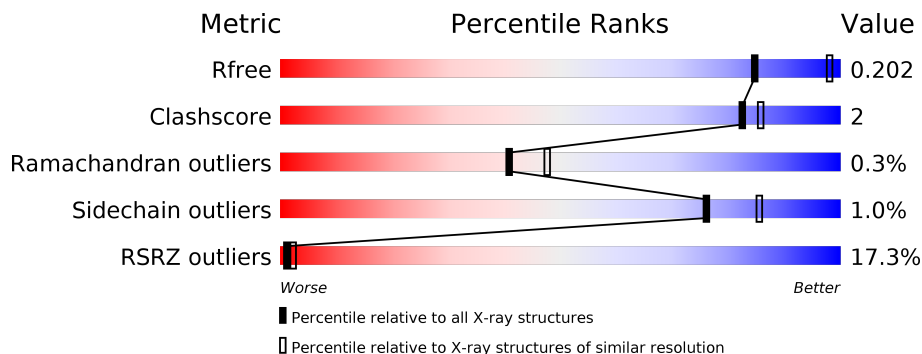
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



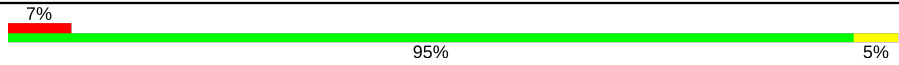
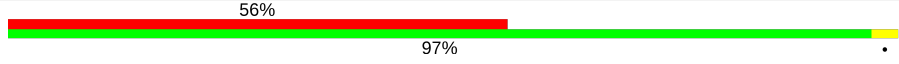

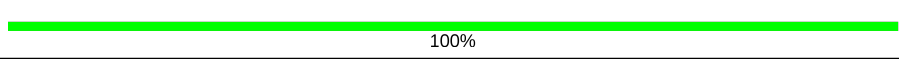
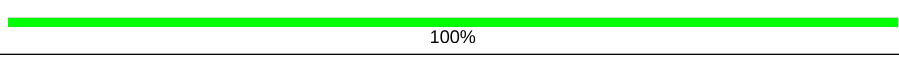
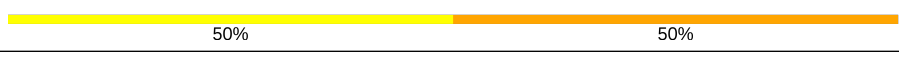

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	457	 93% 6%
1	C	457	 2% 94% 5%
2	B	472	 15% 89% 10%
2	D	472	 25% 74% 22%
3	E	221	 2% 93% 5%
3	H	221	 52% 94%

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Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	
5	I	6	
5	J	6	
6	G	6	
7	K	2	
8	M	4	

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
8	MAN	M	4	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 41569 atoms, of which 19764 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
			Total	C	H	N	O	S			
1	A	454	Total	C	H	N	O	S	2	5	0
			6845	2228	3341	600	668	8			
1	C	453	Total	C	H	N	O	S	1	6	0
			6840	2227	3337	602	666	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	469	Total	C	H	N	O	S	0	7	0
			7218	2275	3569	619	721	34			
2	D	367	Total	C	H	N	O	S	0	6	0
			5806	1834	2896	487	570	19			

- Molecule 3 is a protein called 10E5 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			

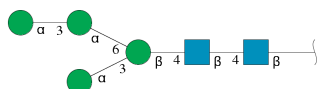
- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	214	Total	C	H	N	O	S	0	2	0
			3222	1028	1569	273	343	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

- Molecule 5 is a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	I	6	111	32	52	15	12	0	3	0
5	J	6	74	22	34	9	9	0	0	0

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



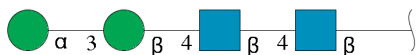
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
6	G	6	133	40	61	2	30	0	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
7	K	2	53	16	25	2	10	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-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
			Total	C	H	N	O			
8	M	4	93	28	43	2	20	0	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	A	1	14	3	8	3	0	0
9	A	1	14	3	8	3	0	0
9	C	1	14	3	8	3	0	0
9	C	1	14	3	8	3	0	0
9	C	1	14	3	8	3	0	0
9	C	1	14	3	8	3	0	0
9	E	1	14	3	8	3	0	0
9	F	1	14	3	8	3	0	0
9	F	1	14	3	8	3	0	0
9	J	1	14	3	8	3	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	4	Total Ca 4 4	0	0
11	C	4	Total Ca 4 4	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	3	Total Mn 3 3	0	0
12	D	3	Total Mn 3 3	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
13	C	1	27	8	13	1	5	0	0

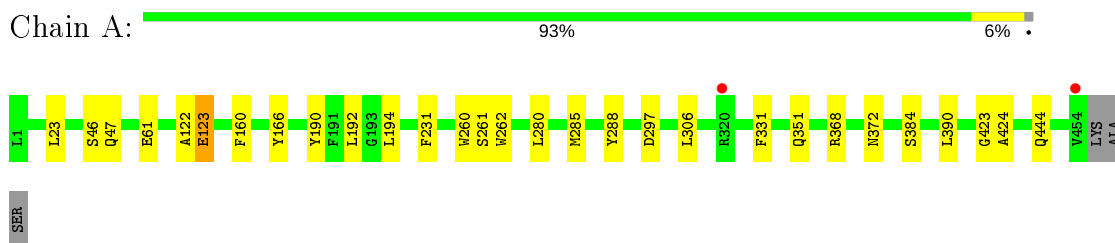
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	483	Total	O	0	0
			483	483		
14	B	211	Total	O	0	0
			211	211		
14	C	283	Total	O	0	0
			283	283		
14	D	107	Total	O	0	0
			107	107		
14	E	129	Total	O	0	0
			129	129		
14	F	68	Total	O	0	0
			68	68		
14	H	18	Total	O	0	0
			18	18		
14	I	2	Total	O	0	0
			2	2		
14	J	2	Total	O	0	0
			2	2		
14	L	15	Total	O	0	0
			15	15		

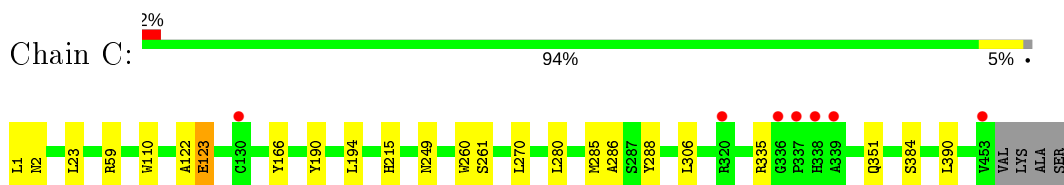
3 Residue-property plots [i](#)

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.

