



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 05:11 PM EDT

PDB ID : 3NIG
Title : The Closed Headpiece of Integrin IIB 3 and its Complex with an IIB 3 -Specific Antagonist That Does Not Induce Opening
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on : 2010-06-15
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

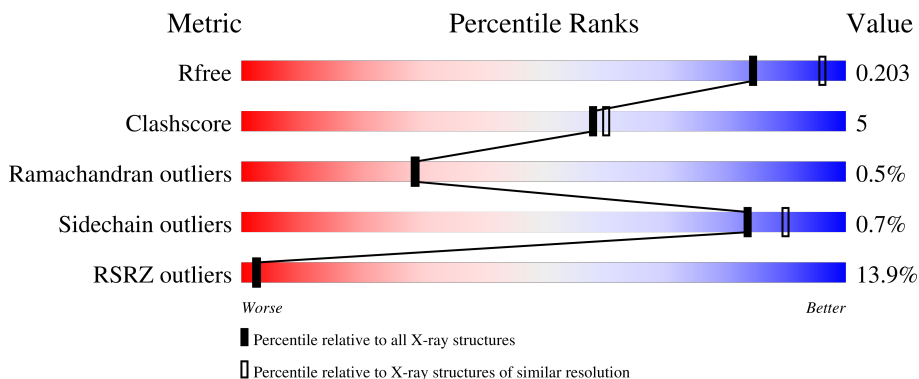
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	457	 96%
1	C	457	 92% 7%
2	B	471	 16% 86% 12%
2	D	471	 8% 88% 11%
3	E	221	 49% 74% 22%

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	3	
5	J	3	
6	I	2	
6	K	2	

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
5	MAN	G	3	X	-	-	-
5	MAN	J	3	X	-	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 22226 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	Total	C	N	O	S	0	3	0
			3515	2235	605	667	8			
1	C	453	Total	C	N	O	S	0	3	0
			3489	2217	601	663	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	466	Total	C	N	O	S	0	0	0
			3590	2236	613	708	33			
2	D	471	Total	C	N	O	S	0	1	0
			3634	2265	620	715	34			

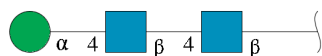
- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Ca	0	0
			4	4		
7	B	2	Total	Ca	0	0
			2	2		
7	C	4	Total	Ca	0	0
			4	4		
7	D	2	Total	Ca	0	0
			2	2		

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



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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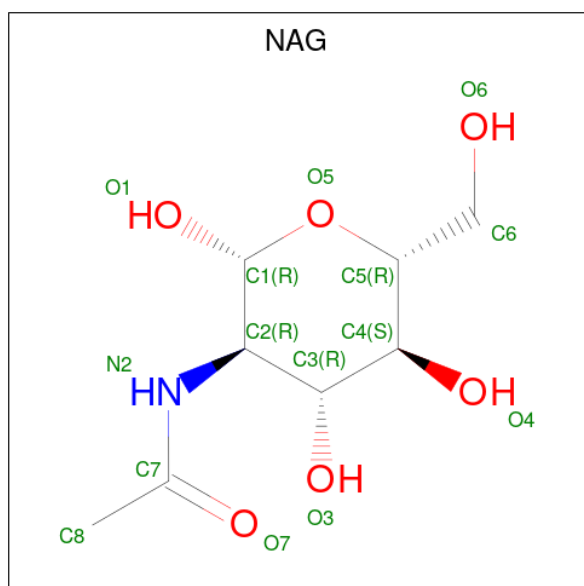
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
9	A	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0
9	D	1	Total 5	O 4	S 1	0	0
9	L	1	Total 5	O 4	S 1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
10	B	1	Total 1	Mg 1	0	0
10	D	1	Total 1	Mg 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

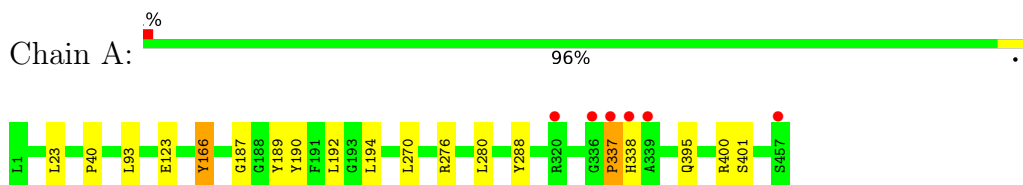
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	446	Total O 446 446	0	0
12	B	231	Total O 231 231	0	0
12	C	259	Total O 259 259	0	0
12	D	191	Total O 191 191	0	0
12	E	9	Total O 9 9	0	0
12	F	12	Total O 12 12	0	0
12	H	32	Total O 32 32	0	0
12	L	47	Total O 47 47	0	0

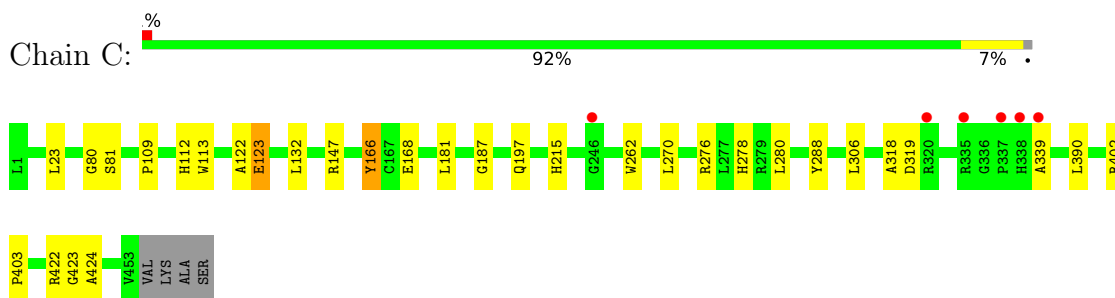
3 Residue-property plots [i](#)

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.

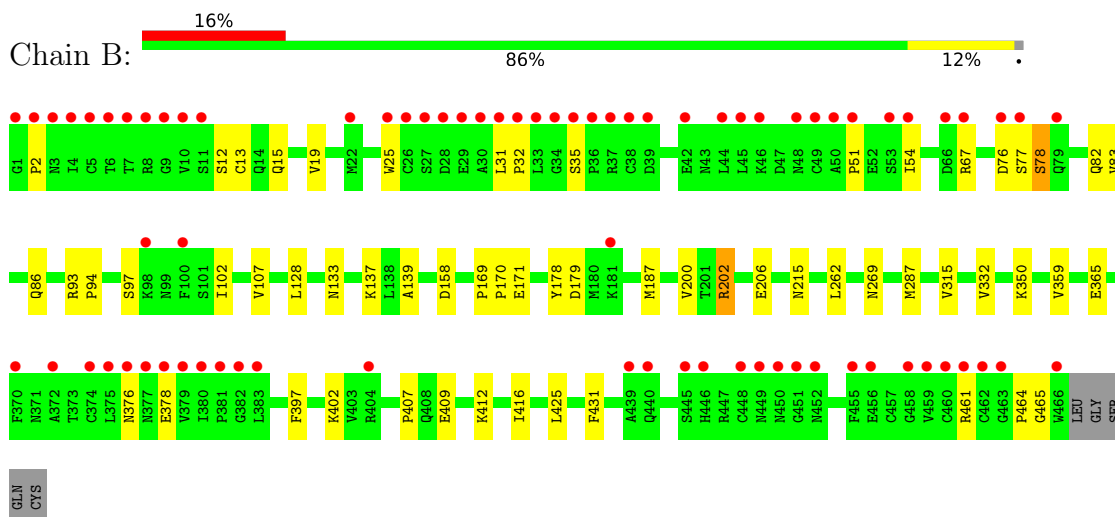
- Molecule 1: Integrin alpha-IIb



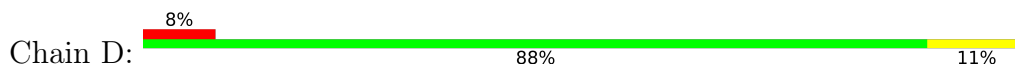
- Molecule 1: Integrin alpha-IIb

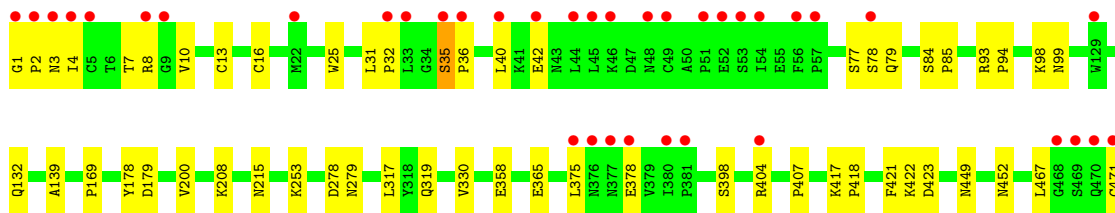


- Molecule 2: Integrin beta-3

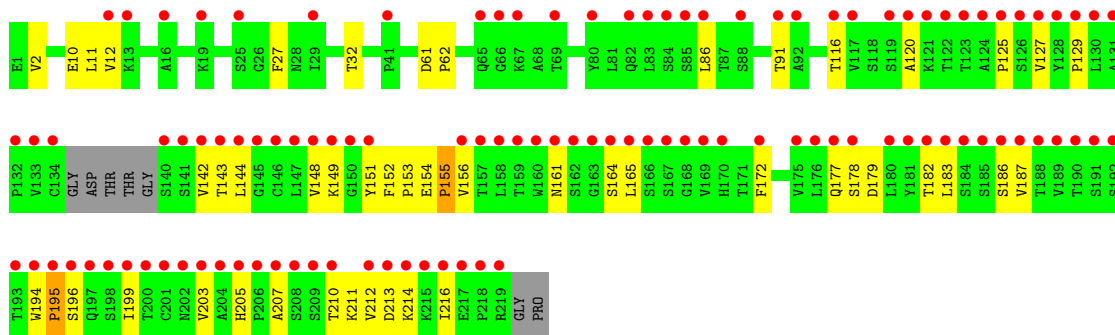
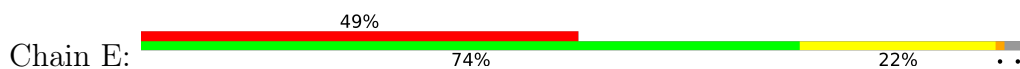


