



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 02:29 PM EDT

PDB ID : 7UDH
Title : Integrin α IIb β 3 complex with BMS4-3
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2022-03-19
Resolution : 2.00 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:

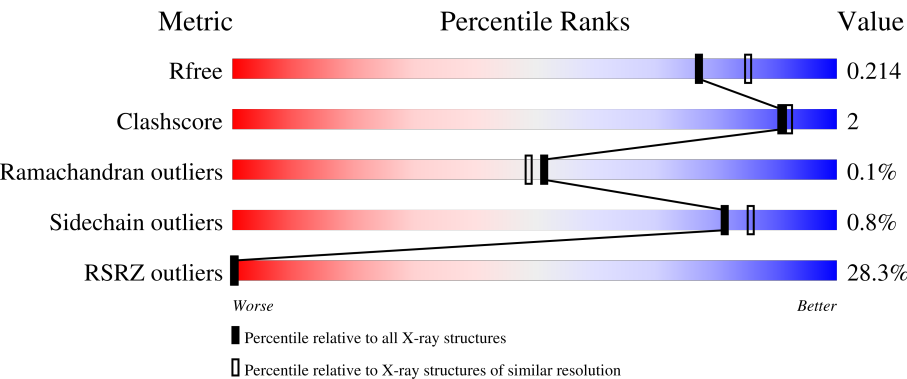
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	<div><div>28%</div><div>95%</div><div>..</div></div>
1	C	457	<div><div>14%</div><div>96%</div><div>..</div></div>
2	B	472	<div><div>26%</div><div>93%</div><div>6% .</div></div>
2	D	472	<div><div>20%</div><div>94%</div><div>5%</div></div>
3	E	221	<div><div>62%</div><div>94%</div><div>..</div></div>

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	I	1	-	-	X	-
7	NAG	J	1	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 22567 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	4	0
			3499	2226	601	664	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	3	0
			3610	2248	616	712	34			
2	D	471	Total	C	N	O	S	3	0	0
			3623	2255	619	715	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 10E5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



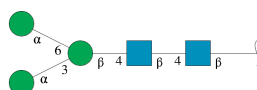
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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 an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
7	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

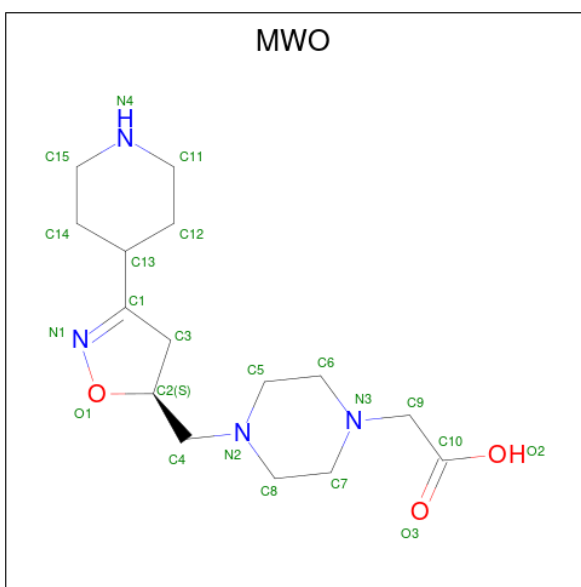
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

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



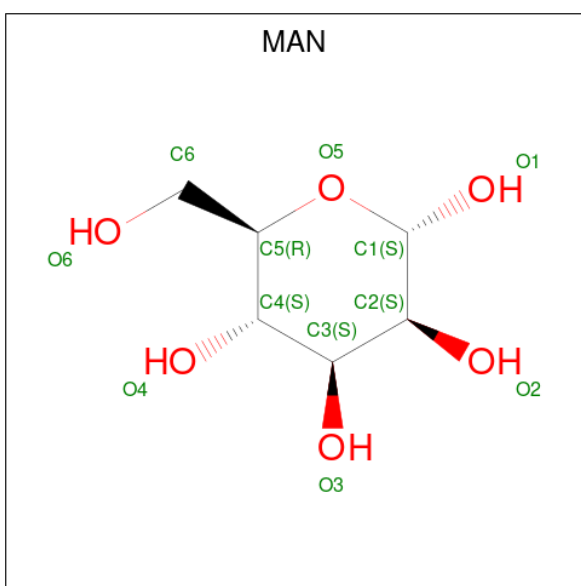
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is (4-{[(5S)-3-(piperidin-4-yl)-4,5-dihydro-1,2-oxazol-5-yl]methyl}piperazin-1-yl)acetic acid (three-letter code: MWO) (formula: C₁₅H₂₆N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			22	15	4	3		
12	D	1	Total	C	N	O	0	0
			22	15	4	3		

- Molecule 13 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	2	Total	Cl	0	0
			2	2		
14	D	1	Total	Cl	0	0
			1	1		

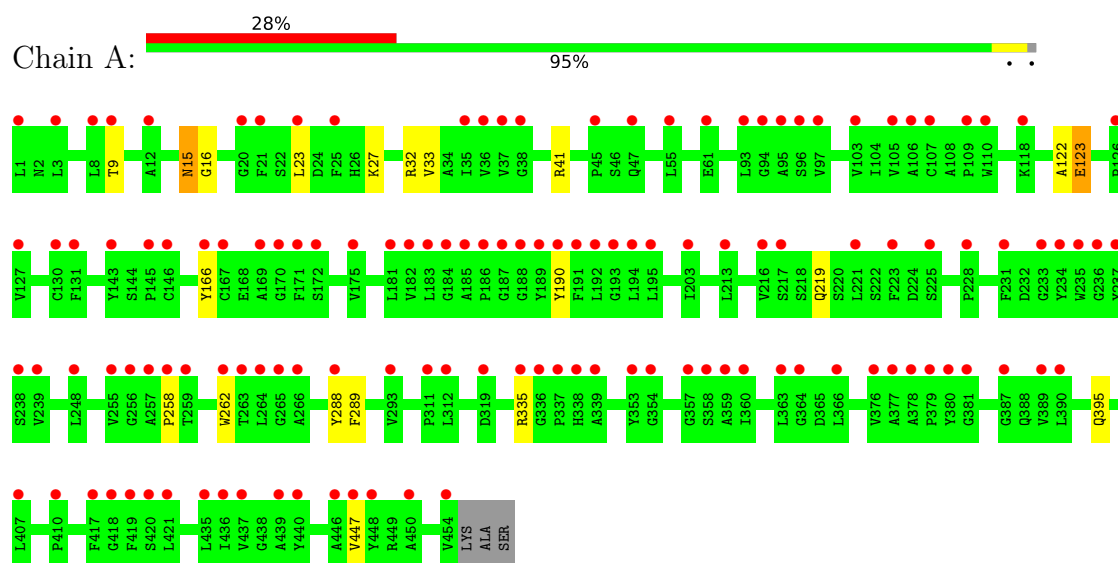
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	542	Total	O	0	0
			542	542		
15	B	319	Total	O	0	0
			319	319		
15	C	232	Total	O	0	0
			232	232		
15	D	200	Total	O	0	0
			200	200		
15	E	29	Total	O	0	0
			29	29		
15	F	20	Total	O	0	0
			20	20		
15	H	45	Total	O	0	0
			45	45		
15	L	87	Total	O	0	0
			87	87		

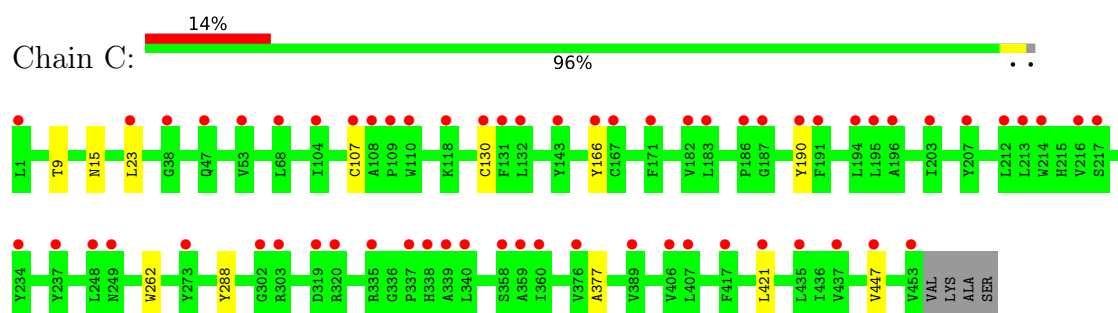
3 Residue-property plots [i](#)

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.