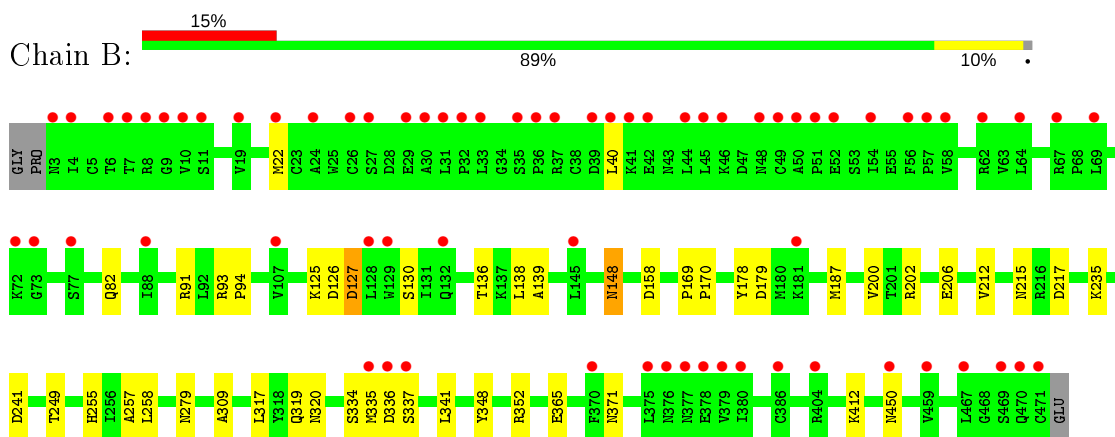
- Molecule 1: INTEGRIN ALPHA-IIB



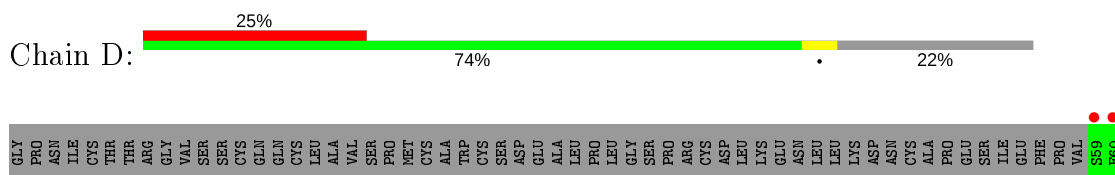
- Molecule 1: INTEGRIN ALPHA-IIB

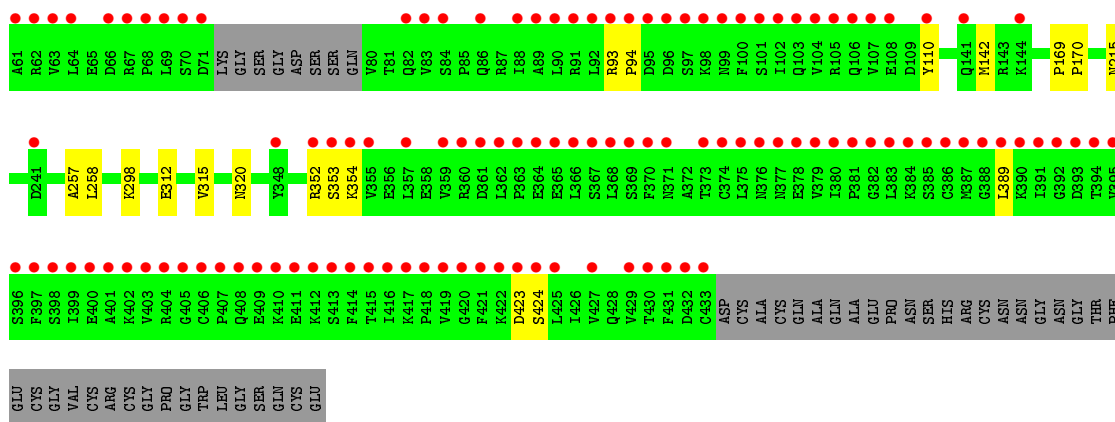


- Molecule 2: INTEGRIN BETA-3

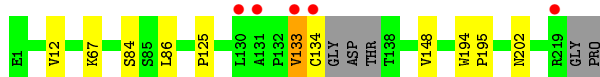
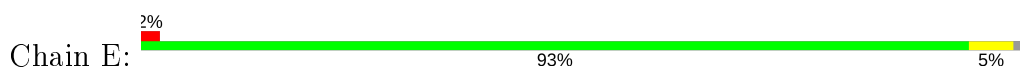


- Molecule 2: INTEGRIN BETA-3

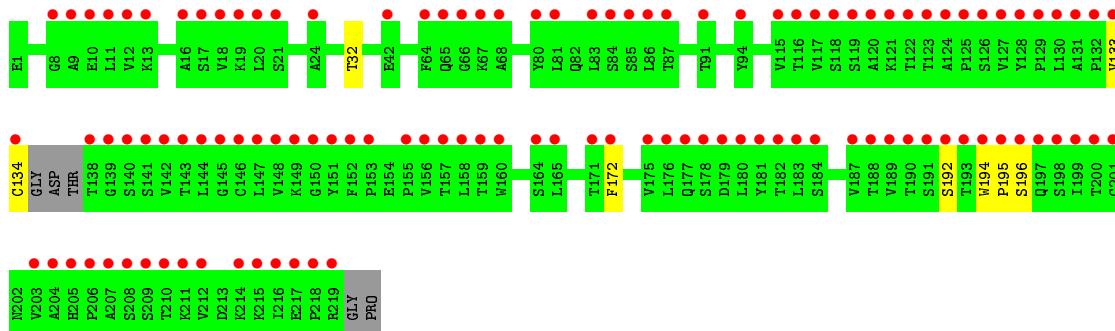
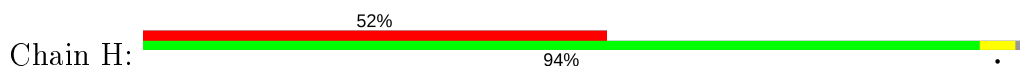




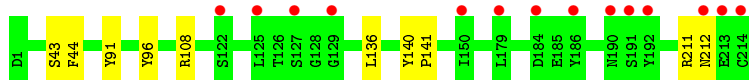
- Molecule 3: 10E5 FAB HEAVY CHAIN



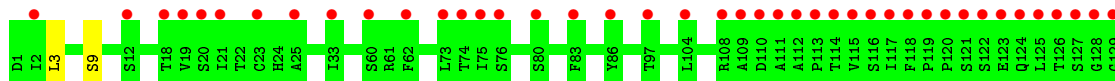
- Molecule 3: 10E5 FAB HEAVY CHAIN

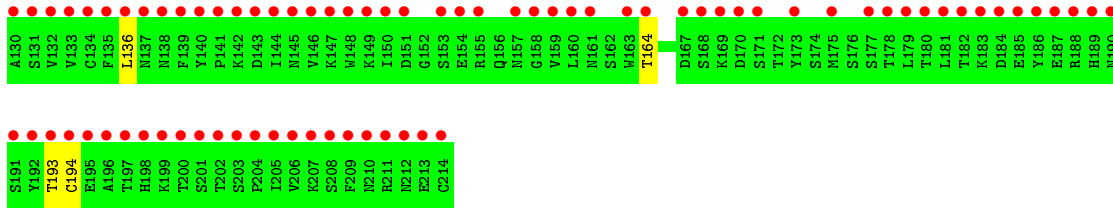


- Molecule 4: 10E5 FAB LIGHT CHAIN



- Molecule 4: 10E5 FAB LIGHT CHAIN





- Molecule 5: RGD PEPTIDE



- Molecule 5: RGD PEPTIDE



There are no outlier residues recorded for this chain.

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



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	233.21Å 143.56Å 104.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.02 – 2.35 54.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.02-2.35) 100.0 (54.02-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.204 0.174 , 0.202	Depositor DCC
R_{free} test set	1017 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	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	41569	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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, BMA, NAG, CA, MN, SO4, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3612	0.44	0/4923
1	C	0.23	0/3615	0.41	0/4927
2	B	0.22	0/3737	0.40	0/5066
2	D	0.22	0/2976	0.39	0/4031
3	E	0.23	0/1684	0.42	0/2305
3	H	0.21	0/1684	0.38	0/2305
4	F	0.23	0/1692	0.41	0/2294
4	L	0.22	0/1673	0.37	0/2269
5	I	0.20	0/59	0.40	0/76
5	J	0.18	0/40	0.39	0/52
All	All	0.23	0/20772	0.41	0/28248

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

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	3504	3341	3348	20	0
1	C	3503	3337	3345	18	0
2	B	3649	3569	3575	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2910	2896	2900	11	0
3	E	1642	1597	1600	5	0
3	H	1642	1597	1600	5	0
4	F	1653	1569	1571	6	0
4	L	1637	1550	1553	4	0
5	I	59	52	51	6	0
5	J	40	34	34	0	0
6	G	72	61	61	0	0
7	K	28	25	25	2	0
8	M	50	43	43	0	0
9	A	12	16	16	0	0
9	C	24	32	32	1	0
9	E	6	8	8	0	0
9	F	12	16	16	0	0
9	J	6	8	8	0	0
10	A	10	0	0	1	0
11	A	4	0	0	0	0
11	C	4	0	0	0	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	C	14	13	13	0	0
14	A	483	0	0	6	1
14	B	211	0	0	6	0
14	C	283	0	0	6	1
14	D	107	0	0	1	0
14	E	129	0	0	0	0
14	F	68	0	0	0	0
14	H	18	0	0	0	0
14	I	2	0	0	0	0
14	J	2	0	0	0	0
14	L	15	0	0	1	0
All	All	21805	19764	19799	99	1