- Molecule 2: Integrin beta-3

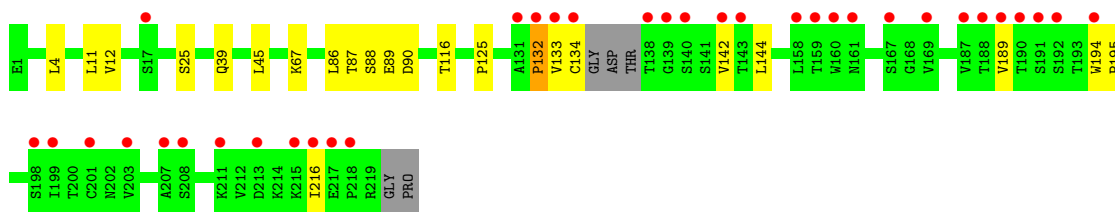
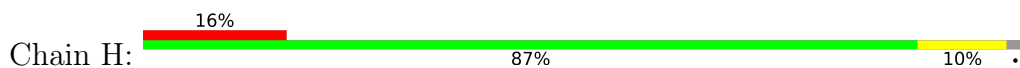




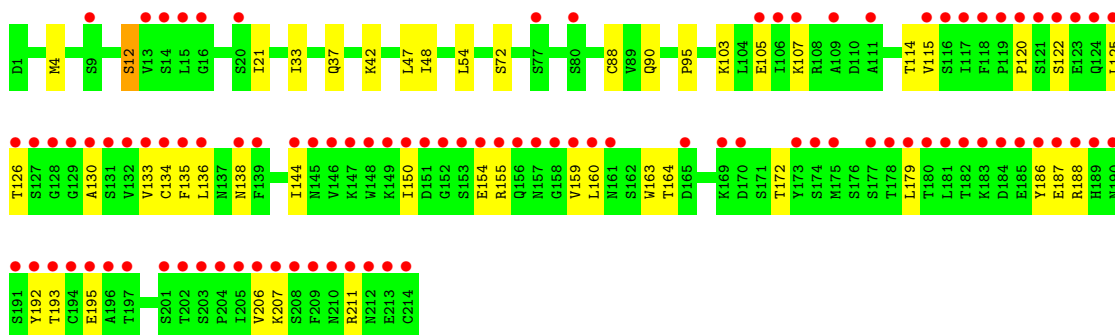
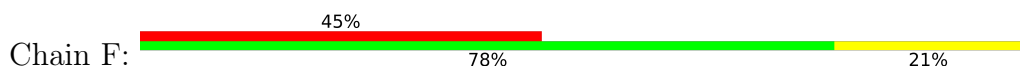
• Molecule 3: Monoclonal antibody 10E5 heavy chain



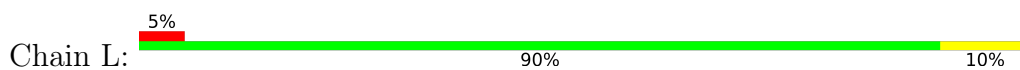
• Molecule 3: Monoclonal antibody 10E5 heavy chain



• Molecule 4: Monoclonal antibody 10E5 light chain



• Molecule 4: Monoclonal antibody 10E5 light chain





- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

MAG1
MAG2
MAN3

- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%

MAG1
MAG2
MAN3

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	260.67Å 145.17Å 104.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.25 48.49 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.49-2.25) 99.9 (48.49-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.24Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.172 , 0.212 0.161 , 0.203	Depositor DCC
R_{free} test set	1009 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22226	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, MG, GOL, MAN, SO4

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	0.63	0/3621	0.68	1/4934 (0.0%)
1	C	0.49	0/3595	0.60	0/4899
2	B	0.50	0/3657	0.62	3/4959 (0.1%)
2	D	0.45	0/3706	0.55	0/5026
3	E	0.28	0/1673	0.46	0/2290
3	H	0.35	0/1684	0.51	0/2305
4	F	0.29	0/1673	0.46	0/2269
4	L	0.36	0/1673	0.54	0/2269
All	All	0.47	0/21282	0.58	4/28951 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	B	202	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	280	LEU	CA-CB-CG	-5.67	102.25	115.30
2	B	262	LEU	CA-CB-CG	-5.51	102.62	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	78	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3515	0	3361	9	0
1	C	3489	0	3327	23	0
2	B	3590	0	3511	36	0
2	D	3634	0	3551	34	0
3	E	1631	0	1590	36	0
3	H	1642	0	1600	14	0
4	F	1637	0	1553	32	0
4	L	1637	0	1553	13	0
5	G	39	0	34	0	0
5	J	39	0	34	2	0
6	I	28	0	25	1	0
6	K	28	0	25	1	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
8	A	12	0	16	3	0
8	C	6	0	8	2	0
9	A	10	0	0	1	0
9	C	10	0	0	0	0
9	D	5	0	0	0	0
9	L	5	0	0	1	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	A	446	0	0	1	0
12	B	231	0	0	1	0
12	C	259	0	0	2	0
12	D	191	0	0	2	0
12	E	9	0	0	1	0
12	F	12	0	0	0	0
12	H	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	47	0	0	1	0
All	All	22226	0	20214	197	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 5.