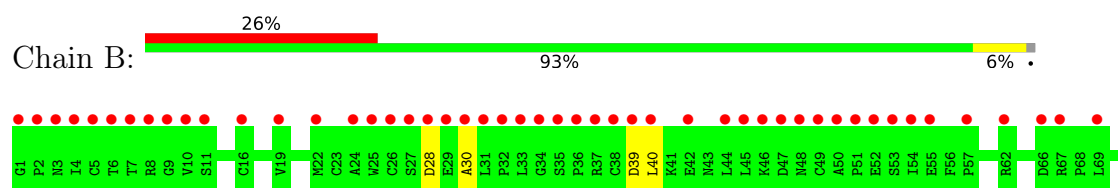
- Molecule 1: Integrin alpha-IIb heavy chain

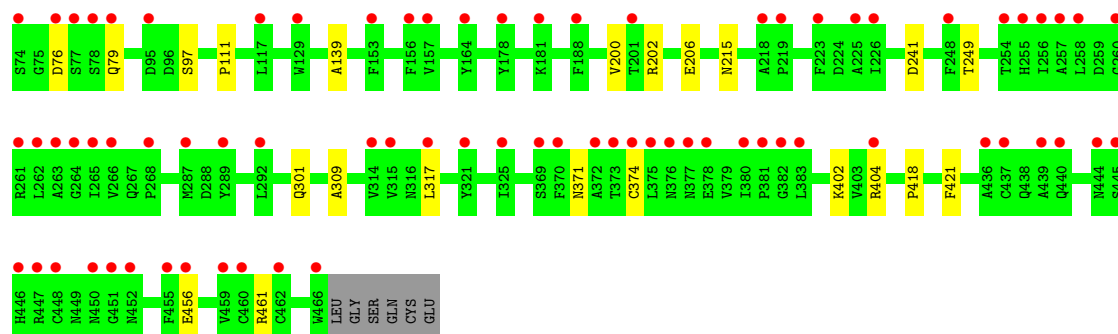


- Molecule 1: Integrin alpha-IIb heavy chain

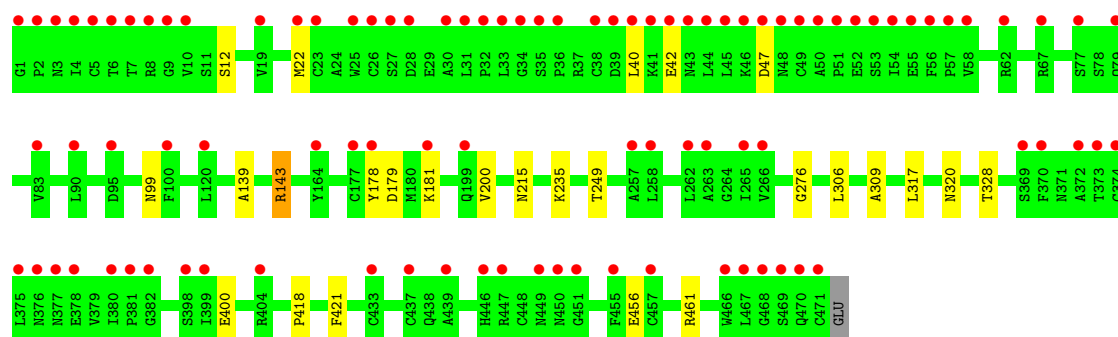


- Molecule 2: Isoform Beta-3C of Integrin beta-3

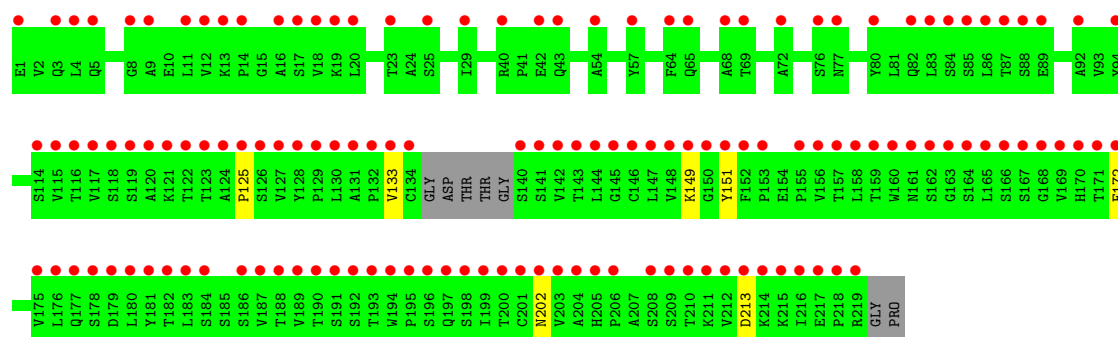




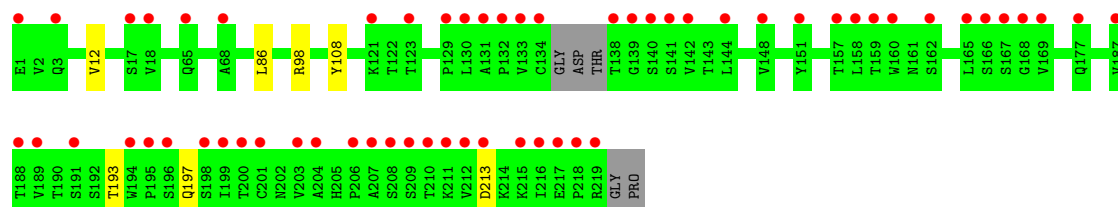
• Molecule 2: Isoform Beta-3C of Integrin beta-3



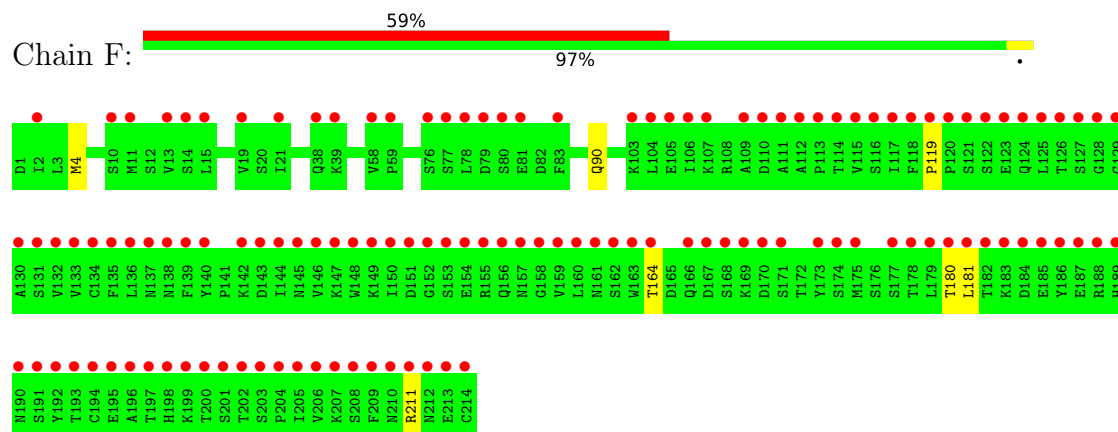
• Molecule 3: 10E5 Fab heavy chain



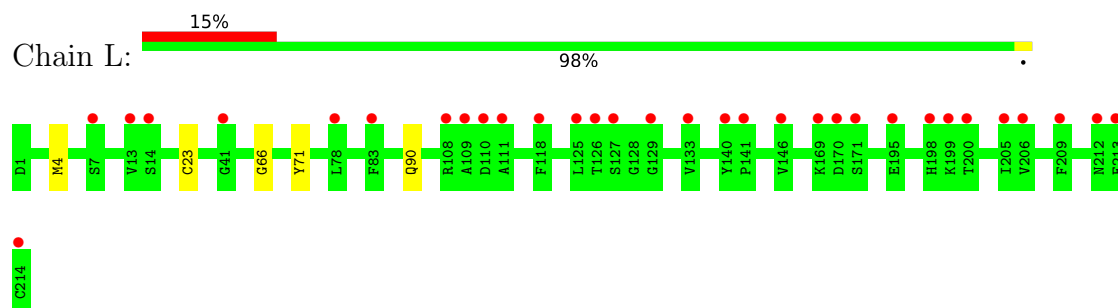
• Molecule 3: 10E5 Fab heavy chain



- Molecule 4: 10E5 Fab light chain



- Molecule 4: 10E5 Fab light chain



- Molecule 5: 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 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  40% 60%