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 (99) 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)
14:A:3238:HOH:O	5:I:492[B]:GLY:N	2.03	0.90
14:A:3222:HOH:O	5:I:493[A]:ARG:NH2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:SER:OG	14:C:3243:HOH:O	2.05	0.74
1:A:384:SER:OG	14:A:3430:HOH:O	2.06	0.73
10:A:1457:SO4:O3	14:A:3482:HOH:O	2.09	0.70
2:B:148:ASN:OD1	14:B:3048:HOH:O	2.10	0.70
2:B:335:MET:O	14:B:3040:HOH:O	2.10	0.68
1:C:249:ASN:ND2	14:C:3170:HOH:O	2.27	0.68
1:C:2[B]:ASN:OD1	14:C:3001:HOH:O	2.12	0.67
2:B:126:ASP:OD1	14:B:3039:HOH:O	2.13	0.67
1:C:351:GLN:OE1	14:C:3221:HOH:O	2.13	0.66
2:B:130[B]:SER:OG	2:B:336:ASP:OD2	2.14	0.65
2:B:319[B]:GLN:OE1	14:B:3169:HOH:O	2.13	0.65
1:C:1:LEU:N	1:C:2[B]:ASN:HA	2.11	0.65
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.32	0.62
7:K:1:NAG:O3	7:K:2:NAG:O5	2.13	0.62
1:C:1:LEU:N	1:C:2[A]:ASN:HA	2.12	0.60
2:B:82:GLN:NE2	14:B:3017:HOH:O	2.36	0.56
1:A:122:ALA:O	1:A:123:GLU:HB2	2.06	0.56
1:C:122:ALA:O	1:C:123:GLU:HB2	2.06	0.55
2:B:178[B]:TYR:CD1	2:B:179:ASP:N	2.74	0.55
2:B:235:LYS:NZ	14:B:3109:HOH:O	2.36	0.55
1:C:335:ARG:NH2	14:C:3212:HOH:O	2.40	0.55
1:A:192:LEU:HD13	5:I:493[A]:ARG:NH1	2.22	0.55
1:C:59:ARG:NH1	14:C:3050:HOH:O	2.39	0.55
2:B:130[A]:SER:OG	2:B:337[A]:SER:OG	2.25	0.55
2:D:423:ASP:OD1	2:D:424:SER:N	2.40	0.55
1:A:280[B]:LEU:HD23	1:A:331:PHE:CZ	2.44	0.53
2:B:127:ASP:N	2:B:127:ASP:OD1	2.41	0.52
4:L:9:SER:OG	14:L:3004:HOH:O	2.19	0.52
1:A:351:GLN:OE1	14:A:3394:HOH:O	2.19	0.51
2:B:450:ASN:ND2	2:B:450:ASN:O	2.44	0.51
1:A:280[B]:LEU:HD23	1:A:331:PHE:CE1	2.45	0.51
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.93	0.51
3:H:192:SER:O	3:H:196:SER:OG	2.29	0.50
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.42	0.50
2:D:257:ALA:O	2:D:258:LEU:HB2	2.12	0.50
3:E:133:VAL:O	3:E:134:CYS:SG	2.70	0.50
2:D:298:LYS:NZ	14:D:3079:HOH:O	2.43	0.48
2:B:257:ALA:O	2:B:258:LEU:HB2	2.14	0.48
1:A:122:ALA:O	1:A:123:GLU:CB	2.62	0.48
2:B:158:ASP:HB3	2:B:187:MET:CE	2.44	0.48
2:B:371:ASN:ND2	7:K:1:NAG:C7	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280[A]:LEU:CD1	1:A:306:LEU:HD23	2.44	0.48
2:B:249[B]:THR:HG22	2:B:309:ALA:HB3	1.95	0.47
1:C:122:ALA:O	1:C:123:GLU:CB	2.63	0.47
3:E:194:TRP:CG	3:E:195:PRO:HA	2.49	0.47
1:A:160:PHE:HB2	5:I:493[B]:ARG:HD3	1.97	0.46
1:A:280[B]:LEU:HD12	1:A:280[B]:LEU:N	2.30	0.46
3:H:194:TRP:CG	3:H:195:PRO:HA	2.50	0.46
2:D:110:TYR:OH	2:D:354:LYS:O	2.25	0.46
2:B:22:MET:HG2	2:B:40:LEU:CD2	2.46	0.45
1:A:46:SER:O	1:A:47:GLN:HB2	2.17	0.45
3:H:172:PHE:CD2	4:L:164:THR:HG23	2.51	0.45
2:D:352:ARG:O	2:D:352:ARG:CG	2.64	0.45
2:D:169:PRO:HB2	2:D:170:PRO:HD2	1.98	0.45
1:A:285:MET:SD	2:B:320:ASN:HB3	2.57	0.45
5:I:492[B]:GLY:O	5:I:494[B]:GLY:N	2.50	0.45
1:C:194:LEU:C	1:C:194:LEU:HD12	2.38	0.44
1:C:280:LEU:CD1	1:C:306:LEU:HD23	2.46	0.44
1:C:390:LEU:HD12	1:C:390:LEU:N	2.32	0.44
3:E:67:LYS:NZ	3:E:84:SER:O	2.50	0.44
4:L:136:LEU:N	4:L:136:LEU:HD12	2.33	0.43
2:D:312:GLU:HA	2:D:315:VAL:HG23	2.00	0.43
1:A:390:LEU:N	1:A:390:LEU:HD12	2.34	0.43
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.99	0.43
2:B:235:LYS:CE	2:B:279:ASN:OD1	2.67	0.43
2:B:348:TYR:CZ	2:B:352:ARG:HD2	2.53	0.43
2:B:125:LYS:HA	2:B:212:VAL:HG11	2.01	0.43
4:F:91:TYR:HB2	4:F:96:TYR:CZ	2.53	0.43
1:C:215:HIS:CE1	3:H:32:THR:HG22	2.53	0.43
3:H:133:VAL:O	3:H:134:CYS:SG	2.77	0.43
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.49	0.43
1:A:192:LEU:HD11	1:A:231:PHE:CD1	2.53	0.43
5:I:492[B]:GLY:C	5:I:494[B]:GLY:N	2.72	0.43
1:C:260:TRP:CE3	1:C:261:SER:HB2	2.54	0.42
1:C:285:MET:SD	2:D:320:ASN:HB3	2.59	0.42
2:B:169:PRO:HB2	2:B:170:PRO:HD2	1.99	0.42
1:A:194:LEU:C	1:A:194:LEU:HD12	2.39	0.42
2:B:138:LEU:HA	2:B:341:LEU:HD13	2.00	0.42
2:D:354:LYS:HG3	2:D:354:LYS:O	2.19	0.42
4:L:193:THR:HG22	4:L:194:CYS:N	2.34	0.42
1:A:260:TRP:CE3	1:A:261:SER:HB2	2.55	0.42
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:211:ARG:NH1	4:F:212:ASN:OD1	2.53	0.42
4:F:43:SER:OG	4:F:44:PHE:N	2.50	0.41
1:A:423:GLY:O	1:A:424:ALA:HB3	2.20	0.41
1:C:285:MET:O	1:C:286:ALA:HB3	2.20	0.41
2:D:353:SER:HB2	2:D:389:LEU:N	2.35	0.41
1:A:444:GLN:NE2	14:A:3478:HOH:O	2.53	0.41
4:F:136:LEU:N	4:F:136:LEU:HD12	2.36	0.41
1:A:262:TRP:HB3	2:B:317:LEU:HD13	2.03	0.41
4:F:140:TYR:CG	4:F:141:PRO:HA	2.56	0.41
2:B:217:ASP:OD2	2:B:255:HIS:NE2	2.55	0.40
2:D:93:ARG:HB2	2:D:94:PRO:HD2	2.03	0.40
2:B:169:PRO:HD2	2:B:178[B]:TYR:CE1	2.56	0.40
4:F:211:ARG:O	4:F:212:ASN:HB2	2.22	0.40
1:A:297:ASP:O	1:A:372:ASN:HB2	2.21	0.40
1:C:110:TRP:HB3	9:C:1457:GOL:H31	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:3480:HOH:O	14:C:3252:HOH:O[1_554]	2.18	0.02