All (197) 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)
2:D:365:GLU:HG3	2:D:407:PRO:HG3	1.66	0.76
2:D:78:SER:HB3	2:D:422:LYS:HE2	1.75	0.68
3:E:161:ASN:HB2	3:E:164:SER:HB2	1.77	0.66
2:D:375:LEU:O	2:D:378:GLU:HB2	1.95	0.65
1:C:402:ARG:HD2	12:C:574:HOH:O	1.98	0.64
3:H:87:THR:HG22	3:H:88:SER:N	2.15	0.62
2:B:102:ILE:HD13	2:B:425:LEU:HD22	1.80	0.62
2:B:82:GLN:HG2	2:B:107:VAL:CG2	2.30	0.61
3:E:125:PRO:HA	3:E:151:TYR:HB3	1.81	0.61
3:E:129:PRO:HB3	3:E:216:ILE:HD13	1.81	0.61
9:A:461:SO4:O3	12:A:1036:HOH:O	2.13	0.60
2:B:67:ARG:H	2:B:86:GLN:HE22	1.50	0.59
4:F:150:ILE:HD11	4:F:155:ARG:HD2	1.84	0.59
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.85	0.59
3:H:133:VAL:O	3:H:134:CYS:SG	2.62	0.57
4:L:155:ARG:HA	9:L:215:SO4:O3	2.05	0.57
2:B:365:GLU:HG3	2:B:407:PRO:HG3	1.85	0.57
2:B:82:GLN:HG2	2:B:107:VAL:HG23	1.87	0.56
1:C:122:ALA:O	1:C:123:GLU:HB2	2.05	0.55
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.88	0.55
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.88	0.55
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.35	0.55
3:H:194:TRP:CG	3:H:195:PRO:HA	2.41	0.54
2:B:97:SER:HB3	2:B:402:LYS:HG2	1.89	0.54
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.43	0.54
1:A:337:PRO:O	1:A:338:HIS:CD2	2.61	0.54
12:H:1009:HOH:O	4:L:160:LEU:HD12	2.08	0.54
4:F:4:MET:HE2	4:F:90:GLN:HB3	1.90	0.53
2:B:83:VAL:CG1	2:B:102:ILE:HD11	2.38	0.53
2:D:79:GLN:N	2:D:79:GLN:OE1	2.42	0.53
3:E:183:LEU:C	3:E:183:LEU:HD23	2.29	0.53
2:D:4:ILE:O	2:D:8:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:194:TRP:HA	3:E:196:SER:H	1.74	0.52
2:D:358:GLU:HG2	2:D:417:LYS:O	2.09	0.52
1:C:132:LEU:N	1:C:132:LEU:HD12	2.25	0.52
8:C:458:GOL:O3	8:C:458:GOL:O1	2.26	0.52
3:E:142:VAL:HG22	3:E:143:THR:N	2.25	0.52
5:J:1:NAG:H61	5:J:2:NAG:C1	2.40	0.51
2:B:51:PRO:HA	2:B:54:ILE:HD13	1.93	0.51
5:J:2:NAG:O3	5:J:3:MAN:H61	2.11	0.51
1:C:112:HIS:CE1	8:C:458:GOL:H12	2.46	0.51
2:D:178:TYR:CG	2:D:179:ASP:N	2.79	0.51
4:L:136:LEU:HD12	4:L:136:LEU:N	2.26	0.51
2:B:102:ILE:HG22	2:B:397:PHE:HB2	1.93	0.51
4:L:85:ASP:OD1	4:L:103:LYS:HG3	2.11	0.50
2:D:98:LYS:HD3	2:D:99:ASN:H	1.76	0.50
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.46	0.50
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.45	0.50
4:F:193:THR:HG23	4:F:206:VAL:HG13	1.92	0.50
3:E:172:PHE:CD1	4:F:164:THR:HG23	2.46	0.50
1:C:270:LEU:HD23	1:C:276:ARG:HA	1.94	0.49
4:L:167:ASP:HB3	4:L:170:ASP:OD1	2.11	0.49
1:A:400:ARG:CD	8:A:459:GOL:H12	2.42	0.49
1:A:400:ARG:HD2	8:A:459:GOL:H12	1.94	0.49
1:A:40:PRO:HA	1:A:93:LEU:O	2.12	0.49
2:B:407:PRO:HG2	2:B:431:PHE:CE1	2.48	0.49
2:B:31:LEU:HG	2:B:35:SER:HB2	1.94	0.49
1:C:318:ALA:O	1:C:319:ASP:HB2	2.13	0.49
3:E:120:ALA:HB2	3:E:179:ASP:HB3	1.93	0.49
2:B:67:ARG:N	2:B:86:GLN:HE22	2.10	0.49
3:E:186:SER:HB3	4:F:135:PHE:CE1	2.48	0.49
3:H:11:LEU:HD12	3:H:116:THR:HB	1.94	0.49
3:E:152:PHE:CE2	3:E:153:PRO:HG3	2.47	0.49
1:C:113:TRP:CZ3	1:C:147:ARG:HD3	2.48	0.48
2:D:84:SER:HA	2:D:85:PRO:C	2.33	0.48
4:L:211:ARG:O	4:L:212:ASN:HB2	2.13	0.48
2:B:359:VAL:HG22	2:B:416:ILE:HD13	1.96	0.48
1:C:166:TYR:O	1:C:187:GLY:HA3	2.14	0.47
3:E:149:LYS:HG2	3:E:182:THR:HG23	1.96	0.47
2:D:398:SER:OG	6:K:1:NAG:H81	2.14	0.47
3:E:129:PRO:CG	3:E:214:LYS:HB3	2.44	0.47
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.97	0.47
1:C:280:LEU:CD1	1:C:306:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:PRO:HA	2:B:465:GLY:HA2	1.67	0.47
3:E:194:TRP:CD1	3:E:195:PRO:HA	2.50	0.47
3:E:199:ILE:HB	12:E:1010:HOH:O	2.14	0.47
2:B:171:GLU:HB2	12:B:1219:HOH:O	2.15	0.47
3:H:87:THR:CG2	3:H:88:SER:N	2.77	0.47
2:B:102:ILE:CG2	2:B:397:PHE:HB2	2.45	0.47
4:F:144:ILE:HD11	4:F:163:TRP:HE1	1.80	0.47
4:F:150:ILE:HG23	4:F:192:TYR:CE2	2.50	0.47
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.98	0.46
2:B:82:GLN:HG2	2:B:107:VAL:HG21	1.95	0.46
4:L:125:LEU:O	4:L:183:LYS:HD2	2.15	0.46
1:A:270:LEU:HD23	1:A:276:ARG:HA	1.97	0.46
1:C:390:LEU:HD12	1:C:390:LEU:N	2.30	0.46
2:B:133:ASN:ND2	2:B:137:LYS:HD2	2.31	0.46
1:A:194:LEU:HD12	1:A:194:LEU:C	2.36	0.46
4:F:21:ILE:O	4:F:72:SER:HA	2.15	0.46
2:B:77:SER:HA	2:B:78:SER:HA	1.51	0.46
2:D:31:LEU:HD12	2:D:32:PRO:HD2	1.97	0.46
3:E:154:GLU:OE1	3:E:155:PRO:HA	2.16	0.46
4:F:125:LEU:HD23	4:F:130:ALA:HB2	1.98	0.45
2:B:178:TYR:CE2	2:B:179:ASP:HB3	2.52	0.45
3:E:205:HIS:CE1	3:E:207:ALA:HB3	2.52	0.45
4:F:115:VAL:O	4:F:207:LYS:HE3	2.16	0.45
4:F:138:ASN:HA	4:F:172:THR:OG1	2.17	0.45
1:A:166:TYR:O	1:A:187:GLY:HA3	2.17	0.45
2:B:178:TYR:CG	2:B:179:ASP:N	2.83	0.45
4:F:133:VAL:HG12	4:F:134:CYS:N	2.31	0.45
4:L:135:PHE:C	4:L:136:LEU:HD12	2.37	0.45
3:E:12:VAL:HG21	3:E:86:LEU:HD13	1.98	0.45
3:H:4:LEU:HD12	3:H:4:LEU:N	2.31	0.45
3:E:212:VAL:HG12	3:E:213:ASP:N	2.32	0.45
4:F:115:VAL:HG12	4:F:207:LYS:HG3	1.97	0.45
1:C:122:ALA:O	1:C:123:GLU:CB	2.64	0.45
4:F:159:VAL:HG22	4:F:179:LEU:HD13	1.98	0.45
1:C:278[B]:HIS:NE2	1:C:339:ALA:HA	2.32	0.45
2:D:93:ARG:HB2	2:D:94:PRO:CD	2.47	0.45
2:D:423:ASP:HB3	12:D:1208:HOH:O	2.16	0.45
1:A:189:TYR:O	1:A:192:LEU:HD13	2.17	0.44
2:D:3:ASN:O	2:D:7:THR:HG23	2.17	0.44
2:D:77:SER:HA	2:D:78:SER:HA	1.59	0.44
2:B:83:VAL:HG12	2:B:102:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:33:ILE:HD11	4:F:88:CYS:HB2	2.00	0.44
4:F:187:GLU:HA	4:F:211:ARG:HD2	1.99	0.44
3:H:67:LYS:HE3	3:H:90:ASP:OD2	2.17	0.44
4:F:120:PRO:CG	4:F:130:ALA:HB1	2.47	0.44
1:A:401:SER:H	8:A:459:GOL:H2	1.83	0.44
3:E:10:GLU:C	3:E:11:LEU:HD12	2.38	0.44
3:E:91:THR:HG23	3:E:116:THR:HA	1.99	0.44
2:B:178:TYR:CD2	2:B:179:ASP:N	2.86	0.44
4:L:13:VAL:HG11	4:L:19:VAL:HG11	2.00	0.44
4:F:186:TYR:C	4:F:188:ARG:H	2.21	0.43
2:D:319:GLN:HA	2:D:330:VAL:HG21	2.01	0.43
6:I:1:NAG:H62	6:I:2:NAG:C1	2.49	0.43
3:E:11:LEU:HD21	3:E:153:PRO:HB3	2.01	0.43
3:E:125:PRO:HD2	3:E:210:THR:HG21	1.99	0.43
3:E:156:VAL:HG12	3:E:205:HIS:HD2	1.83	0.43
4:F:150:ILE:CD1	4:F:155:ARG:HD2	2.49	0.43
3:H:132:PRO:HD3	3:H:144:LEU:HD22	2.00	0.43
3:E:149:LYS:HE3	3:E:182:THR:OG1	2.19	0.43
2:B:269:ASN:HA	2:B:287:MET:CG	2.48	0.43
2:B:169:PRO:HB2	2:B:170:PRO:HD2	2.00	0.43
1:C:278[A]:HIS:CD2	1:C:339:ALA:HB1	2.54	0.43
2:D:467:LEU:O	2:D:471:CYS:HA	2.19	0.42
4:F:206:VAL:HG12	4:F:207:LYS:N	2.34	0.42
2:B:315:VAL:HG21	2:B:332:VAL:HG22	2.01	0.42
1:C:181:LEU:O	1:C:197:GLN:HA	2.19	0.42
4:F:12:SER:HB2	4:F:107:LYS:HG2	2.00	0.42
4:F:136:LEU:HD12	4:F:136:LEU:N	2.35	0.42
1:C:262:TRP:HB3	2:D:317:LEU:HD13	2.02	0.42
3:H:87:THR:HG22	3:H:89:GLU:H	1.84	0.42
4:L:4:MET:HE1	4:L:90:GLN:HB3	1.99	0.42
1:C:422:ARG:NH2	12:C:804:HOH:O	2.52	0.42
3:E:144:LEU:HD21	3:E:194:TRP:CZ3	2.54	0.42
2:B:139:ALA:HB2	2:B:200:VAL:HG11	2.00	0.42
2:D:3:ASN:ND2	2:D:40:LEU:HG	2.34	0.42
2:D:139:ALA:HB2	2:D:200:VAL:HG11	2.01	0.42
2:D:278:ASP:O	2:D:279:ASN:HB2	2.20	0.42
3:E:210:THR:C	3:E:211:LYS:HG3	2.40	0.42
2:B:376:ASN:C	2:B:378:GLU:N	2.71	0.42
2:D:404:ARG:HG3	12:D:547:HOH:O	2.20	0.42
3:E:125:PRO:CA	3:E:151:TYR:HB3	2.47	0.42
3:H:132:PRO:HD3	3:H:144:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:54:LEU:HD21	4:L:60:SER:HA	2.01	0.42
4:F:114:THR:O	4:F:114:THR:HG22	2.19	0.41
2:B:158:ASP:HB3	2:B:187:MET:CE	2.50	0.41
3:E:125:PRO:HB3	3:E:148:VAL:CG1	2.50	0.41
4:F:195:GLU:HG2	4:F:206:VAL:HG22	2.01	0.41
1:C:280:LEU:CD1	1:C:306:LEU:CD2	2.97	0.41
2:D:42:GLU:H	2:D:42:GLU:CD	2.23	0.41
3:E:165:LEU:HD23	3:E:187:VAL:HG21	2.02	0.41
3:E:205:HIS:HB3	3:E:210:THR:HG22	2.01	0.41
4:F:37:GLN:HB2	4:F:47:LEU:HD11	2.01	0.41
4:L:124:GLN:HG2	4:L:129:GLY:O	2.20	0.41
1:C:390:LEU:HD23	1:C:403:PRO:HG3	2.03	0.41
3:E:177:GLN:OE1	4:F:160:LEU:HD11	2.20	0.41
4:F:48:ILE:HD11	4:F:54:LEU:HD23	2.03	0.41
3:H:144:LEU:HD13	3:H:216:ILE:HG21	2.01	0.41
1:C:109:PRO:O	1:C:168:GLU:HA	2.21	0.41
1:C:280:LEU:HD11	1:C:306:LEU:HD23	2.02	0.41
4:F:103:LYS:HG2	4:F:105:GLU:HG3	2.02	0.41
2:D:1:GLY:HA2	2:D:2:PRO:HD3	1.89	0.41
4:F:186:TYR:CE2	4:F:211:ARG:HG3	2.55	0.41
2:B:15:GLN:O	2:B:19:VAL:HG23	2.21	0.41
2:B:409:GLU:HB2	2:B:412:LYS:HE3	2.03	0.41
2:D:132:GLN:OE1	2:D:208:LYS:HG2	2.21	0.41
3:H:142:VAL:CG1	3:H:189:VAL:HG23	2.51	0.41
2:D:35:SER:HA	2:D:36:PRO:HD3	1.97	0.41
2:D:10:VAL:HG21	2:D:16:CYS:HB2	2.03	0.40
3:E:61:ASP:OD1	3:E:62:PRO:HD2	2.21	0.40
1:C:80:GLY:O	1:C:81:SER:HB2	2.21	0.40
1:C:423:GLY:O	1:C:424:ALA:HB3	2.21	0.40
2:D:13:CYS:SG	2:D:25:TRP:CG	3.14	0.40
2:D:449:ASN:CB	2:D:452:ASN:HB2	2.52	0.40
3:E:2:VAL:HG13	3:E:27:PHE:CE1	2.56	0.40
4:F:154:GLU:HG2	4:F:155:ARG:N	2.37	0.40
4:L:45:MET:HG3	12:L:1094:HOH:O	2.21	0.40
2:B:13:CYS:SG	2:B:25:TRP:CD1	3.15	0.40
2:B:350:LYS:HE3	2:B:350:LYS:HB2	1.92	0.40
2:D:169:PRO:HD3	2:D:178:TYR:OH	2.21	0.40
2:D:178:TYR:CD2	2:D:179:ASP:N	2.90	0.40
3:E:127:VAL:HG22	3:E:203:VAL:HG21	2.03	0.40
4:F:42:LYS:HD2	4:F:42:LYS:N	2.37	0.40
4:F:122:SER:O	4:F:126:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:CYS:SG	2:D:25:TRP:CD1	3.14	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	458/457 (100%)	440 (96%)	16 (4%)	2 (0%)	34	37
1	C	454/457 (99%)	439 (97%)	14 (3%)	1 (0%)	47	55
2	B	464/471 (98%)	439 (95%)	22 (5%)	3 (1%)	25	25
2	D	470/471 (100%)	455 (97%)	14 (3%)	1 (0%)	47	55
3	E	210/221 (95%)	183 (87%)	24 (11%)	3 (1%)	11	7
3	H	212/221 (96%)	195 (92%)	16 (8%)	1 (0%)	29	29
4	F	212/214 (99%)	194 (92%)	18 (8%)	0	100	100
4	L	212/214 (99%)	204 (96%)	6 (3%)	2 (1%)	17	14
All	All	2692/2726 (99%)	2549 (95%)	130 (5%)	13 (0%)	29	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	GLU
3	E	178	SER
1	A	123	GLU
2	B	2	PRO
2	B	76	ASP
3	E	195	PRO
4	L	212	ASN
1	A	337	PRO
2	D	253	LYS