MAG1	MAG2	EMJ3	MAM4	MAM5
------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	258.33Å 144.67Å 105.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.99 – 2.00 48.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.99-2.00) 97.4 (48.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.185 , 0.214 0.185 , 0.214	Depositor DCC
R_{free} test set	2000 reflections (0.78%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22567	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: MWO, MN, BMA, CA, CL, MAN, NAG, 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	0.30	0/3608	0.53	0/4918
1	C	0.27	0/3605	0.50	0/4912
2	B	0.28	0/3680	0.48	0/4989
2	D	0.26	0/3690	0.47	0/5003
3	E	0.24	0/1673	0.45	0/2290
3	H	0.25	0/1684	0.48	0/2305
4	F	0.24	0/1673	0.44	0/2269
4	L	0.25	0/1673	0.47	0/2269
All	All	0.27	0/21286	0.48	0/28955

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3499	0	3345	9	0
1	C	3502	0	3334	4	0
2	B	3610	0	3531	19	0
2	D	3623	0	3541	28	0
3	E	1631	0	1590	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	4	0
4	F	1637	0	1553	5	0
4	L	1637	0	1553	3	0
5	G	50	0	42	0	0
6	I	28	0	25	7	0
6	K	28	0	25	1	0
7	J	61	0	52	8	0
8	A	20	0	0	0	0
8	C	20	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	B	3	0	0	0	0
10	D	3	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	5	0
12	B	22	0	0	0	0
12	D	22	0	0	0	0
13	C	11	0	10	0	0
14	C	2	0	0	0	0
14	D	1	0	0	0	0
15	A	542	0	0	3	1
15	B	319	0	0	2	0
15	C	232	0	0	0	1
15	D	200	0	0	2	0
15	E	29	0	0	0	0
15	F	20	0	0	1	0
15	H	45	0	0	0	0
15	L	87	0	0	1	0
All	All	22567	0	20227	72	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 (72) 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:320:ASN:HD21	7:J:1:NAG:C1	0.99	1.59
2:D:99:ASN:ND2	11:D:2004:NAG:C1	1.68	1.56
2:B:371:ASN:HD21	6:I:1:NAG:C1	0.97	1.53
2:B:371:ASN:ND2	6:I:1:NAG:C1	1.73	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:ASN:ND2	7:J:1:NAG:C1	1.76	1.45
2:B:371:ASN:HD21	6:I:1:NAG:C2	1.63	1.10
2:B:371:ASN:ND2	6:I:1:NAG:C2	2.16	1.07
2:D:320:ASN:HD21	7:J:1:NAG:C2	1.75	1.00
2:D:99:ASN:CG	11:D:2004:NAG:C1	2.39	0.91
2:B:371:ASN:CG	6:I:1:NAG:C1	2.41	0.88
2:D:320:ASN:CG	7:J:1:NAG:C1	2.44	0.85
2:D:99:ASN:ND2	11:D:2004:NAG:O5	2.10	0.82
2:B:371:ASN:ND2	6:I:1:NAG:H2	1.96	0.81
4:L:23:CYS:SG	15:L:457:HOH:O	2.47	0.72
2:D:320:ASN:ND2	7:J:1:NAG:C2	2.45	0.71
2:D:99:ASN:ND2	11:D:2004:NAG:C2	2.53	0.70
4:F:211:ARG:NH2	15:F:301:HOH:O	2.26	0.69
2:D:181:LYS:NZ	15:D:2101:HOH:O	2.26	0.67
2:D:143:ARG:NH1	15:D:2103:HOH:O	2.30	0.64
2:B:301:GLN:NE2	15:B:2103:HOH:O	2.29	0.63
2:B:371:ASN:OD1	6:I:1:NAG:C1	2.48	0.62
2:B:404:ARG:NH1	15:B:2105:HOH:O	2.33	0.62
2:D:320:ASN:ND2	7:J:1:NAG:O5	2.30	0.60
2:D:99:ASN:OD1	11:D:2004:NAG:C1	2.51	0.59
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.85	0.59
2:D:320:ASN:OD1	7:J:1:NAG:C1	2.51	0.58
1:A:335:ARG:NH2	15:A:607:HOH:O	2.37	0.57
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.40	0.55
2:B:97:SER:HB3	2:B:402:LYS:HG2	1.92	0.52
2:D:22:MET:HG2	2:D:40:LEU:HD22	1.94	0.50
1:A:9:THR:HB	1:A:447:VAL:HB	1.95	0.49
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.94	0.49
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.95	0.48
2:D:456:GLU:OE2	2:D:461:ARG:NH1	2.47	0.48
1:A:32:ARG:NH2	15:A:616:HOH:O	2.47	0.47
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.97	0.47
3:H:213:ASP:OD1	3:H:213:ASP:N	2.47	0.47
1:A:27:LYS:HG2	1:A:33:VAL:HG22	1.97	0.47
3:E:133:VAL:HG22	4:F:119:PRO:HD3	1.96	0.47
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.49	0.46
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.52	0.45
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.45
2:D:178:TYR:CG	2:D:179:ASP:N	2.85	0.44
2:B:249:THR:HA	2:B:309:ALA:O	2.17	0.44
2:B:28:ASP:OD1	2:B:30:ALA:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ASP:OD1	2:B:40:LEU:N	2.48	0.43
2:D:249:THR:HA	2:D:309:ALA:O	2.17	0.43
1:C:9:THR:HB	1:C:447:VAL:HB	2.00	0.43
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.98	0.43
3:H:12:VAL:HG21	3:H:86:LEU:HD13	2.00	0.43
2:D:235:LYS:HE3	2:D:276:GLY:O	2.18	0.43
2:D:42:GLU:OE2	2:D:42:GLU:N	2.51	0.43
4:L:4:MET:HE2	4:L:90:GLN:HB3	2.01	0.43
4:L:66:GLY:HA3	4:L:71:TYR:HA	2.01	0.43
1:C:107:CYS:HA	1:C:130:CYS:HA	2.01	0.43
1:A:15:ASN:HD22	1:A:16:GLY:N	2.17	0.43
1:A:122:ALA:O	1:A:123:GLU:HB2	2.19	0.43
2:B:111:PRO:HG2	2:B:241:ASP:O	2.18	0.43
2:B:139:ALA:HB2	2:B:200:VAL:HG11	2.01	0.42
4:F:4:MET:HE2	4:F:90:GLN:HB3	2.00	0.42
1:C:377:ALA:HB2	1:C:421:LEU:HD11	2.00	0.42
2:D:320:ASN:ND2	7:J:1:NAG:H2	2.30	0.42
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.35	0.42
1:A:41:ARG:NH1	15:A:623:HOH:O	2.49	0.42
2:D:139:ALA:HB2	2:D:200:VAL:HG11	2.02	0.41
2:D:400:GLU:HB2	6:K:1:NAG:H83	2.02	0.41
3:H:193:THR:O	3:H:197:GLN:N	2.50	0.41
1:A:258:PRO:HA	1:A:289:PHE:O	2.21	0.41
2:B:418:PRO:HB2	2:B:421:PHE:CD1	2.55	0.41
3:H:98:ARG:HG3	3:H:108:TYR:HB2	2.03	0.41
2:D:249:THR:HG22	2:D:309:ALA:HB3	2.03	0.40
3:E:125:PRO:HB3	3:E:151:TYR:HB3	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)
15:A:1035:HOH:O	15:C:786:HOH:O[1_554]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/457 (100%)	440 (96%)	15 (3%)	1 (0%)	47	44
1	C	455/457 (100%)	441 (97%)	14 (3%)	0	100	100
2	B	467/472 (99%)	452 (97%)	14 (3%)	1 (0%)	47	44
2	D	469/472 (99%)	451 (96%)	18 (4%)	0	100	100
3	E	210/221 (95%)	196 (93%)	14 (7%)	0	100	100
3	H	212/221 (96%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2693/2728 (99%)	2587 (96%)	104 (4%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	76	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/364 (100%)	359 (98%)	7 (2%)	57	61
1	C	365/364 (100%)	360 (99%)	5 (1%)	67	72
2	B	415/417 (100%)	412 (99%)	3 (1%)	84	88
2	D	416/417 (100%)	413 (99%)	3 (1%)	84	88
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2311/2318 (100%)	2292 (99%)	19 (1%)	81	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	219	GLN
1	A	288	TYR
1	A	395	GLN
2	B	79	GLN
2	B	215	ASN
2	B	374	CYS
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
2	D	47	ASP
2	D	143	ARG
2	D	215	ASN
4	F	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
2	B	280	HIS
2	B	301	GLN
2	B	371	ASN
2	D	82	GLN
2	D	301	GLN
2	D	320	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	G	1	5,2	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	G	2	5	14,14,15	0.34	0	17,19,21	0.35	0
5	BMA	G	3	5	11,11,12	1.05	1 (9%)	15,15,17	0.96	1 (6%)
5	MAN	G	4	5	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
6	NAG	I	1	6	14,14,15	0.24	0	17,19,21	0.46	0
6	NAG	I	2	6	14,14,15	0.27	0	17,19,21	0.38	0
7	NAG	J	1	7	14,14,15	0.32	0	17,19,21	0.45	0
7	NAG	J	2	7	14,14,15	0.33	0	17,19,21	0.40	0
7	BMA	J	3	7	11,11,12	0.99	0	15,15,17	0.73	0
7	MAN	J	4	7	11,11,12	0.78	0	15,15,17	0.95	2 (13%)
7	MAN	J	5	7	11,11,12	0.78	1 (9%)	15,15,17	1.16	2 (13%)
6	NAG	K	1	6	14,14,15	0.24	0	17,19,21	0.38	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	BMA	O5-C1	-2.48	1.39	1.43
7	J	5	MAN	C1-C2	2.12	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	5	MAN	C1-O5-C5	3.41	116.81	112.19
5	G	4	MAN	C1-O5-C5	2.46	115.52	112.19
7	J	4	MAN	C1-O5-C5	2.30	115.31	112.19
5	G	4	MAN	O2-C2-C3	-2.29	105.55	110.14
7	J	4	MAN	O2-C2-C3	-2.26	105.61	110.14
5	G	3	BMA	C3-C4-C5	2.20	114.17	110.24
7	J	5	MAN	O2-C2-C3	-2.08	105.98	110.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	4	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	K	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
7	J	5	MAN	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