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	457/457 (100%)	445 (97%)	11 (2%)	1 (0%)	47 56
1	C	457/457 (100%)	440 (96%)	16 (4%)	1 (0%)	47 56
2	B	474/472 (100%)	460 (97%)	13 (3%)	1 (0%)	47 56
2	D	369/472 (78%)	355 (96%)	13 (4%)	1 (0%)	41 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	29	32
3	H	212/221 (96%)	200 (94%)	12 (6%)	0	100	100
4	F	214/214 (100%)	206 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	I	6/6 (100%)	2 (33%)	0	4 (67%)	0	0
5	J	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2617/2740 (96%)	2514 (96%)	94 (4%)	9 (0%)	41	47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	D	142	MET
1	C	123	GLU
5	I	493[A]	ARG
5	I	493[B]	ARG
2	B	334	SER
5	I	494[A]	GLY
5	I	494[B]	GLY
3	E	133	VAL

5.3.2 Protein sidechains [i](#)

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	367/364 (101%)	361 (98%)	6 (2%)	62	75
1	C	367/364 (101%)	362 (99%)	5 (1%)	67	78
2	B	422/417 (101%)	416 (99%)	6 (1%)	67	78
2	D	336/417 (81%)	335 (100%)	1 (0%)	92	96
3	E	187/190 (98%)	186 (100%)	1 (0%)	88	94
3	H	187/190 (98%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	190/188 (101%)	188 (99%)	2 (1%)	73	84
4	L	188/188 (100%)	187 (100%)	1 (0%)	88	94
5	I	5/4 (125%)	3 (60%)	2 (40%)	0	0
5	J	4/4 (100%)	4 (100%)	0	100	100
All	All	2253/2326 (97%)	2229 (99%)	24 (1%)	76	84

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	190	TYR
1	A	288	TYR
1	A	368	ARG
2	B	91	ARG
2	B	127	ASP
2	B	136	THR
2	B	148	ASN
2	B	215	ASN
2	B	241	ASP
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	270	LEU
1	C	288	TYR
2	D	215	ASN
3	E	202	ASN
4	F	108[A]	ARG
4	F	108[B]	ARG
5	I	493[A]	ARG
5	I	493[B]	ARG
4	L	3	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
2	B	450	ASN
1	C	338	HIS

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Mol	Chain	Res	Type
2	D	316	ASN
3	E	202	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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	G	1	2,6	14,14,15	0.62	0	17,19,21	0.67	0
6	NAG	G	2	6	14,14,15	0.56	0	17,19,21	0.77	0
6	BMA	G	3	6	11,11,12	0.63	0	15,15,17	0.77	0
6	MAN	G	4	6	11,11,12	0.65	0	15,15,17	0.76	0
6	MAN	G	5	6	11,11,12	0.65	0	15,15,17	0.64	0
6	MAN	G	6	6	11,11,12	0.65	0	15,15,17	0.69	0
7	NAG	K	1	7	14,14,15	0.52	0	17,19,21	0.87	1 (5%)
7	NAG	K	2	7	14,14,15	0.55	0	17,19,21	0.62	0
8	NAG	M	1	8,2	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
8	NAG	M	2	8	14,14,15	0.62	0	17,19,21	0.93	1 (5%)
8	BMA	M	3	8	11,11,12	0.64	0	15,15,17	0.76	0
8	MAN	M	4	8	11,11,12	0.61	0	15,15,17	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	0/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
8	NAG	M	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
8	BMA	M	3	8	-	2/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	1	NAG	O5-C5-C6	2.56	111.22	107.20
8	M	2	NAG	O5-C5-C6	2.33	110.85	107.20
8	M	1	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

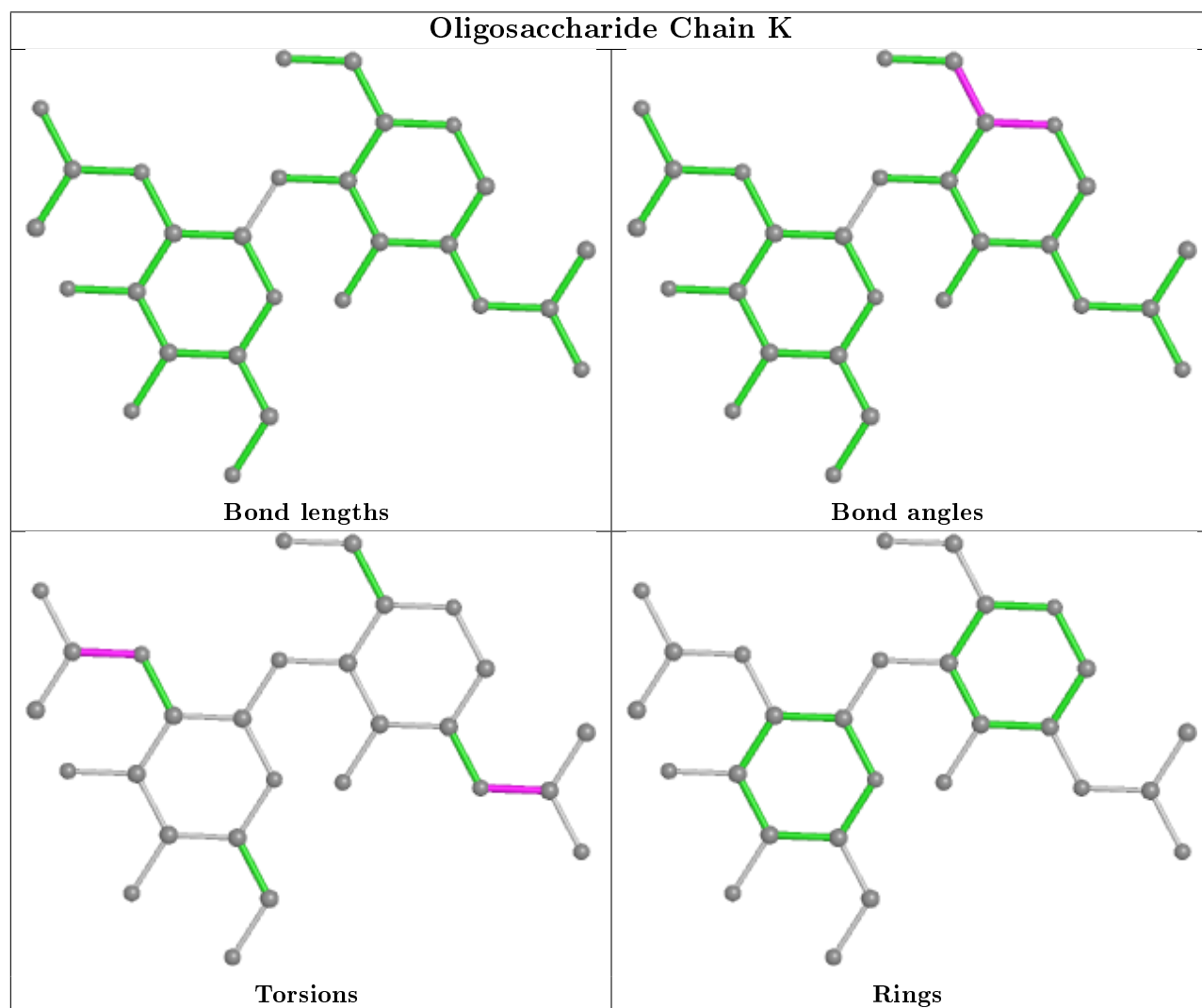
Mol	Chain	Res	Type	Atoms
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2
8	M	3	BMA	O5-C5-C6-O6
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
8	M	3	BMA	C4-C5-C6-O6