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Mol	Chain	Res	Type
4	L	213	GLU
2	B	32	PRO
3	H	132	PRO
3	E	155	PRO

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%)	362 (99%)	5 (1%)	67	76
1	C	364/364 (100%)	361 (99%)	3 (1%)	81	88
2	B	412/416 (99%)	410 (100%)	2 (0%)	88	92
2	D	417/416 (100%)	415 (100%)	2 (0%)	88	92
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	185 (99%)	2 (1%)	73	82
4	F	188/188 (100%)	186 (99%)	2 (1%)	73	82
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2309/2316 (100%)	2293 (99%)	16 (1%)	84	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	288	TYR
1	A	395	GLN
2	B	128	LEU
2	B	215	ASN
1	C	23	LEU
1	C	166	TYR
1	C	288	TYR
2	D	35	SER

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Mol	Chain	Res	Type
2	D	215	ASN
4	F	12	SER
4	F	95	PRO
3	H	25	SER
3	H	125	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
2	B	86	GLN
2	B	438	GLN
2	B	440	GLN
1	C	197	GLN
1	C	338	HIS
1	C	451	GLN
2	D	274	HIS
2	D	452	ASN
3	H	82	GLN

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](#)

10 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	NAG	G	1	2,5	14,14,15	0.75	1 (7%)	17,19,21	0.97	0
5	NAG	G	2	5	14,14,15	0.64	0	17,19,21	3.20	6 (35%)
5	MAN	G	3	5	11,11,12	0.53	0	15,15,17	1.23	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.58	0	17,19,21	1.12	2 (11%)
6	NAG	I	2	6	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
5	NAG	J	1	2,5	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
5	NAG	J	2	5	14,14,15	0.54	0	17,19,21	1.38	1 (5%)
5	MAN	J	3	5	11,11,12	0.52	0	15,15,17	1.38	3 (20%)
6	NAG	K	1	2,6	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
6	NAG	K	2	6	14,14,15	0.55	0	17,19,21	0.94	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	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	MAN	G	3	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
5	NAG	J	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	MAN	J	3	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	NAG	O5-C1	-2.04	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2	NAG	C1-O5-C5	10.07	125.84	112.19
5	G	2	NAG	O5-C5-C6	-5.94	97.89	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2	NAG	C1-O5-C5	4.76	118.64	112.19
5	G	3	MAN	C1-O5-C5	3.19	116.52	112.19
5	J	3	MAN	C1-O5-C5	3.13	116.44	112.19
5	J	1	NAG	O5-C5-C6	3.12	112.10	107.20
5	J	1	NAG	C1-O5-C5	2.96	116.20	112.19
5	G	2	NAG	C3-C4-C5	2.70	115.06	110.24
6	K	1	NAG	C2-N2-C7	-2.53	119.31	122.90
6	I	2	NAG	C8-C7-N2	2.48	120.29	116.10
5	G	2	NAG	O4-C4-C3	-2.47	104.64	110.35
5	G	2	NAG	O5-C5-C4	2.25	116.30	110.83
5	J	3	MAN	O5-C1-C2	-2.23	107.33	110.77
5	G	3	MAN	C2-C3-C4	-2.22	107.05	110.89
6	I	1	NAG	C1-O5-C5	2.19	115.16	112.19
5	J	3	MAN	O2-C2-C1	2.18	113.62	109.15
6	I	1	NAG	C4-C3-C2	2.15	114.17	111.02
6	K	2	NAG	C2-N2-C7	-2.14	119.86	122.90
5	G	2	NAG	C4-C3-C2	2.08	114.06	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	3	MAN	C1
5	J	3	MAN	C1

All (12) torsion outliers are listed below:

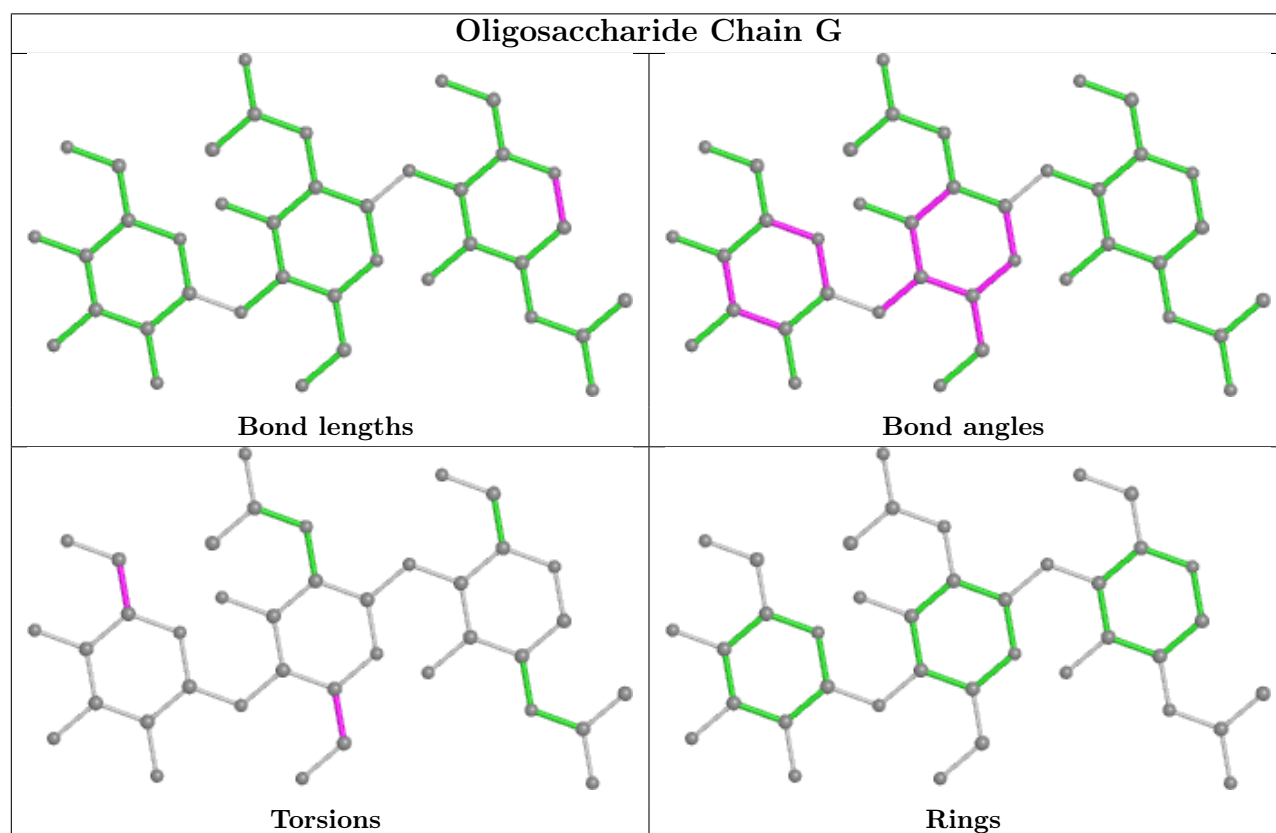
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C8-C7-N2-C2
5	G	3	MAN	C4-C5-C6-O6
5	J	3	MAN	O5-C5-C6-O6
5	G	3	MAN	O5-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C4-C5-C6-O6
5	J	3	MAN	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6