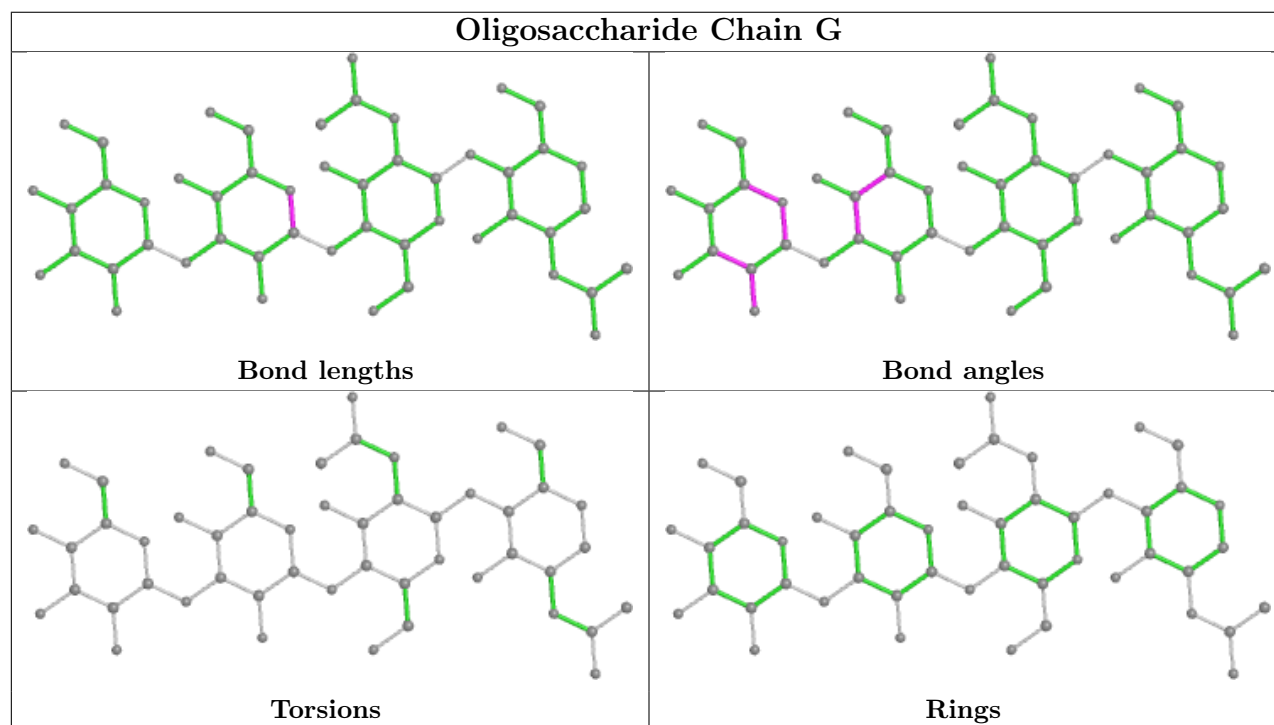
Mol	Chain	Res	Type	Atoms
7	J	3	BMA	O5-C5-C6-O6

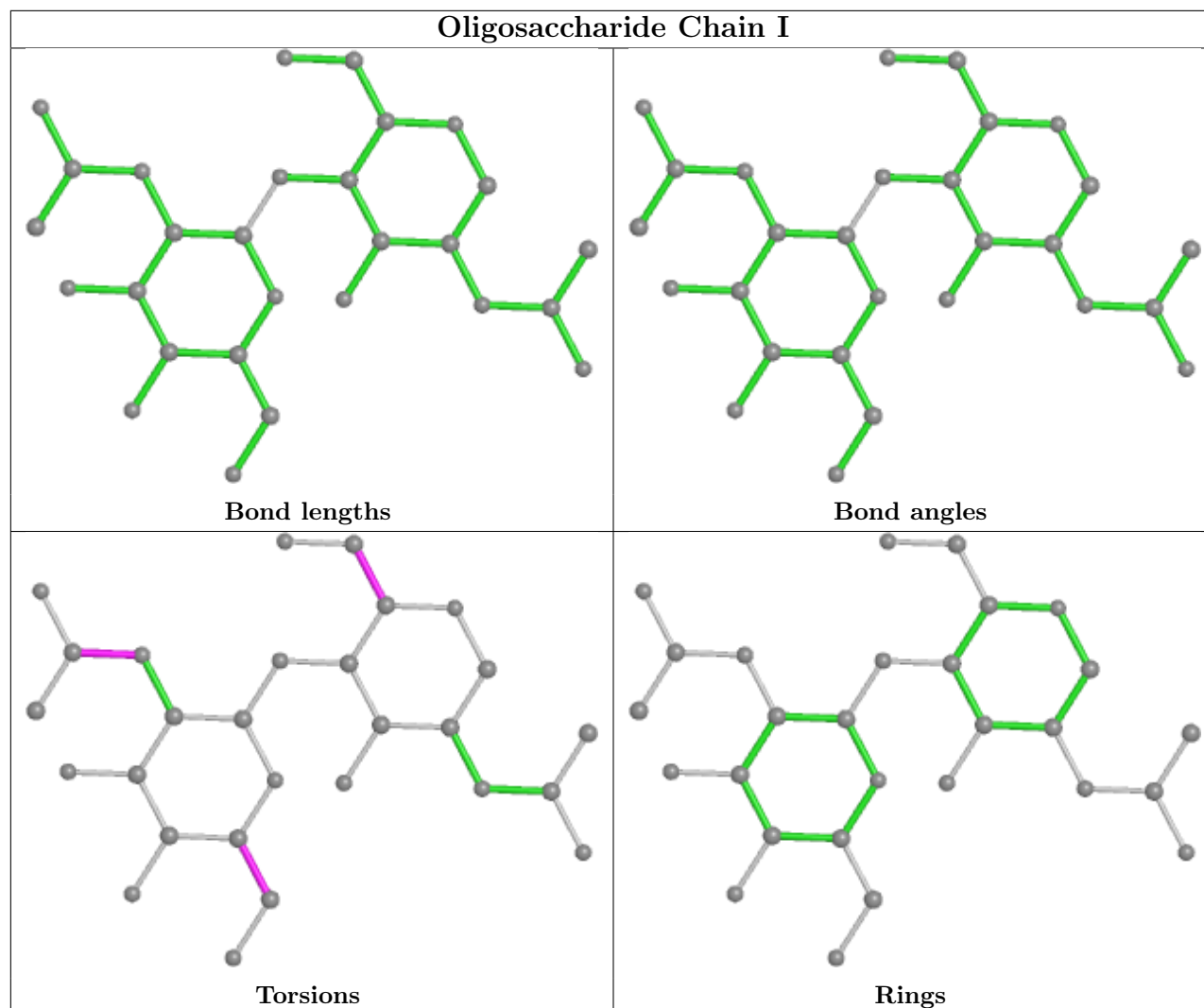
There are no ring outliers.