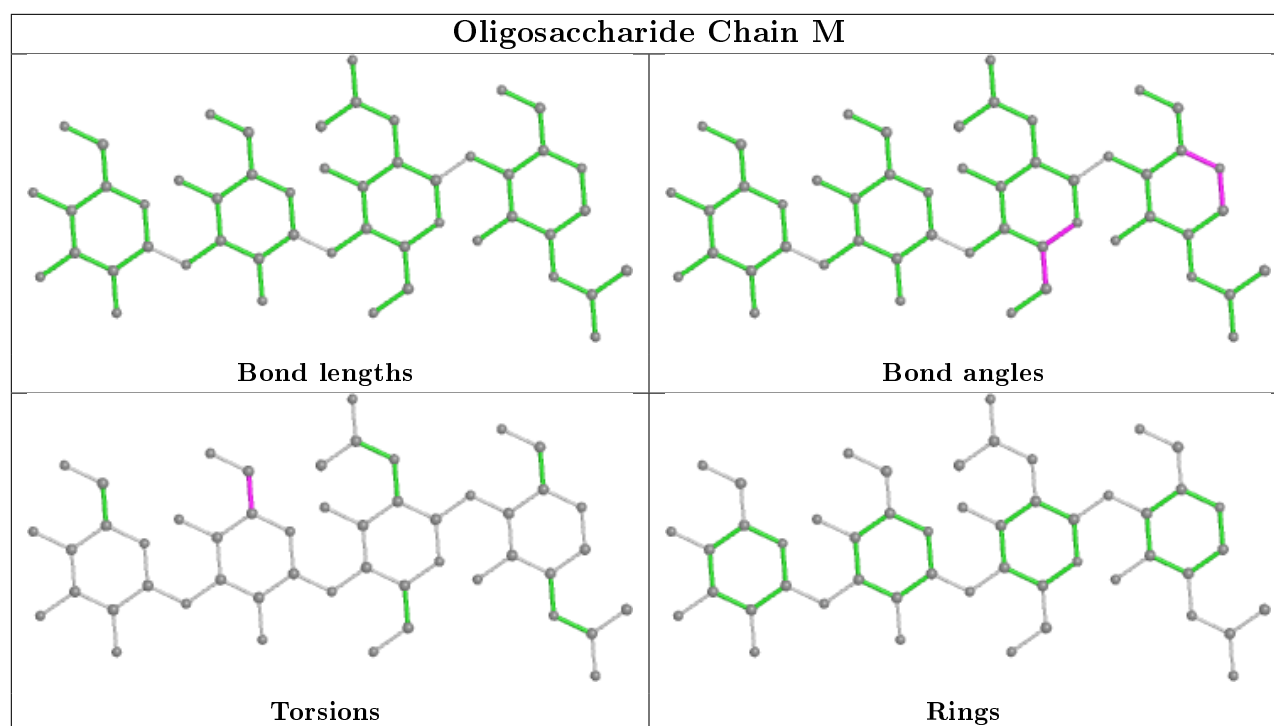
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	1	NAG	2	0
7	K	2	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 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	$\# Z > 2$
9	GOL	A	1455	-	5,5,5	0.39	0	5,5,5	0.10	0
9	GOL	C	1455	-	5,5,5	0.37	0	5,5,5	0.24	0
10	SO4	A	1457	-	4,4,4	0.14	0	6,6,6	0.11	0
9	GOL	J	1498	-	5,5,5	0.36	0	5,5,5	0.27	0
9	GOL	C	1454	-	5,5,5	0.37	0	5,5,5	0.29	0
10	SO4	A	1458	-	4,4,4	0.14	0	6,6,6	0.06	0
9	GOL	C	1457	-	5,5,5	0.38	0	5,5,5	0.17	0
9	GOL	F	1215	-	5,5,5	0.39	0	5,5,5	0.22	0
13	NAG	C	2015	1	14,14,15	0.55	0	17,19,21	0.75	0
9	GOL	F	1216	-	5,5,5	0.36	0	5,5,5	0.25	0
9	GOL	A	1456	-	5,5,5	0.37	0	5,5,5	0.18	0
9	GOL	C	1456	-	5,5,5	0.37	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	E	1220	-	5,5,5	0.39	0	5,5,5	0.22	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
9	GOL	A	1455	-	-	3/4/4/4	-
9	GOL	C	1455	-	-	2/4/4/4	-
9	GOL	J	1498	-	-	2/4/4/4	-
9	GOL	C	1454	-	-	2/4/4/4	-
9	GOL	C	1457	-	-	2/4/4/4	-
9	GOL	F	1215	-	-	2/4/4/4	-
13	NAG	C	2015	1	-	3/6/23/26	0/1/1/1
9	GOL	F	1216	-	-	2/4/4/4	-
9	GOL	A	1456	-	-	2/4/4/4	-
9	GOL	C	1456	-	-	2/4/4/4	-
9	GOL	E	1220	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1456	GOL	O1-C1-C2-C3
9	F	1215	GOL	C1-C2-C3-O3
9	A	1455	GOL	O1-C1-C2-C3
9	C	1457	GOL	O1-C1-C2-C3
9	F	1216	GOL	O1-C1-C2-O2
9	F	1216	GOL	O1-C1-C2-C3
9	E	1220	GOL	C1-C2-C3-O3
13	C	2015	NAG	C8-C7-N2-C2
13	C	2015	NAG	O7-C7-N2-C2
9	F	1215	GOL	O2-C2-C3-O3
9	C	1454	GOL	O1-C1-C2-C3
9	A	1456	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	C	1455	GOL	O1-C1-C2-C3
9	E	1220	GOL	O1-C1-C2-C3
9	C	1456	GOL	O1-C1-C2-O2
9	A	1455	GOL	O1-C1-C2-O2
9	C	1457	GOL	O1-C1-C2-O2
9	E	1220	GOL	O1-C1-C2-O2
9	C	1454	GOL	O1-C1-C2-O2
9	C	1455	GOL	O1-C1-C2-O2
9	A	1455	GOL	C1-C2-C3-O3
9	E	1220	GOL	O2-C2-C3-O3
13	C	2015	NAG	O5-C5-C6-O6
9	J	1498	GOL	O1-C1-C2-C3
9	J	1498	GOL	O1-C1-C2-O2
9	A	1456	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1457	SO4	1	0
9	C	1457	GOL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	454/457 (99%)	0.36	2 (0%) 92 96	15, 26, 52, 116	4 (0%)
1	C	453/457 (99%)	0.27	7 (1%) 73 81	22, 38, 72, 130	1 (0%)
2	B	469/472 (99%)	0.89	69 (14%) 2 3	16, 48, 118, 193	127 (27%)
2	D	367/472 (77%)	2.11	119 (32%) 0 0	23, 53, 179, 217	76 (20%)
3	E	216/221 (97%)	0.04	5 (2%) 60 70	26, 42, 70, 107	0
3	H	216/221 (97%)	2.73	115 (53%) 0 0	49, 107, 160, 211	0
4	F	214/214 (100%)	0.44	14 (6%) 18 27	30, 48, 86, 192	2 (0%)
4	L	214/214 (100%)	3.12	119 (55%) 0 0	59, 114, 205, 233	1 (0%)
5	I	6/6 (100%)	1.60	2 (33%) 0 0	27, 33, 51, 56	0
5	J	6/6 (100%)	0.69	0 100 100	31, 38, 70, 72	0
All	All	2615/2740 (95%)	1.09	452 (17%) 1 2	15, 45, 157, 233	211 (8%)

All (452) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	409	GLU	23.6
4	L	181	LEU	21.1
4	L	214	CYS	15.9
4	L	130	ALA	15.5
2	D	395	VAL	14.1
2	D	391	ILE	13.1
2	B	7	THR	13.0
2	D	401	ALA	12.9
2	D	375	LEU	12.8
2	D	433	CYS	12.6
4	F	214	CYS	12.4
4	L	193	THR	12.2
3	H	133	VAL	12.1