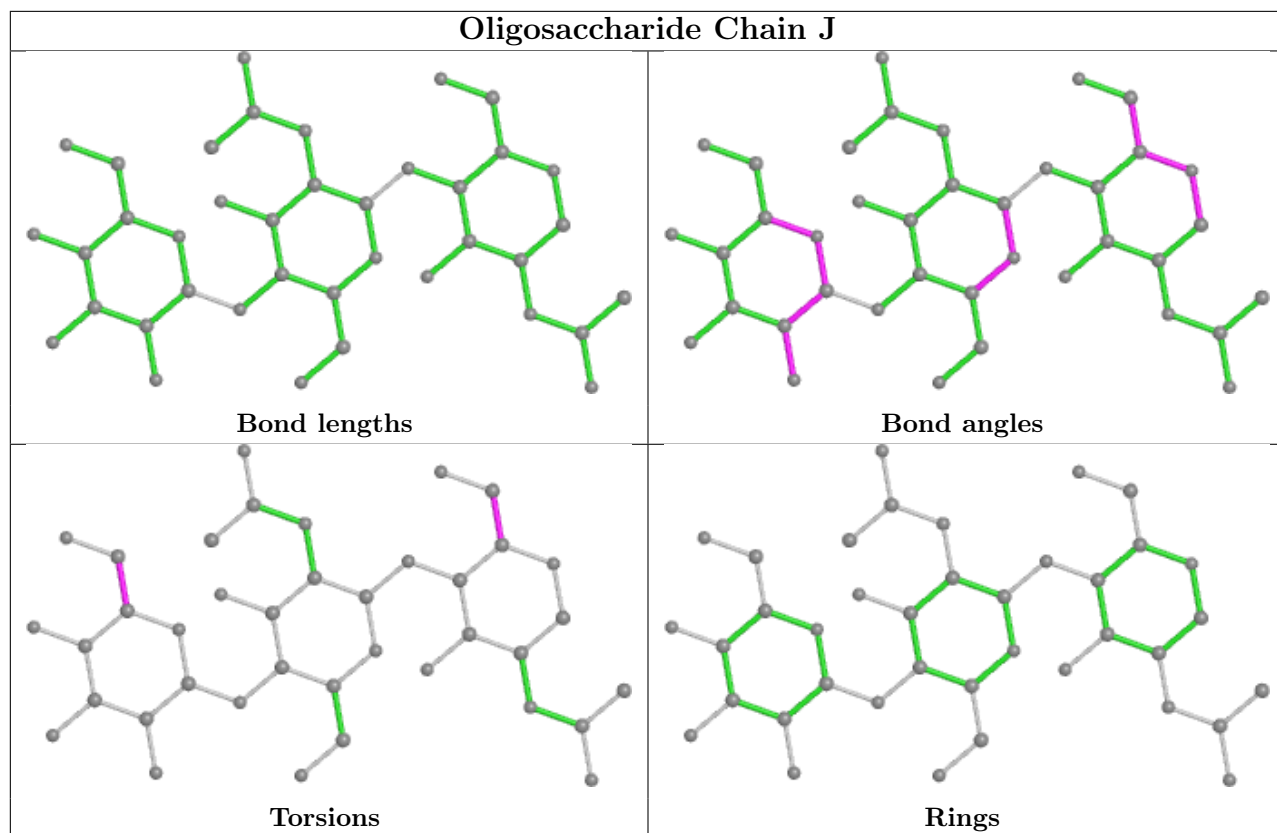
There are no ring outliers.

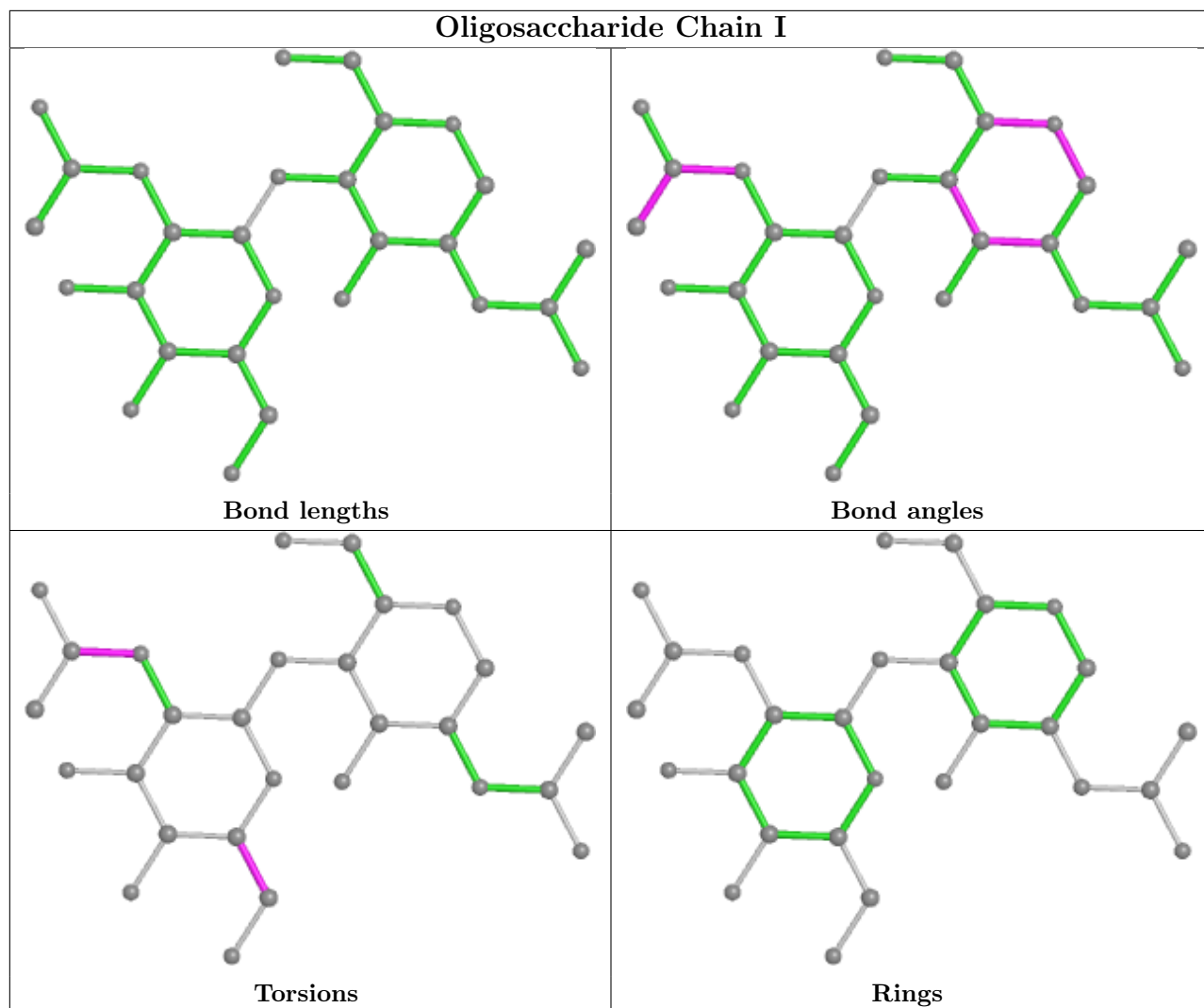
6 monomers are involved in 4 short contacts:

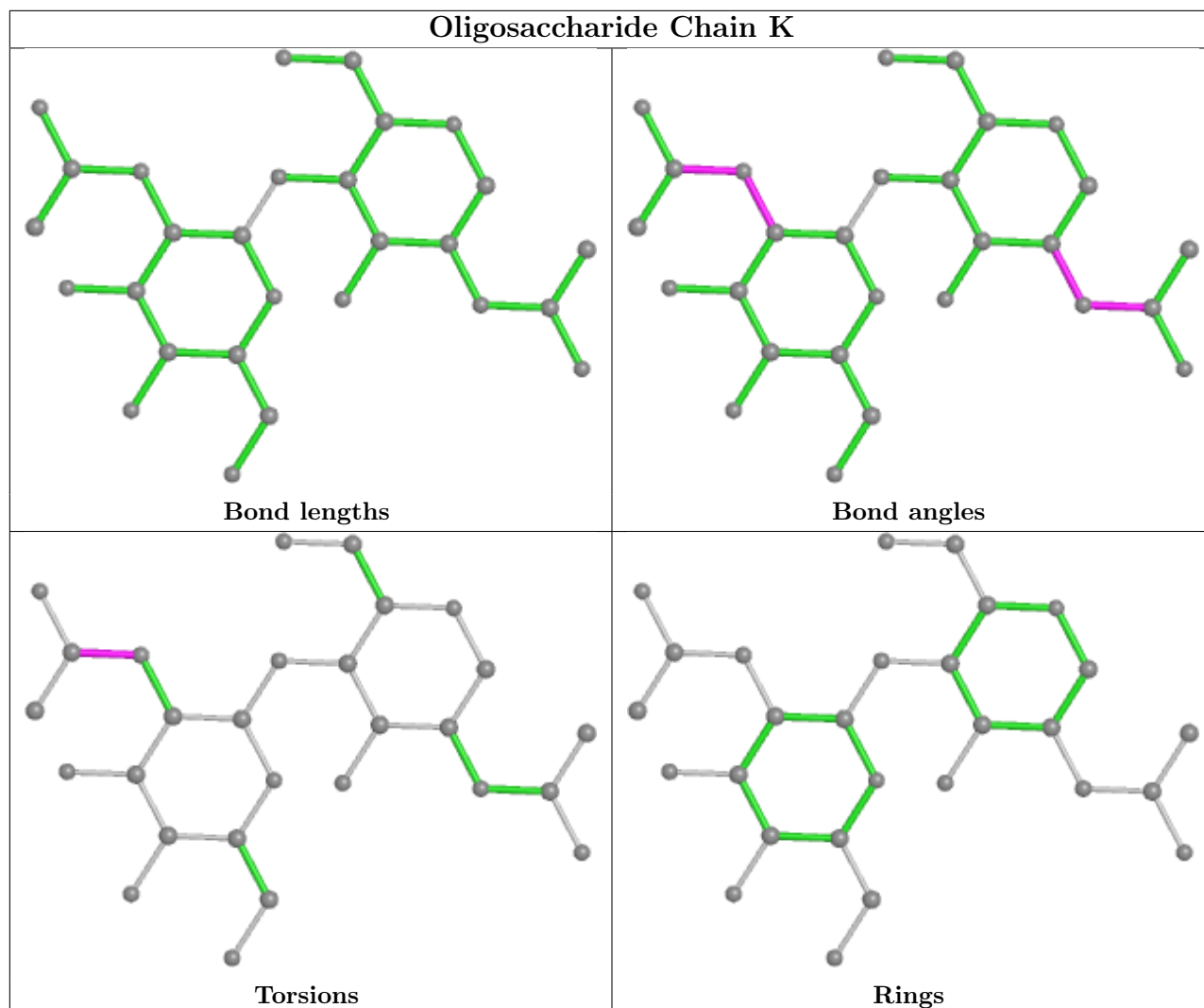
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0
6	I	1	NAG	1	0
5	J	2	NAG	2	0
5	J	3	MAN	1	0
6	I	2	NAG	1	0
5	J	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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	SO4	A	460	-	4,4,4	0.24	0	6,6,6	0.38	0
9	SO4	C	460	-	4,4,4	0.25	0	6,6,6	0.46	0
9	SO4	A	461	-	4,4,4	0.26	0	6,6,6	1.24	0
11	NAG	D	3099	2	14,14,15	0.60	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	C	459	-	4,4,4	0.18	0	6,6,6	0.44	0
9	SO4	L	215	-	4,4,4	0.18	0	6,6,6	0.26	0
11	NAG	B	3099	2	14,14,15	0.55	0	17,19,21	0.64	0
8	GOL	A	458	-	5,5,5	0.23	0	5,5,5	0.47	0
8	GOL	C	458	-	5,5,5	0.25	0	5,5,5	0.79	0
8	GOL	A	459	-	5,5,5	0.44	0	5,5,5	0.34	0
9	SO4	D	472	-	4,4,4	0.24	0	6,6,6	0.54	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
11	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
11	NAG	B	3099	2	-	4/6/23/26	0/1/1/1
8	GOL	A	458	-	-	0/4/4/4	-
8	GOL	C	458	-	-	2/4/4/4	-
8	GOL	A	459	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	459	GOL	O1-C1-C2-C3
8	C	458	GOL	O1-C1-C2-O2
8	C	458	GOL	O1-C1-C2-C3
11	B	3099	NAG	O5-C5-C6-O6
8	A	459	GOL	O2-C2-C3-O3
8	A	459	GOL	C1-C2-C3-O3
8	A	459	GOL	O1-C1-C2-O2
11	B	3099	NAG	C4-C5-C6-O6
11	B	3099	NAG	C8-C7-N2-C2
11	B	3099	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	461	SO4	1	0
9	L	215	SO4	1	0
8	C	458	GOL	2	0
8	A	459	GOL	3	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	457/457 (100%)	0.25	6 (1%) 77 79	15, 27, 61, 131	0
1	C	453/457 (99%)	0.12	6 (1%) 77 79	21, 42, 76, 121	0
2	B	466/471 (98%)	0.81	76 (16%) 1 1	18, 56, 134, 196	0
2	D	471/471 (100%)	0.33	38 (8%) 12 13	24, 54, 118, 159	0
3	E	214/221 (96%)	2.70	109 (50%) 0 0	47, 110, 196, 236	0
3	H	216/221 (97%)	0.50	35 (16%) 1 1	30, 77, 138, 181	0
4	F	214/214 (100%)	2.12	96 (44%) 0 0	49, 98, 187, 249	1 (0%)
4	L	214/214 (100%)	0.23	10 (4%) 31 34	36, 67, 102, 164	1 (0%)
All	All	2705/2726 (99%)	0.70	376 (13%) 2 2	15, 55, 142, 249	2 (0%)

All (376) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	216	ILE	15.7
3	E	199	ILE	13.9
3	E	198	SER	13.8
3	E	133	VAL	12.6
3	E	215	LYS	12.0
3	E	212	VAL	12.0
4	F	214	CYS	11.5
2	D	469	SER	11.5
3	E	128	TYR	11.3
3	E	194	TRP	10.6
3	E	219	ARG	10.4
3	E	142	VAL	10.3
4	F	181	LEU	10.3
3	E	130	LEU	9.9
3	E	134	CYS	9.7
4	F	130	ALA	9.6