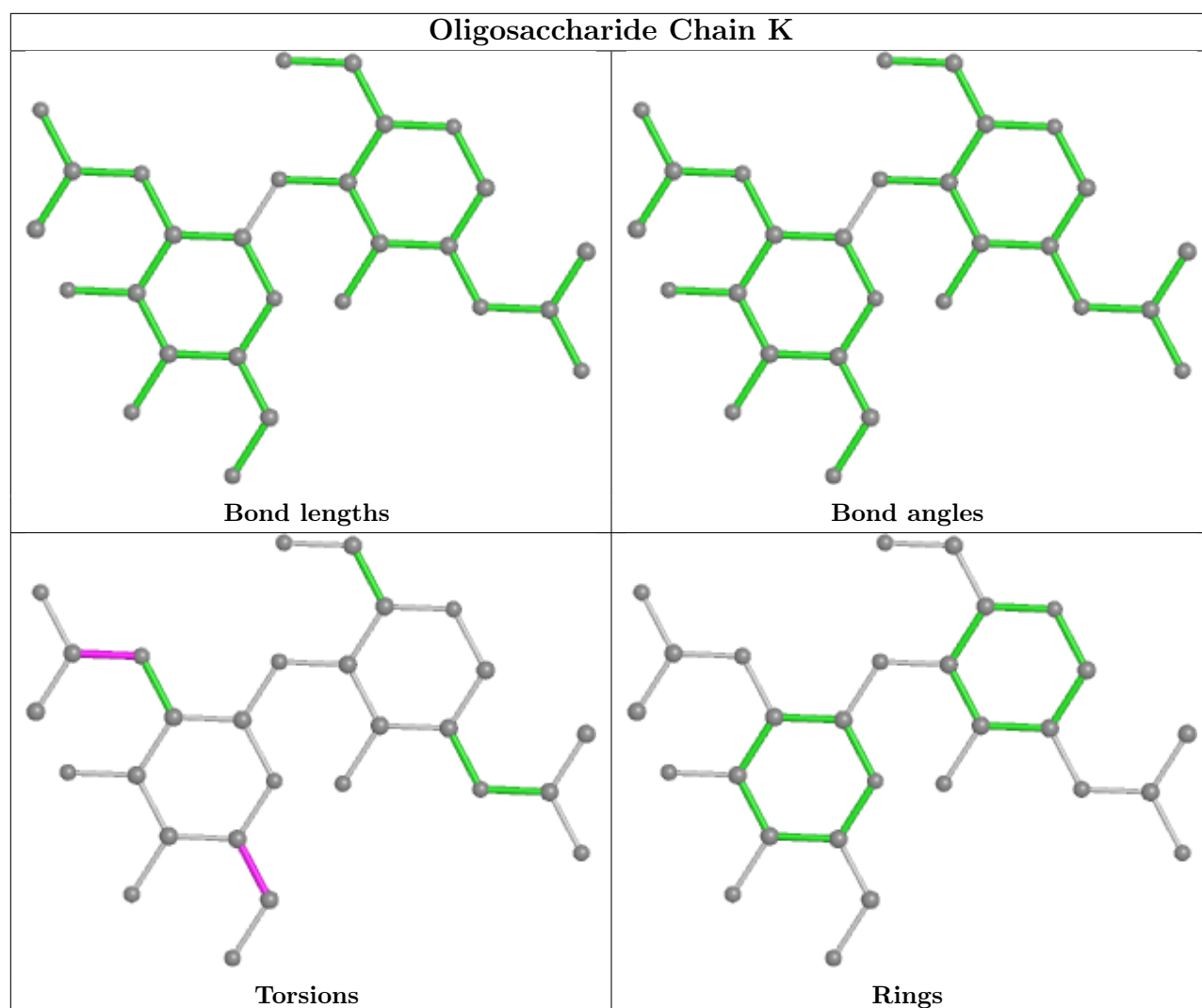
3 monomers are involved in 16 short contacts:

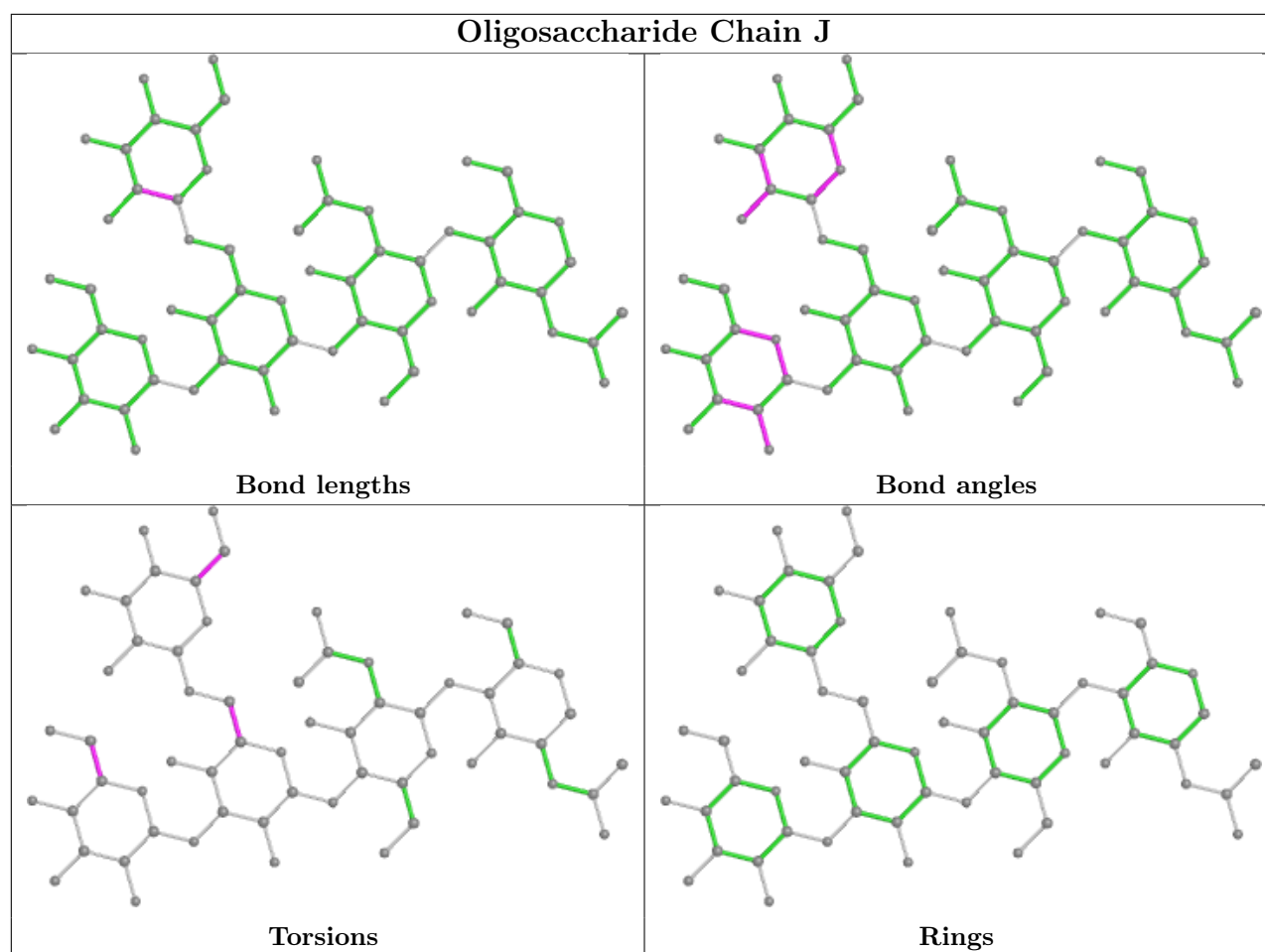
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1	NAG	8	0
6	I	1	NAG	7	0
6	K	1	NAG	1	0