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Mol	Chain	Res	Type	RSRZ
4	L	148	TRP	12.0
2	D	412	LYS	11.3
3	H	147	LEU	11.0
2	D	431	PHE	10.9
2	D	389	LEU	10.8
2	D	419	VAL	10.8
2	D	103	GLN	10.7
4	L	136	LEU	10.6
2	D	93	ARG	10.1
2	D	407	PRO	9.9
4	L	209	PHE	9.9
2	D	399	ILE	9.8
2	D	397	PHE	9.5
2	D	363	PRO	9.5
2	D	92	LEU	9.2
2	D	381	PRO	9.0
4	F	212	ASN	8.9
3	H	217	GLU	8.9
2	D	405	GLY	8.8
2	B	469	SER	8.8
2	D	408	GLN	8.8
3	H	128	TYR	8.7
3	H	130	LEU	8.7
3	H	131	ALA	8.5
4	L	129	GLY	8.4
2	D	376	ASN	8.2
3	H	11	LEU	8.2
2	D	106	GLN	8.2
2	D	420	GLY	8.2
3	H	134	CYS	8.1
4	L	213	GLU	8.1
2	D	425	LEU	8.1
3	H	209	SER	8.1
2	D	429	VAL	8.1
3	H	132	PRO	8.0
4	L	186	TYR	7.8
2	D	100	PHE	7.8
3	H	156	VAL	7.8
4	L	150	ILE	7.8
3	H	219	ARG	7.7
2	D	380	ILE	7.7
2	D	102	ILE	7.6

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Mol	Chain	Res	Type	RSRZ
2	B	471	CYS	7.6
3	H	216	ILE	7.6
2	D	410	LYS	7.5
2	D	62	ARG	7.5
4	L	117	ILE	7.5
4	L	192	TYR	7.5
3	H	218	PRO	7.5
2	D	400	GLU	7.4
2	D	99	ASN	7.2
2	D	88	ILE	7.2
3	H	138	THR	7.2
2	D	390	LYS	7.1
2	D	104	VAL	7.1
3	H	140	SER	7.1
4	L	125	LEU	7.1
4	L	203	SER	7.0
2	D	406	CYS	7.0
3	H	199	ILE	7.0
4	L	155	ARG	7.0
4	L	206	VAL	6.9
4	L	119	PRO	6.9
4	L	128	GLY	6.8
4	L	160	LEU	6.8
2	D	71	ASP	6.8
4	L	145	ASN	6.8
4	L	183	LYS	6.8
2	D	90	LEU	6.7
2	D	352	ARG	6.7
3	H	152	PHE	6.7
2	D	392	GLY	6.7
2	D	403	VAL	6.7
4	L	208	SER	6.6
2	D	94	PRO	6.6
4	L	115	VAL	6.6
2	D	64	LEU	6.6
2	D	105	ARG	6.6
3	H	144	LEU	6.5
3	H	18	VAL	6.5
2	D	61	ALA	6.5
2	B	33	LEU	6.5
1	C	337	PRO	6.5
4	L	190	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
4	L	212	ASN	6.5
4	L	114	THR	6.4
2	D	364	GLU	6.4
3	H	200	THR	6.4
2	D	404	ARG	6.4
4	L	205	ILE	6.4
4	L	158	GLY	6.4
2	B	335	MET	6.4
2	B	470	GLN	6.3
4	L	132	VAL	6.3
3	H	151	TYR	6.3
4	L	197	THR	6.3
2	D	377	ASN	6.3
3	H	148	VAL	6.3
2	B	9	GLY	6.3
3	H	17	SER	6.3
4	L	196	ALA	6.3
2	B	32	PRO	6.2
2	B	8	ARG	6.2
3	H	127	VAL	6.2
2	D	379	VAL	6.2
2	D	83	VAL	6.1
2	D	386	CYS	6.1
2	D	402	LYS	6.1
2	B	129	TRP	6.1
2	B	10	VAL	6.0
4	L	194	CYS	6.0
4	L	126	THR	6.0
2	D	427	VAL	6.0
2	D	432	ASP	6.0
4	L	180	THR	6.0
3	H	146	CYS	6.0
3	H	121	LYS	5.9
3	H	176	LEU	5.9
4	L	182	THR	5.9
2	D	107	VAL	5.8
2	D	371	ASN	5.8
3	H	158	LEU	5.8
4	L	146	VAL	5.8
2	D	370	PHE	5.7
2	D	394	THR	5.7
2	D	416	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
3	H	159	THR	5.7
3	H	117	VAL	5.7
4	L	144	ILE	5.7
2	D	101	SER	5.7
4	L	113	PRO	5.6
2	D	97	SER	5.6
4	L	159	VAL	5.6
4	L	120	PRO	5.6
2	D	393	ASP	5.6
4	L	195	GLU	5.5
2	B	54	ILE	5.5
2	D	366	LEU	5.5
2	D	84	SER	5.5
4	L	179	LEU	5.5
2	D	430	THR	5.5
2	D	423	ASP	5.5
4	L	131	SER	5.4
3	H	194	TRP	5.4
3	H	189	VAL	5.4
2	D	383	LEU	5.4
2	B	50	ALA	5.4
2	B	51	PRO	5.4
4	L	188	ARG	5.3
4	L	154	GLU	5.3
4	L	175	MET	5.3
3	H	177	GLN	5.2
2	D	108	GLU	5.2
2	D	387	MET	5.1
4	L	121	SER	5.1
2	D	368	LEU	5.1
3	H	205	HIS	5.1
4	L	211	ARG	5.1
2	D	374	CYS	5.1
2	D	369	SER	5.0
3	H	210	THR	5.0
2	D	355	VAL	5.0
4	L	210	ASN	5.0
4	L	135	PHE	5.0
2	D	96	ASP	5.0
2	D	396	SER	5.0
3	H	126	SER	5.0
4	L	122	SER	5.0