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Mol	Chain	Res	Type	RSRZ
2	B	36	PRO	9.5
3	E	144	LEU	9.3
4	F	125	LEU	9.2
3	E	200	THR	8.8
4	F	132	VAL	8.8
2	B	33	LEU	8.7
3	E	165	LEU	8.6
2	B	1	GLY	8.6
3	E	131	ALA	8.4
4	F	118	PHE	8.2
3	E	129	PRO	8.2
4	F	193	THR	8.1
4	F	122	SER	8.1
4	F	179	LEU	7.8
3	E	217	GLU	7.7
4	F	194	CYS	7.7
2	B	34	GLY	7.6
2	B	10	VAL	7.3
4	F	180	THR	7.3
3	E	195	PRO	7.1
3	E	160	TRP	7.1
4	F	119	PRO	7.0
3	E	132	PRO	6.9
3	E	201	CYS	6.8
2	B	31	LEU	6.8
4	F	182	THR	6.8
2	B	28	ASP	6.6
3	E	147	LEU	6.6
4	F	117	ILE	6.5
4	F	210	ASN	6.5
3	E	189	VAL	6.3
4	L	214	CYS	6.3
4	F	209	PHE	6.2
4	F	133	VAL	6.2
3	E	218	PRO	6.1
4	F	186	TYR	6.1
2	B	44	LEU	6.1
4	F	126	THR	6.1
3	E	145	GLY	6.0
4	F	115	VAL	6.0
2	D	78	SER	6.0
4	F	129	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
4	F	213	GLU	5.9
2	B	2	PRO	5.9
4	F	120	PRO	5.9
3	E	214	LYS	5.9
3	E	143	THR	5.8
4	F	158	GLY	5.8
4	F	192	TYR	5.8
3	E	146	CYS	5.7
4	F	127	SER	5.7
4	F	148	TRP	5.7
4	F	124	GLN	5.7
2	B	51	PRO	5.6
2	B	32	PRO	5.6
2	D	2	PRO	5.5
3	E	149	LYS	5.5
2	B	376	ASN	5.5
2	D	470	GLN	5.5
3	E	187	VAL	5.4
3	E	163	GLY	5.4
4	F	136	LEU	5.4
4	F	152	GLY	5.3
4	F	150	ILE	5.3
3	E	164	SER	5.3
4	F	208	SER	5.3
4	F	135	PHE	5.2
2	B	450	ASN	5.1
2	B	4	ILE	5.1
2	B	30	ALA	5.1
4	F	156	GLN	5.1
2	B	375	LEU	5.0
3	E	117	VAL	5.0
2	B	35	SER	5.0
2	D	35	SER	5.0
3	E	213	ASP	5.0
3	H	133	VAL	5.0
2	B	383	LEU	5.0
4	F	212	ASN	5.0
3	H	217	GLU	5.0
3	E	207	ALA	4.9
3	E	210	THR	4.9
3	E	124	ALA	4.9
3	E	208	SER	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	8	ARG	4.9
1	A	337	PRO	4.8
4	F	159	VAL	4.8
3	H	134	CYS	4.8
2	D	44	LEU	4.8
3	E	169	VAL	4.7
3	H	189	VAL	4.7
4	F	191	SER	4.6
2	B	466	TRP	4.6
3	E	183	LEU	4.6
3	E	176	LEU	4.6
4	F	151	ASP	4.6
2	B	462	CYS	4.5
3	E	12	VAL	4.5
2	B	456	GLU	4.5
2	B	5	CYS	4.4
4	F	178	THR	4.4
2	D	376	ASN	4.4
4	L	212	ASN	4.4
4	F	121	SER	4.4
2	B	39	ASP	4.4
3	E	204	ALA	4.4
2	B	382	GLY	4.3
3	E	188	THR	4.3
3	E	140	SER	4.3
4	F	128	GLY	4.3
3	E	127	VAL	4.3
4	F	184	ASP	4.3
2	D	468	GLY	4.2
3	E	161	ASN	4.2
4	F	188	ARG	4.2
4	F	116	SER	4.2
3	E	123	THR	4.2
2	D	33	LEU	4.2
4	F	206	VAL	4.2
2	B	29	GLU	4.2
2	B	46	LYS	4.1
3	E	126	SER	4.1
4	F	155	ARG	4.1
3	E	178	SER	4.1
2	B	381	PRO	4.1
4	F	190	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
3	E	192	SER	4.1
2	D	471	CYS	4.1
2	B	50	ALA	4.1
3	E	83	LEU	4.1
3	H	160	TRP	4.0
4	F	131	SER	4.0
1	C	335	ARG	4.0
3	E	196	SER	4.0
4	F	154	GLU	4.0
3	H	199	ILE	3.9
3	E	159	THR	3.9
2	B	458	GLY	3.9
2	B	6	THR	3.9
4	F	185	GLU	3.9
3	H	216	ILE	3.9
2	D	42	GLU	3.8
2	D	36	PRO	3.8
3	H	201	CYS	3.8
3	E	191	SER	3.8
2	B	7	THR	3.8
2	B	379	VAL	3.8
4	F	157	ASN	3.8
3	E	185	SER	3.7
2	B	37	ARG	3.7
2	B	38	CYS	3.7
3	E	25	SER	3.7
4	F	187	GLU	3.7
3	E	86	LEU	3.7
2	D	380	ILE	3.7
3	E	141	SER	3.7
3	H	138	THR	3.7
2	B	45	LEU	3.6
4	F	146	VAL	3.6
2	B	53	SER	3.6
3	E	186	SER	3.6
4	F	174	SER	3.6
3	E	88	SER	3.6
2	B	9	GLY	3.6
3	E	65	GLN	3.6
2	B	374	CYS	3.6
3	E	193	THR	3.5
4	F	207	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
3	E	150	GLY	3.5
2	B	49	CYS	3.5
3	E	148	VAL	3.5
4	F	134	CYS	3.5
3	E	84	SER	3.5
2	B	377	ASN	3.4
1	A	339	ALA	3.4
2	D	129[A]	TRP	3.4
4	F	123	GLU	3.4
4	F	205	ILE	3.4
2	D	51	PRO	3.4
2	B	460	CYS	3.4
3	E	85	SER	3.4
3	E	157	THR	3.4
3	H	188	THR	3.4
4	F	144	ILE	3.4
2	D	45	LEU	3.4
1	A	336	GLY	3.4
4	F	196	ALA	3.4
2	D	54	ILE	3.3
4	F	161	ASN	3.3
2	B	76	ASP	3.3
2	D	48	ASN	3.3
2	D	40	LEU	3.3
3	H	142	VAL	3.3
2	B	48	ASN	3.2
2	B	446	HIS	3.2
4	F	160	LEU	3.2
4	F	173	TYR	3.2
2	D	4	ILE	3.2
2	B	452	ASN	3.2
2	D	378	GLU	3.2
3	E	190	THR	3.2
3	E	202	ASN	3.2
4	F	189	HIS	3.2
1	C	339	ALA	3.2
3	E	162	SER	3.2
2	B	77	SER	3.2
3	E	16	ALA	3.2
2	B	67	ARG	3.2
2	B	54	ILE	3.1
3	H	218	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	66	GLY	3.1
3	E	122	THR	3.1
4	F	147	LYS	3.1
4	F	149	LYS	3.1
4	F	195	GLU	3.1
4	F	177	SER	3.1
3	E	120	ALA	3.1
2	B	370	PHE	3.1
3	E	172	PHE	3.1
2	B	79	GLN	3.1
4	F	145	ASN	3.1
2	D	46	LYS	3.1
2	D	8	ARG	3.1
3	E	67	LYS	3.0
2	D	1	GLY	3.0
3	E	166	SER	3.0
1	A	320	ARG	3.0
3	E	82	GLN	3.0
2	D	56	PHE	3.0
1	C	246	GLY	3.0
2	B	463	GLY	3.0
3	E	177	GLN	3.0
4	F	183	LYS	3.0
2	D	22	MET	2.9
2	B	26	CYS	2.9
4	F	169	LYS	2.9
2	D	381	PRO	2.9
2	B	11	SER	2.9
3	E	180	LEU	2.9
3	E	13	LYS	2.9
2	B	3	ASN	2.9
3	E	203	VAL	2.9
4	F	13	VAL	2.9
4	F	202	THR	2.9
2	B	448	CYS	2.9
3	H	169	VAL	2.9
2	B	372	ALA	2.9
2	D	375	LEU	2.9
2	B	449	ASN	2.8
1	C	320	ARG	2.8
3	E	197	GLN	2.8
4	F	153	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	338	HIS	2.8
3	H	158	LEU	2.8
2	B	445	SER	2.8
4	F	211	ARG	2.8
1	C	337	PRO	2.8
3	H	211	LYS	2.8
2	B	25	TRP	2.8
1	C	338	HIS	2.8
3	E	151	TYR	2.8
4	F	139	PHE	2.7
3	E	205	HIS	2.7
2	B	22	MET	2.7
4	F	77	SER	2.7
4	F	203	SER	2.7
3	H	132	PRO	2.7
3	H	191	SER	2.7
3	E	181	TYR	2.7
2	B	380	ILE	2.7
3	E	92	ALA	2.7
3	H	187	VAL	2.7
4	L	12	SER	2.7
2	D	9	GLY	2.7
3	E	209	SER	2.6
3	E	206	PRO	2.6
3	H	139	GLY	2.6
4	L	171	SER	2.6
4	F	107	LYS	2.6
2	D	377	ASN	2.6
2	B	455	PHE	2.5
4	L	169	LYS	2.5
4	L	83	PHE	2.5
2	B	440	GLN	2.5
3	H	161	ASN	2.5
3	H	194	TRP	2.5
4	F	9	SER	2.5
3	E	182	THR	2.5
3	H	208	SER	2.4
3	H	159	THR	2.4
2	B	404	ARG	2.4
2	D	53	SER	2.4
4	F	109	ALA	2.4
3	E	41	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	203	VAL	2.4
2	D	3	ASN	2.4
4	F	15	LEU	2.4
2	D	32	PRO	2.4
3	E	175	VAL	2.4
3	H	17	SER	2.4
2	D	5	CYS	2.4
2	B	27	SER	2.4
3	H	198	SER	2.4
4	F	20	SER	2.4
2	B	100	PHE	2.4
3	E	29	ILE	2.3
4	F	197	THR	2.3
2	D	404	ARG	2.3
4	F	80	SER	2.3
4	F	201	SER	2.3
4	F	16	GLY	2.3
3	E	170	HIS	2.3
3	E	80	TYR	2.3
1	A	457	SER	2.3
3	E	125	PRO	2.3
3	H	207	ALA	2.3
3	E	156	VAL	2.3
2	B	461	ARG	2.3
3	E	168	GLY	2.3
2	B	42	GLU	2.3
4	F	204	PRO	2.3
3	E	19	LYS	2.3
3	H	131	ALA	2.3
3	H	190	THR	2.2
2	B	378	GLU	2.2
2	D	52	GLU	2.2
3	E	119	SER	2.2
4	F	106	ILE	2.2
4	F	170	ASP	2.2
4	L	128	GLY	2.2
2	B	439	ALA	2.2
4	F	105	GLU	2.2
4	F	111	ALA	2.2
2	B	98	LYS	2.2
2	B	181	LYS	2.2
3	H	167	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	116	THR	2.2
3	H	143	THR	2.2
2	D	49	CYS	2.1
4	L	7	SER	2.1
3	E	91	THR	2.1
4	F	165	ASP	2.1
3	E	121	LYS	2.1
4	L	106	ILE	2.1
3	E	158	LEU	2.1
4	L	213	GLU	2.1
4	F	175	MET	2.1
2	B	66	ASP	2.1
3	E	69	THR	2.1
2	B	451	GLY	2.1
3	H	192	SER	2.1
2	D	57	PRO	2.1
3	H	215	LYS	2.0
4	F	138	ASN	2.0
3	H	213	ASP	2.0
2	B	459	VAL	2.0
3	E	167	SER	2.0
3	E	184	SER	2.0
3	H	140	SER	2.0
4	F	14	SER	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.

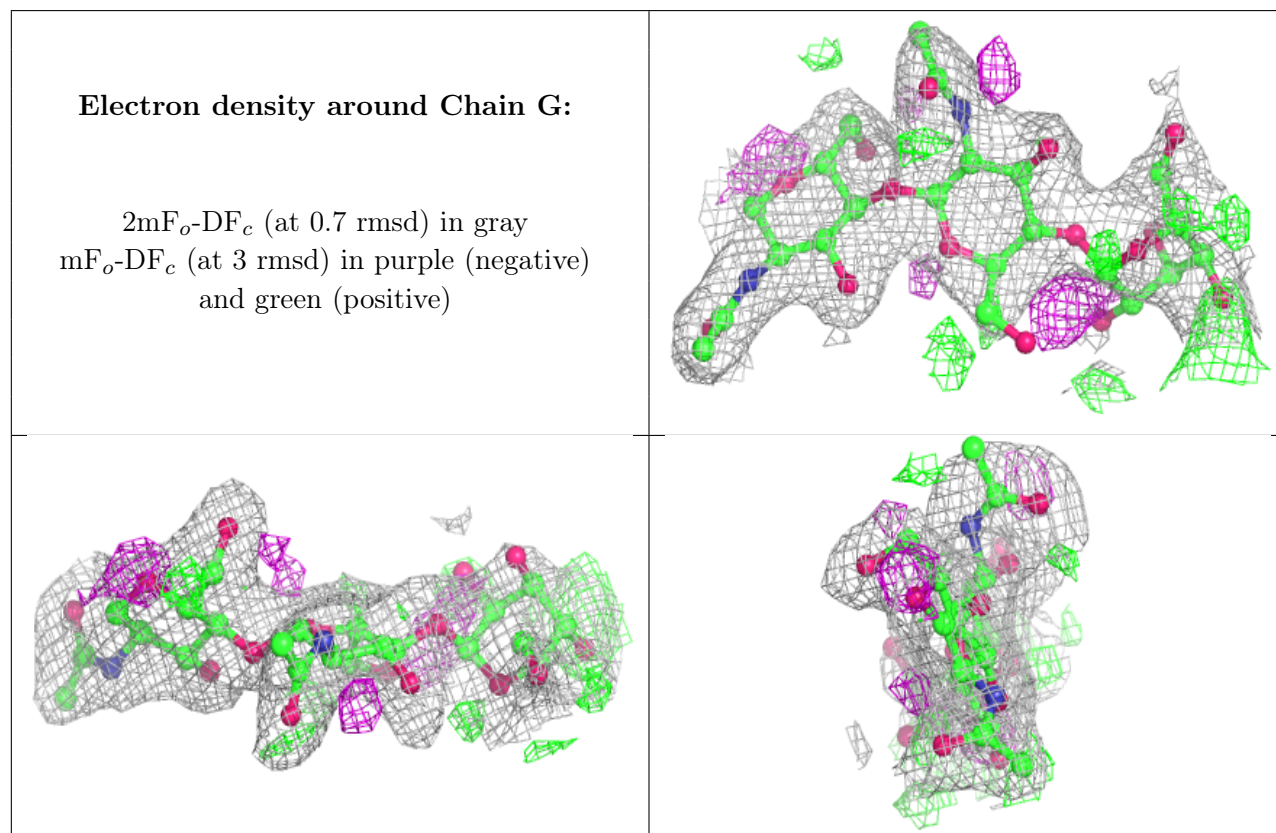
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	G	3	11/12	0.48	0.30	132,140,144,145	0
5	MAN	J	3	11/12	0.57	0.36	125,131,134,134	0
5	NAG	J	2	14/15	0.78	0.23	58,95,109,117	0
6	NAG	I	1	14/15	0.79	0.28	90,114,122,124	0