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 31 ligands modelled in this entry, 17 are monoatomic - leaving 14 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	$\# Z > 2$
8	SO4	A	507	-	4,4,4	0.15	0	6,6,6	0.08	0
11	NAG	B	2004	2	14,14,15	0.16	0	17,19,21	0.44	0
8	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.06	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
13	MAN	C	501	-	11,11,12	0.80	0	15,15,17	1.09	2 (13%)
8	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.04	0
8	SO4	C	511	-	4,4,4	0.14	0	6,6,6	0.06	0
12	MWO	D	2006	10	23,24,24	3.15	9 (39%)	27,32,32	2.19	8 (29%)
11	NAG	D	2004	-	14,14,15	0.21	0	17,19,21	0.40	0
12	MWO	B	2005	10	23,24,24	3.16	9 (39%)	27,32,32	2.12	6 (22%)

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	B	2004	2	-	2/6/23/26	0/1/1/1
13	MAN	C	501	-	-	2/2/19/22	0/1/1/1
12	MWO	D	2006	10	-	3/12/39/39	0/3/3/3
11	NAG	D	2004	-	-	0/6/23/26	0/1/1/1
12	MWO	B	2005	10	-	3/12/39/39	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2006	MWO	C4-N2	-8.43	1.31	1.47
12	B	2005	MWO	C4-N2	-8.38	1.31	1.47
12	B	2005	MWO	O1-C2	-7.45	1.36	1.46
12	D	2006	MWO	O1-C2	-7.34	1.36	1.46
12	D	2006	MWO	C5-N2	-5.11	1.32	1.46
12	B	2005	MWO	C5-N2	-5.09	1.32	1.46
12	D	2006	MWO	C8-N2	-5.08	1.32	1.46
12	B	2005	MWO	C8-N2	-5.00	1.33	1.46
12	B	2005	MWO	C3-C1	4.72	1.59	1.50
12	D	2006	MWO	C3-C1	4.57	1.59	1.50
12	B	2005	MWO	O1-N1	-2.68	1.38	1.42
12	D	2006	MWO	O1-N1	-2.58	1.38	1.42
12	B	2005	MWO	C1-N1	2.51	1.29	1.27
12	D	2006	MWO	C1-N1	2.36	1.29	1.27
12	D	2006	MWO	C14-C13	-2.31	1.47	1.53
12	B	2005	MWO	C14-C13	-2.26	1.47	1.53
12	D	2006	MWO	C12-C13	-2.22	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	MWO	C12-C13	-2.18	1.47	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2005	MWO	C3-C1-N1	-7.25	109.89	114.37
12	D	2006	MWO	C3-C1-N1	-6.27	110.50	114.37
12	D	2006	MWO	O1-C2-C3	5.47	109.41	104.33
12	B	2005	MWO	O1-C2-C3	4.21	108.24	104.33
12	B	2005	MWO	C12-C13-C14	-3.24	103.14	109.97
12	D	2006	MWO	C12-C13-C1	-3.15	105.46	111.88
12	D	2006	MWO	C12-C13-C14	-3.13	103.37	109.97
12	D	2006	MWO	C14-C13-C1	-2.92	105.92	111.88
12	B	2005	MWO	C12-C13-C1	-2.81	106.14	111.88
12	B	2005	MWO	C14-C13-C1	-2.80	106.17	111.88
12	D	2006	MWO	C13-C1-N1	2.60	123.86	119.91
12	D	2006	MWO	O1-N1-C1	2.60	111.50	109.22
12	B	2005	MWO	C13-C1-N1	2.43	123.60	119.91
13	C	501	MAN	C1-O5-C5	2.33	115.35	112.19
12	D	2006	MWO	O2-C10-C9	2.14	121.87	113.45
13	C	501	MAN	O2-C2-C3	-2.01	106.11	110.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

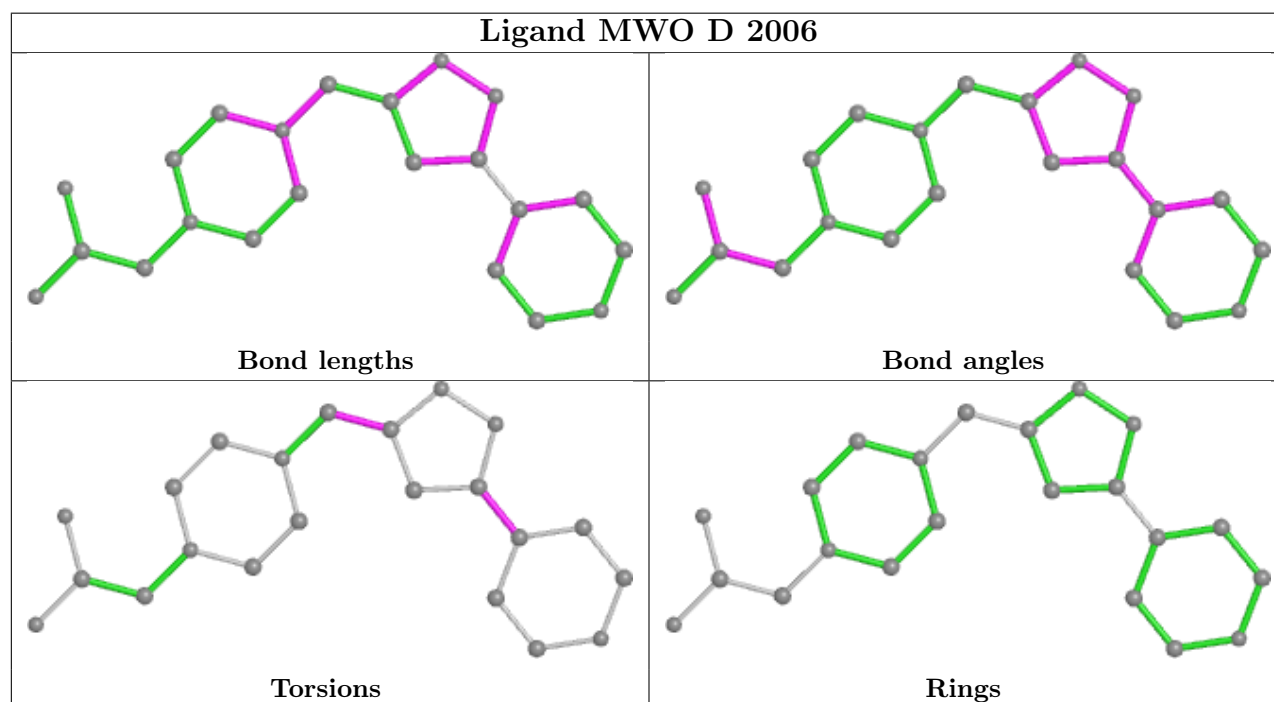
Mol	Chain	Res	Type	Atoms
12	B	2005	MWO	N1-C1-C13-C12
12	B	2005	MWO	C3-C2-C4-N2
12	B	2005	MWO	O1-C2-C4-N2
12	D	2006	MWO	C3-C2-C4-N2
12	D	2006	MWO	O1-C2-C4-N2
11	B	2004	NAG	O5-C5-C6-O6
13	C	501	MAN	O5-C5-C6-O6
11	B	2004	NAG	C4-C5-C6-O6
13	C	501	MAN	C4-C5-C6-O6
12	D	2006	MWO	C3-C1-C13-C14