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Mol	Chain	Res	Type	RSRZ
4	L	118	PHE	5.0
2	B	128	LEU	4.9
2	D	59	SER	4.9
3	H	122	THR	4.9
3	H	157	THR	4.9
2	D	63	VAL	4.9
3	H	203	VAL	4.9
3	H	208	SER	4.9
3	H	215	LYS	4.9
2	B	375	LEU	4.8
2	D	378	GLU	4.8
2	D	362	LEU	4.8
2	D	98	LYS	4.8
2	B	44	LEU	4.8
2	D	357	LEU	4.8
1	C	453	VAL	4.8
4	L	123	GLU	4.7
2	D	95	ASP	4.7
3	H	118	SER	4.7
2	D	373	THR	4.7
3	H	149	LYS	4.7
4	L	111	ALA	4.7
4	L	149	LYS	4.7
1	A	454	VAL	4.7
2	B	3	ASN	4.7
1	C	336	GLY	4.7
3	H	198	SER	4.7
2	B	31	LEU	4.7
3	H	125	PRO	4.6
2	D	110	TYR	4.6
3	H	201	CYS	4.6
3	H	86	LEU	4.6
2	B	4	ILE	4.5
5	I	492[A]	GLY	4.5
4	L	147	LYS	4.5
2	B	48	ASN	4.5
2	B	36	PRO	4.5
4	L	199	LYS	4.5
4	L	207	LYS	4.5
3	H	212	VAL	4.5
3	H	24	ALA	4.5
3	H	142	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	49	CYS	4.5
4	L	127	SER	4.4
3	H	191	SER	4.4
3	H	211	LYS	4.4
3	H	180	LEU	4.4
4	L	201	SER	4.4
4	L	178	THR	4.4
2	B	35	SER	4.4
3	H	195	PRO	4.4
2	B	6	THR	4.3
3	H	141	SER	4.3
4	L	204	PRO	4.3
2	D	354	LYS	4.3
2	D	398	SER	4.3
2	D	382	GLY	4.3
4	L	177	SER	4.3
2	D	82	GLN	4.2
3	H	8	GLY	4.2
3	H	12	VAL	4.2
2	B	39	ASP	4.1
3	H	145	GLY	4.1
1	C	320	ARG	4.1
2	D	60	GLU	4.1
4	L	164	THR	4.1
2	B	450	ASN	4.0
2	D	68	PRO	4.0
2	B	22	MET	4.0
2	B	404	ARG	4.0
2	D	421	PHE	4.0
3	H	182	THR	4.0
4	L	124	GLN	4.0
4	L	168	SER	3.9
4	L	133	VAL	3.9
2	D	86	GLN	3.9
4	L	184	ASP	3.9
4	L	142	LYS	3.9
3	H	123	THR	3.9
3	H	119	SER	3.9
2	D	415	THR	3.8
3	H	115	VAL	3.8
2	B	336	ASP	3.8
3	H	83	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
4	L	141	PRO	3.8
3	H	184	SER	3.8
5	I	493[A]	ARG	3.7
4	L	163	TRP	3.7
4	L	139	PHE	3.7
2	B	30	ALA	3.7
2	D	353	SER	3.7
4	L	134	CYS	3.6
2	B	337[A]	SER	3.6
4	L	189	HIS	3.6
2	B	379	VAL	3.6
3	H	150	GLY	3.6
2	B	37	ARG	3.6
2	B	459	VAL	3.5
4	L	187	GLU	3.5
2	D	70	SER	3.5
2	D	385	SER	3.5
3	H	13	LYS	3.5
3	H	183	LEU	3.5
2	D	367	SER	3.5
3	H	21	SER	3.5
4	L	191	SER	3.5
3	E	133	VAL	3.5
4	L	200	THR	3.5
3	H	129	PRO	3.5
3	H	94	TYR	3.5
4	L	169	LYS	3.5
3	H	64	PHE	3.4
3	H	139	GLY	3.4
3	H	206	PRO	3.4
2	D	89	ALA	3.4
4	L	151	ASP	3.4
4	F	129	GLY	3.4
2	B	41	LYS	3.4
4	L	202	THR	3.4
3	H	81	LEU	3.4
4	F	122	SER	3.4
2	B	376	ASN	3.4
3	H	153	PRO	3.3
4	L	25	ALA	3.3
2	B	45	LEU	3.3
3	H	175	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	213	GLU	3.3
4	L	20	SER	3.2
4	L	83	PHE	3.2
2	D	91	ARG	3.2
2	B	40	LEU	3.2
3	H	160	TRP	3.2
4	L	198	HIS	3.2
2	B	26	CYS	3.2
3	H	214	LYS	3.2
4	L	109	ALA	3.2
3	H	143	THR	3.2
3	H	192	SER	3.1
3	E	134	CYS	3.1
3	H	42	GLU	3.1
4	L	185	GLU	3.1
3	H	193	THR	3.1
2	D	413	SER	3.1
4	F	191	SER	3.1
4	L	137	ASN	3.1
4	L	157	ASN	3.1
4	L	21	ILE	3.1
2	D	414	PHE	3.1
3	E	131	ALA	3.1
3	H	207	ALA	3.1
3	H	172	PHE	3.1
2	B	42	GLU	3.1
3	H	84	SER	3.1
2	B	46	LYS	3.1
2	B	19	VAL	3.1
4	L	171	SER	3.0
3	H	20	LEU	3.0
3	H	116	THR	3.0
4	L	19	VAL	3.0
4	L	86	TYR	3.0
3	H	187	VAL	2.9
2	D	422	LYS	2.9
2	D	69	LEU	2.9
3	H	120	ALA	2.9
4	F	186	TYR	2.9
4	L	140	TYR	2.9
2	B	29	GLU	2.9
2	B	52	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
4	L	143	ASP	2.9
3	H	155	PRO	2.9
2	D	241	ASP	2.8
4	L	12	SER	2.8
3	H	91	THR	2.8
3	E	130	LEU	2.8
2	D	411	GLU	2.8
4	F	190	ASN	2.8
2	B	77	SER	2.7
2	B	72	LYS	2.7
2	B	24	ALA	2.7
4	F	184	ASP	2.7
2	D	424	SER	2.7
3	H	68	ALA	2.7
2	D	417	LYS	2.7
2	B	11	SER	2.7
2	B	380	ILE	2.7
4	L	112	ALA	2.7
2	D	365	GLU	2.7
3	H	188	THR	2.7
4	L	110	ASP	2.6
3	H	197	GLN	2.6
2	B	107	VAL	2.6
4	L	73	LEU	2.6
3	H	181	TYR	2.6
4	L	116	SER	2.6
2	B	73	GLY	2.6
4	L	76	SER	2.6
4	L	153	SER	2.6
2	B	378	GLU	2.6
4	F	192	TYR	2.6
4	L	2	ILE	2.6
2	B	64	LEU	2.5
3	H	165	LEU	2.5
3	H	66	GLY	2.5
3	H	67	LYS	2.5
3	H	204	ALA	2.5
4	L	161	ASN	2.5
4	F	150	ILE	2.5
2	B	132	GLN	2.5
2	D	67	ARG	2.5
3	E	219	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	10	GLU	2.5
3	H	9	ALA	2.5
3	H	164	SER	2.5
4	L	18	THR	2.5
2	D	388	GLY	2.4
3	H	190	THR	2.4
2	D	384	LYS	2.4
4	L	75	ILE	2.4
3	H	171	THR	2.4
4	L	167	ASP	2.4
4	L	62	PHE	2.4
2	B	67	ARG	2.4
2	D	360	ARG	2.4
2	B	58	VAL	2.3
4	L	170	ASP	2.3
3	H	80	TYR	2.3
2	D	144	LYS	2.3
2	B	88	ILE	2.3
3	H	85	SER	2.3
4	L	80	SER	2.3
2	B	145	LEU	2.3
2	D	348	TYR	2.3
4	L	138	ASN	2.3
4	L	108	ARG	2.2
2	D	361	ASP	2.2
4	F	179	LEU	2.2
4	L	74	THR	2.2
4	L	173	TYR	2.2
3	H	124	ALA	2.2
4	L	33	ILE	2.2
3	H	179	ASP	2.2
2	D	141	GLN	2.2
2	B	69	LEU	2.2
4	F	125	LEU	2.2
2	D	66	ASP	2.2
2	B	27	SER	2.1
3	H	196	SER	2.1
2	B	386	CYS	2.1
4	L	23	CYS	2.1
1	C	338	HIS	2.1
2	B	370	PHE	2.1
3	H	65	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	320	ARG	2.1
3	H	178	SER	2.1
3	H	19	LYS	2.1
2	B	56	PHE	2.1
2	B	377	ASN	2.1
2	B	467	LEU	2.1
1	C	130	CYS	2.1
2	B	57	PRO	2.1
4	L	104	LEU	2.0
3	H	87	THR	2.0
1	C	339	ALA	2.0
2	B	62	ARG	2.0
2	D	418	PRO	2.0
2	D	359	VAL	2.0
2	B	181	LYS	2.0
4	F	127	SER	2.0
4	L	60	SER	2.0
4	L	97	THR	2.0
3	H	16	ALA	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.