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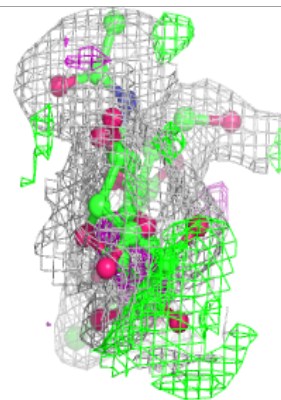
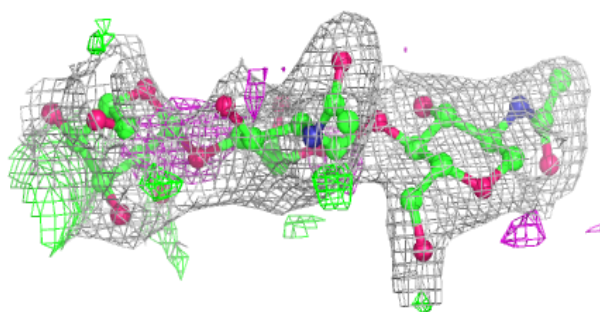
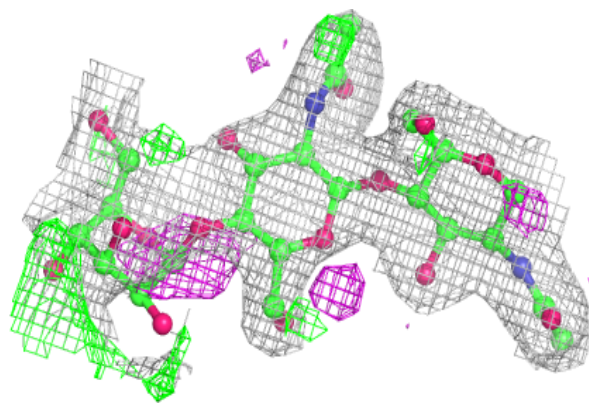
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	I	2	14/15	0.79	0.37	125,129,141,141	0
6	NAG	K	2	14/15	0.80	0.41	134,139,145,145	0
6	NAG	K	1	14/15	0.82	0.29	83,111,133,135	0
5	NAG	G	2	14/15	0.88	0.15	47,74,105,108	0
5	NAG	J	1	14/15	0.93	0.14	44,54,71,72	0
5	NAG	G	1	14/15	0.96	0.12	23,35,51,52	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.



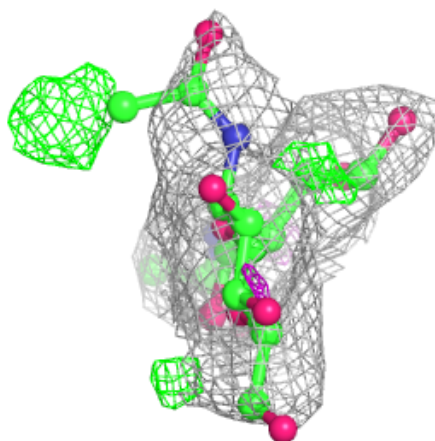
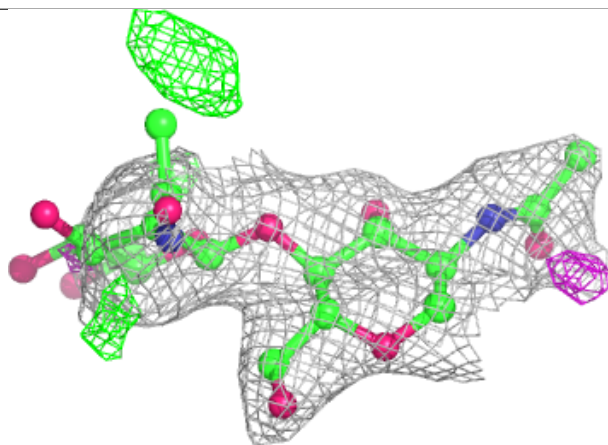
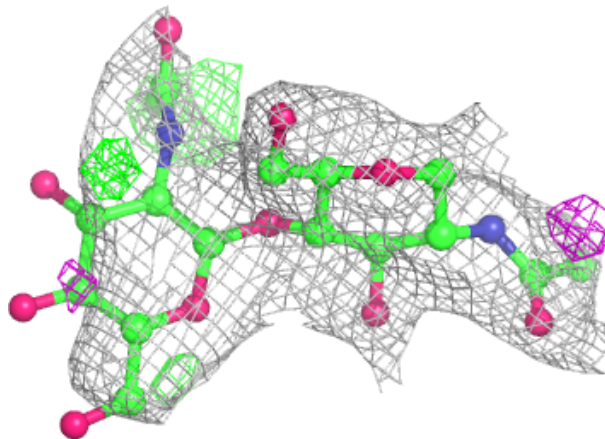
Electron density around Chain J:

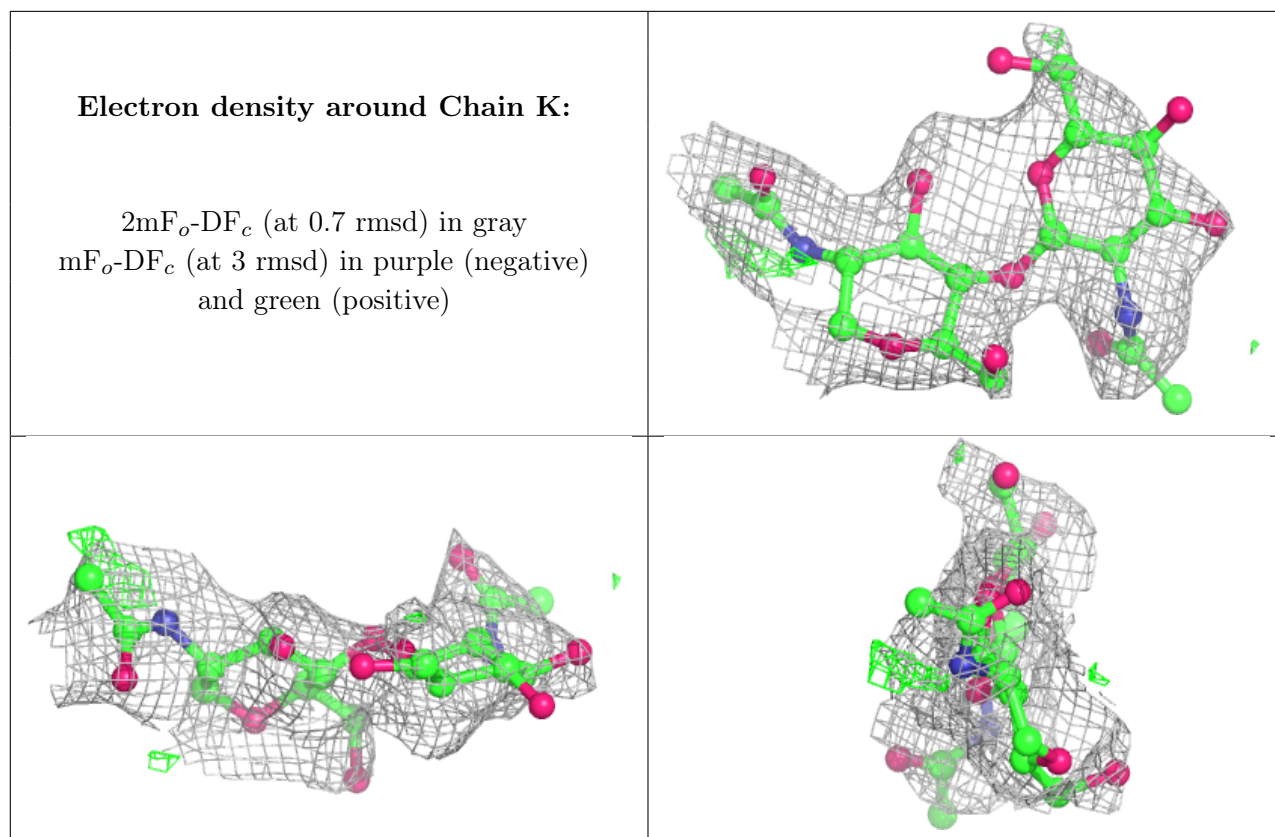
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
11	NAG	D	3099	14/15	0.78	0.34	99,112,115,118	0
9	SO4	C	460	5/5	0.80	0.27	66,66,70,129	0
9	SO4	D	472	5/5	0.84	0.32	62,66,72,133	0
11	NAG	B	3099	14/15	0.89	0.29	108,118,123,123	0
8	GOL	A	459	6/6	0.90	0.19	34,51,67,74	0
9	SO4	A	461	5/5	0.90	0.14	48,49,63,70	0
9	SO4	A	460	5/5	0.91	0.22	57,67,89,90	0
9	SO4	L	215	5/5	0.91	0.23	81,82,86,95	0
8	GOL	A	458	6/6	0.93	0.20	44,55,69,77	0
9	SO4	C	459	5/5	0.94	0.17	56,71,86,96	0
8	GOL	C	458	6/6	0.94	0.13	43,61,65,68	0
10	MG	B	2001	1/1	0.96	0.16	38,38,38,38	0
7	CA	C	2005	1/1	0.96	0.06	44,44,44,44	0
7	CA	C	2004	1/1	0.96	0.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	C	2007	1/1	0.98	0.12	47,47,47,47	0
7	CA	C	2006	1/1	0.99	0.13	41,41,41,41	0
7	CA	B	2002	1/1	0.99	0.06	39,39,39,39	0
7	CA	D	2003	1/1	0.99	0.16	29,29,29,29	0
10	MG	D	2001	1/1	0.99	0.07	42,42,42,42	0
7	CA	A	2004	1/1	0.99	0.08	35,35,35,35	0
7	CA	A	2005	1/1	0.99	0.12	28,28,28,28	0
7	CA	A	2007	1/1	1.00	0.13	23,23,23,23	0
7	CA	D	2002	1/1	1.00	0.11	37,37,37,37	0
7	CA	A	2006	1/1	1.00	0.16	24,24,24,24	0
7	CA	B	2003	1/1	1.00	0.17	20,20,20,20	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.