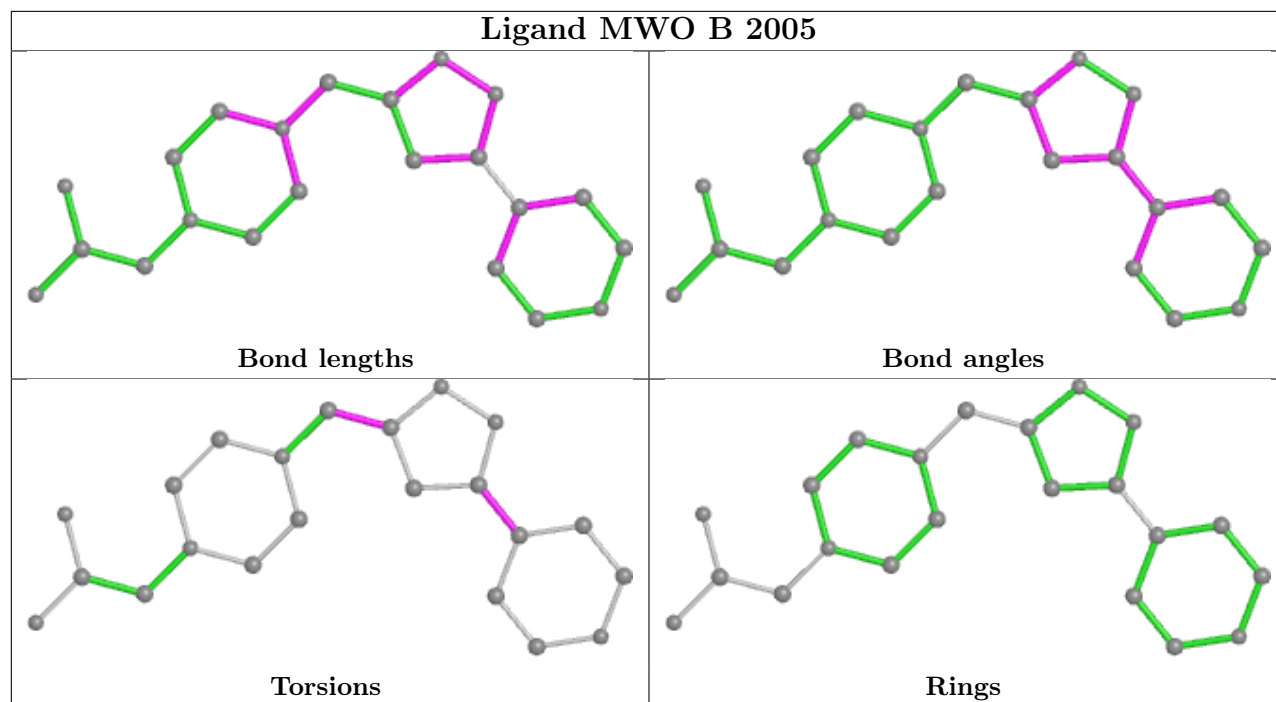
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2004	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	454/457 (99%)	1.43	130 (28%) 0 0	30, 43, 74, 136	0
1	C	453/457 (99%)	1.00	62 (13%) 3 2	38, 57, 90, 138	0
2	B	466/472 (98%)	1.64	124 (26%) 0 0	32, 65, 152, 196	1 (0%)
2	D	471/472 (99%)	1.39	96 (20%) 1 0	40, 74, 147, 199	1 (0%)
3	E	214/221 (96%)	3.56	137 (64%) 0 0	71, 135, 197, 233	0
3	H	216/221 (97%)	1.43	59 (27%) 0 0	49, 102, 162, 187	0
4	F	214/214 (100%)	3.47	126 (58%) 0 0	69, 125, 193, 226	0
4	L	214/214 (100%)	1.14	32 (14%) 2 2	53, 85, 117, 210	0
All	All	2702/2728 (99%)	1.69	766 (28%) 0 0	30, 72, 164, 233	2 (0%)