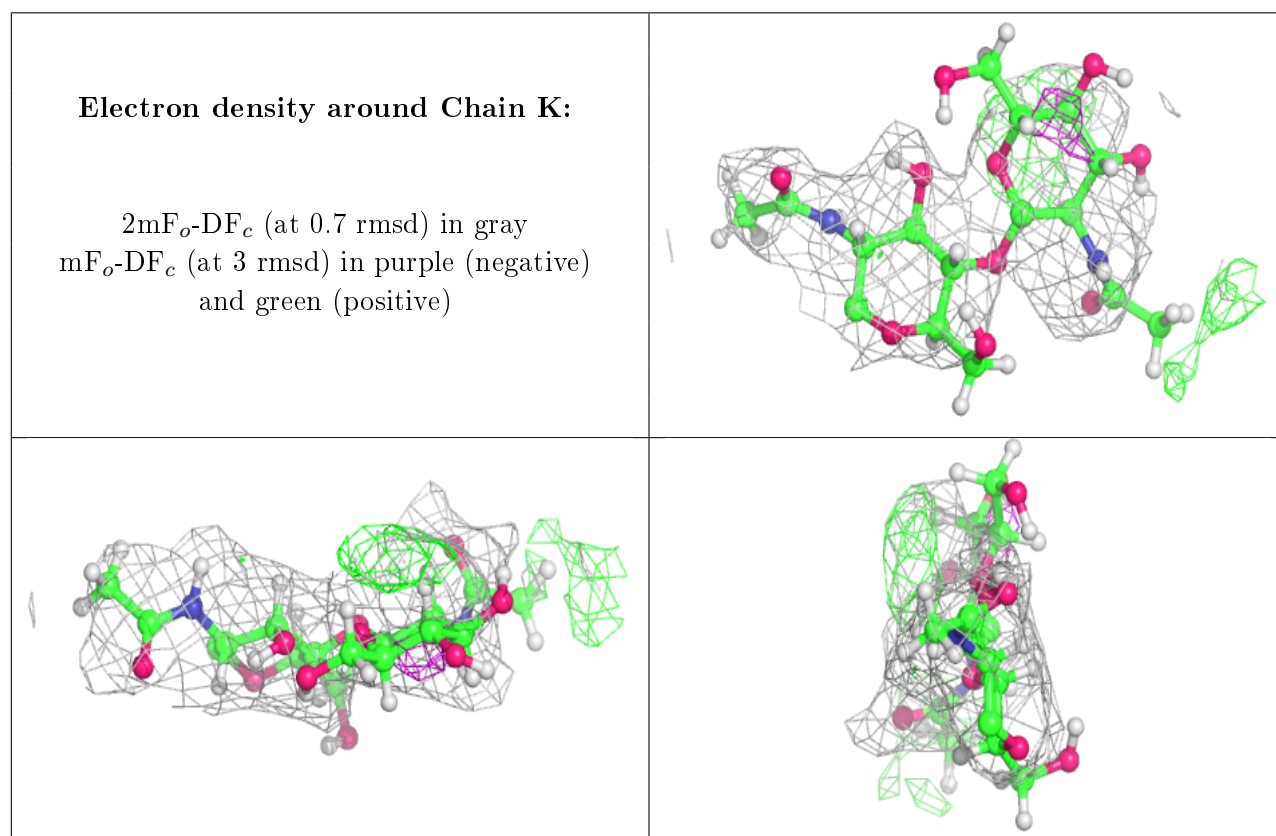
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	K	2	14/15	0.60	0.38	112,122,145,150	0
8	MAN	M	4	11/12	0.69	0.43	106,115,138,138	0
8	BMA	M	3	11/12	0.73	0.30	103,113,135,136	0
6	BMA	G	3	11/12	0.82	0.16	58,74,92,95	0
6	MAN	G	4	11/12	0.84	0.14	65,72,87,89	0
7	NAG	K	1	14/15	0.85	0.24	77,95,114,119	0
6	MAN	G	6	11/12	0.85	0.15	71,78,92,95	0
8	NAG	M	2	14/15	0.85	0.23	66,86,99,105	0
6	MAN	G	5	11/12	0.89	0.15	73,78,93,95	0

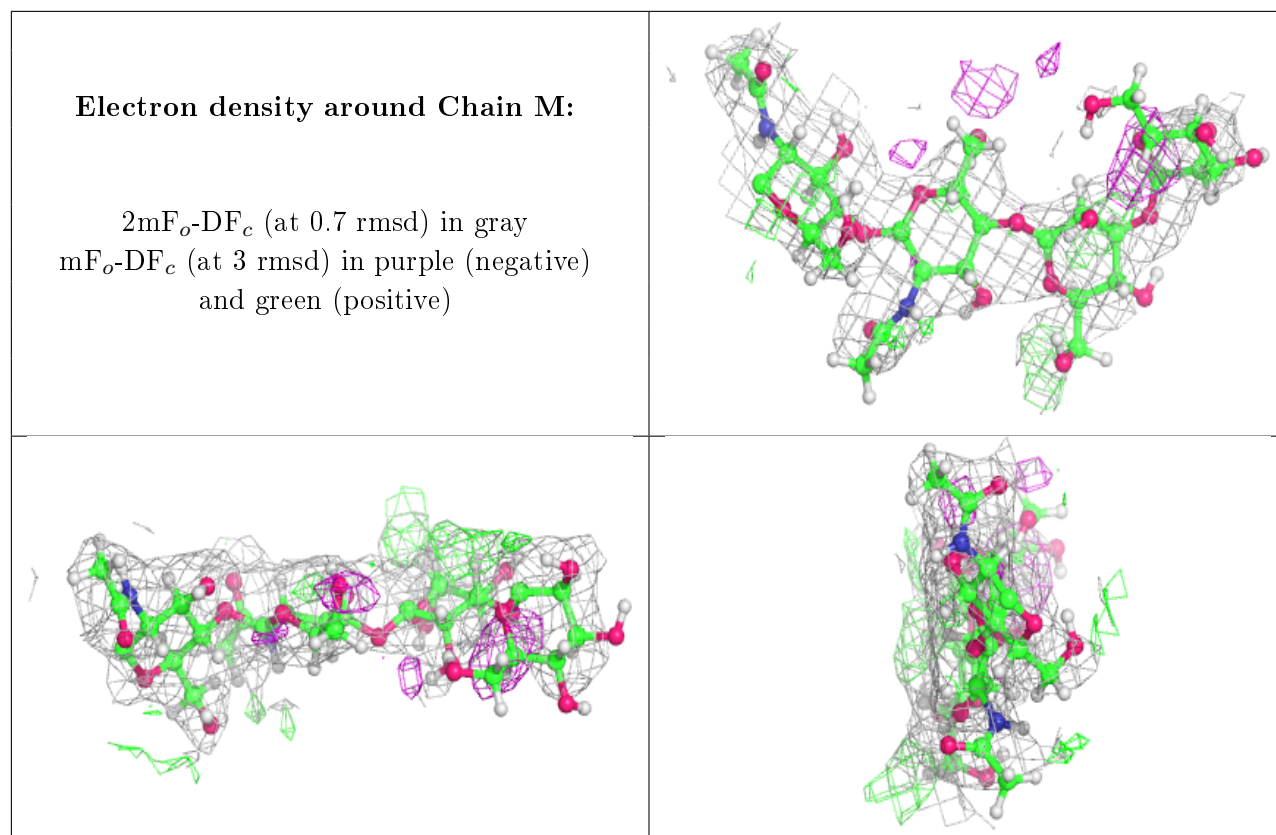
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	M	1	14/15	0.92	0.12	41,55,74,79	0
6	NAG	G	2	14/15	0.96	0.14	34,48,64,68	0
6	NAG	G	1	14/15	0.97	0.16	16,30,47,55	0

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(\AA^2)	Q<0.9
9	GOL	C	1454	6/6	0.64	0.40	86,104,110,114	0
13	NAG	C	2015	14/15	0.66	0.35	86,102,119,129	0
9	GOL	A	1456	6/6	0.68	0.29	64,84,100,103	0
9	GOL	C	1457	6/6	0.72	0.35	65,78,87,92	0
9	GOL	C	1455	6/6	0.81	0.20	85,102,105,107	0
9	GOL	E	1220	6/6	0.83	0.19	67,81,85,85	0
9	GOL	J	1498	6/6	0.84	0.30	68,82,86,88	0
9	GOL	F	1216	6/6	0.85	0.19	58,70,80,83	0
10	SO4	A	1458	5/5	0.87	0.23	95,97,98,102	0
9	GOL	F	1215	6/6	0.88	0.18	70,84,86,86	0
10	SO4	A	1457	5/5	0.88	0.22	72,79,82,82	0
9	GOL	A	1455	6/6	0.89	0.26	56,67,77,79	0
9	GOL	C	1456	6/6	0.92	0.23	62,79,89,95	0
12	MN	B	2002	1/1	0.97	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	CA	C	2007	1/1	0.98	0.14	41,41,41,41	0
11	CA	C	2005	1/1	0.98	0.15	46,46,46,46	0
11	CA	C	2004	1/1	0.98	0.11	53,53,53,53	0
12	MN	D	2003	1/1	0.99	0.12	33,33,33,33	0
11	CA	C	2006	1/1	0.99	0.12	42,42,42,42	0
11	CA	A	2004	1/1	0.99	0.14	27,27,27,27	0
11	CA	A	2006	1/1	0.99	0.17	19,19,19,19	0
12	MN	D	2002	1/1	1.00	0.18	30,30,30,30	0
11	CA	A	2005	1/1	1.00	0.16	23,23,23,23	0
12	MN	B	2001	1/1	1.00	0.20	23,23,23,23	0
11	CA	A	2007	1/1	1.00	0.17	23,23,23,23	0
12	MN	B	2003	1/1	1.00	0.13	28,28,28,28	0
12	MN	D	2001	1/1	1.00	0.20	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.