All (766) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	125	LEU	18.5
3	E	212	VAL	18.4
2	B	77	SER	17.0
4	F	126	THR	15.0
3	E	201	CYS	15.0
4	F	181	LEU	14.3
4	F	206	VAL	13.0
4	L	214	CYS	13.0
4	F	214	CYS	12.8
2	B	33	LEU	12.3
3	E	216	ILE	11.8
4	F	148	TRP	11.7
4	F	122	SER	11.6
4	F	150	ILE	11.6
2	B	30	ALA	11.0
3	E	133	VAL	10.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	471	CYS	10.3
4	F	132	VAL	10.2
3	E	165	LEU	10.0
3	E	144	LEU	10.0
2	D	469	SER	9.7
3	E	210	THR	9.7
2	B	44	LEU	9.5
4	F	136	LEU	9.5
2	B	54	ILE	9.4
4	F	209	PHE	9.3
4	F	118	PHE	9.2
4	F	144	ILE	9.2
3	E	160	TRP	9.1
4	F	120	PRO	9.0
4	F	115	VAL	8.9
3	E	142	VAL	8.9
3	E	194	TRP	8.9
3	E	131	ALA	8.7
4	F	135	PHE	8.7
3	E	147	LEU	8.7
4	F	130	ALA	8.7
4	F	182	THR	8.6
4	F	195	GLU	8.4
3	E	123	THR	8.4
3	E	200	THR	8.4
2	D	375	LEU	8.3
4	F	192	TYR	8.2
3	E	219	ARG	8.2
2	B	4	ILE	8.2
2	D	31	LEU	8.2
3	H	134	CYS	8.1
3	E	134	CYS	8.1
2	B	49	CYS	8.1
2	D	2	PRO	8.0
3	E	128	TYR	8.0
2	B	51	PRO	8.0
4	F	134	CYS	8.0
2	D	8	ARG	7.9
2	B	451	GLY	7.8
4	F	202	THR	7.8
4	F	117	ILE	7.7
2	D	1	GLY	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	194	CYS	7.7
4	F	179	LEU	7.6
3	E	199	ILE	7.6
2	D	470	GLN	7.4
3	E	196	SER	7.4
4	F	193	THR	7.4
3	E	205	HIS	7.4
3	E	16	ALA	7.4
1	A	337	PRO	7.3
2	B	36	PRO	7.3
4	F	213	GLU	7.3
4	F	205	ILE	7.3
2	B	28	ASP	7.3
3	E	12	VAL	7.2
3	H	165	LEU	7.1
2	D	181	LYS	7.1
4	F	208	SER	7.1
3	E	218	PRO	7.1
3	E	86	LEU	7.0
3	H	189	VAL	7.0
2	B	1	GLY	7.0
3	E	192	SER	7.0
2	B	375	LEU	6.9
3	E	140	SER	6.9
3	E	130	LEU	6.8
2	B	46	LYS	6.8
3	E	169	VAL	6.8
4	F	210	ASN	6.8
3	E	25	SER	6.8
3	E	124	ALA	6.8
4	F	180	THR	6.8
2	D	32	PRO	6.7
3	E	117	VAL	6.7
2	B	26	CYS	6.7
2	D	4	ILE	6.7
2	D	9	GLY	6.6
2	D	54	ILE	6.6
3	E	143	THR	6.5
4	F	201	SER	6.5
2	D	46	LYS	6.4
2	D	376	ASN	6.4
3	E	129	PRO	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	452	ASN	6.4
2	D	44	LEU	6.4
3	H	216	ILE	6.4
3	E	203	VAL	6.4
4	F	151	ASP	6.3
4	F	113	PRO	6.3
4	F	200	THR	6.3
2	D	378	GLU	6.3
3	E	183	LEU	6.3
3	E	122	THR	6.3
3	E	178	SER	6.2
4	F	159	VAL	6.2
3	E	145	GLY	6.2
2	B	31	LEU	6.2
2	D	51	PRO	6.2
4	F	204	PRO	6.2
1	A	339	ALA	6.2
3	H	198	SER	6.1
3	E	29	ILE	6.1
3	E	180	LEU	6.1
2	B	32	PRO	6.1
3	H	133	VAL	6.1
2	D	48	ASN	6.1
4	F	119	PRO	6.0
2	B	34	GLY	6.0
2	D	468	GLY	6.0
2	B	437	CYS	5.9
2	D	50	ALA	5.9
3	E	198	SER	5.9
3	E	217	GLU	5.9
4	F	186	TYR	5.8
3	E	127	VAL	5.8
3	E	191	SER	5.8
2	D	36	PRO	5.8
4	F	189	HIS	5.8
4	L	111	ALA	5.7
3	E	11	LEU	5.7
4	F	127	SER	5.7
2	B	50	ALA	5.7
2	D	33	LEU	5.7
4	F	15	LEU	5.7
4	F	197	THR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	42	GLU	5.7
3	H	201	CYS	5.6
2	B	45	LEU	5.6
4	F	174	SER	5.6
4	F	163	TRP	5.6
2	D	446	HIS	5.6
4	F	116	SER	5.6
3	E	158	LEU	5.6
4	F	156	GLN	5.6
3	H	203	VAL	5.5
4	F	106	ILE	5.5
4	F	212	ASN	5.5
3	E	20	LEU	5.5
3	E	189	VAL	5.4
4	F	145	ASN	5.4
4	F	173	TYR	5.4
3	E	132	PRO	5.4
3	H	211	LYS	5.4
3	E	148	VAL	5.4
3	E	126	SER	5.3
3	E	214	LYS	5.3
2	D	40	LEU	5.3
3	H	158	LEU	5.3
2	D	380	ILE	5.3
3	E	13	LYS	5.3
3	E	8	GLY	5.2
3	E	54	ALA	5.2
3	E	215	LYS	5.2
2	B	29	GLU	5.2
4	F	124	GLN	5.2
4	F	160	LEU	5.2
3	E	118	SER	5.1
4	L	212	ASN	5.1
4	F	111	ALA	5.1
4	F	107	LYS	5.1
2	B	445	SER	5.1
3	E	17	SER	5.1
1	A	454	VAL	5.0
2	D	52	GLU	5.0
3	H	167	SER	5.0
2	D	79	GLN	5.0
4	F	147	LYS	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	460	CYS	4.9
2	D	26	CYS	4.9
4	F	157	ASN	4.9
4	F	184	ASP	4.9
3	H	209	SER	4.9
2	B	380	ILE	4.9
4	F	169	LYS	4.9
3	E	92	ALA	4.8
2	B	2	PRO	4.8
3	E	153	PRO	4.8
3	E	85	SER	4.8
4	F	154	GLU	4.8
2	D	5	CYS	4.8
3	E	167	SER	4.8
3	E	208	SER	4.7
3	H	162	SER	4.7
3	E	156	VAL	4.7
3	E	175	VAL	4.7
3	E	161	ASN	4.7
4	F	152	GLY	4.7
2	D	45	LEU	4.6
4	F	146	VAL	4.6
4	F	112	ALA	4.6
2	B	10	VAL	4.6
4	F	149	LYS	4.6
2	D	49	CYS	4.6
3	E	168	GLY	4.6
4	F	133	VAL	4.6
3	E	115	VAL	4.5
4	L	206	VAL	4.5
3	H	217	GLU	4.5
4	F	13	VAL	4.5
2	B	53	SER	4.5
3	E	209	SER	4.5
4	F	131	SER	4.5
2	B	450	ASN	4.5
4	F	207	LYS	4.5
4	F	153	SER	4.5
1	A	217	SER	4.4
4	F	109	ALA	4.4
4	F	155	ARG	4.4
2	B	374	CYS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	399	ILE	4.4
2	B	376	ASN	4.4
3	E	195	PRO	4.4
3	H	160	TRP	4.3
2	D	56	PHE	4.3
2	D	178	TYR	4.3
2	D	58	VAL	4.3
4	F	196	ALA	4.3
2	B	38	CYS	4.3
3	E	40	ARG	4.2
3	H	166	SER	4.2
4	L	200	THR	4.2
4	F	190	ASN	4.2
2	D	53	SER	4.2
4	F	158	GLY	4.2
2	B	35	SER	4.2
3	E	114	SER	4.1
3	E	119	SER	4.1
4	F	191	SER	4.1
2	B	466	TRP	4.1
4	L	125	LEU	4.1
1	A	171	PHE	4.1
2	B	67	ARG	4.1
2	B	76	ASP	4.1
4	F	11	MET	4.1
4	F	14	SER	4.1
2	B	373	THR	4.0
3	E	120	ALA	4.0
2	D	27	SER	4.0
1	C	421	LEU	4.0
4	L	78	LEU	4.0
2	D	39	ASP	4.0
4	F	187	GLU	4.0
2	B	48	ASN	4.0
2	D	3	ASN	4.0
3	E	213	ASP	4.0
2	B	377	ASN	4.0
2	D	35	SER	4.0
4	F	79	ASP	4.0
3	E	82	GLN	4.0
2	D	38	CYS	3.9
4	F	161	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	30	ALA	3.9
3	E	141	SER	3.9
3	E	193	THR	3.9
1	A	336	GLY	3.9
3	E	186	SER	3.9
1	A	436	ILE	3.9
3	E	197	GLN	3.9
4	F	83	PHE	3.9
2	B	383	LEU	3.9
4	L	129	GLY	3.9
2	B	8	ARG	3.8
2	B	381	PRO	3.8
4	F	140	TYR	3.8
4	F	203	SER	3.8
3	E	176	LEU	3.8
2	B	459	VAL	3.8
3	E	181	TYR	3.8
3	E	87	THR	3.8
3	E	172	PHE	3.8
3	E	88	SER	3.8
2	B	42	GLU	3.8
3	E	190	THR	3.8
3	H	157	THR	3.8
2	D	451	GLY	3.8
3	E	164	SER	3.8
3	H	194	TRP	3.7
2	B	178	TYR	3.7
1	C	340	LEU	3.7
2	B	448	CYS	3.7
2	B	444	ASN	3.7
1	C	320	ARG	3.7
2	D	7	THR	3.7
3	E	149	LYS	3.7
1	A	183	LEU	3.7
2	B	378	GLU	3.7
3	H	140	SER	3.7
4	F	168	SER	3.7
1	A	192	LEU	3.6
1	A	389	VAL	3.6
2	B	370	PHE	3.6
3	E	1	GLU	3.6
2	D	398	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	440	GLN	3.6
3	E	121	LYS	3.6
1	C	130	CYS	3.6
3	E	72	ALA	3.6
2	B	446	HIS	3.6
4	F	114	THR	3.6
3	E	42	GLU	3.6
1	A	45	PRO	3.6
1	A	407	LEU	3.6
1	A	421	LEU	3.6
1	C	335	ARG	3.6
3	H	219	ARG	3.6
2	B	455	PHE	3.5
3	H	138	THR	3.5
3	E	64	PHE	3.5
3	H	188	THR	3.5
1	A	194	LEU	3.5
4	F	199	LYS	3.5
1	A	288	TYR	3.5
4	F	166	GLN	3.5
2	B	55	GLU	3.5
2	D	22	MET	3.5
3	E	94	TYR	3.5
1	C	302	GLY	3.5
2	B	262	LEU	3.5
2	D	437	CYS	3.5
1	C	339	ALA	3.4
4	F	185	GLU	3.4
3	H	212	VAL	3.4
3	H	168	GLY	3.4
3	E	162	SER	3.4
2	B	265	ILE	3.4
3	E	177	GLN	3.4
4	F	78	LEU	3.4
1	A	235	TRP	3.4
2	B	129	TRP	3.4
4	F	123	GLU	3.4
4	L	41	GLY	3.4
2	D	404	ARG	3.3
2	B	24	ALA	3.3
2	B	25	TRP	3.3
1	A	338	HIS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	116	THR	3.3
4	F	129	GLY	3.3
4	L	205	ILE	3.3
4	F	178	THR	3.3
4	F	121	SER	3.3
3	H	129	PRO	3.3
3	E	4	LEU	3.3
3	H	187	VAL	3.3
2	D	34	GLY	3.3
3	H	1	GLU	3.3
4	L	146	VAL	3.3
4	F	137	ASN	3.3
3	E	206	PRO	3.3
2	B	9	GLY	3.2
4	F	139	PHE	3.2
4	F	103	LYS	3.2
1	C	453	VAL	3.2
2	B	6	THR	3.2
2	B	164	TYR	3.2
3	E	187	VAL	3.2
3	E	5	GLN	3.2
1	C	132	LEU	3.2
2	B	439	ALA	3.2
1	C	249	ASN	3.2
2	B	258	LEU	3.1
4	L	213	GLU	3.1
1	A	319	ASP	3.1
4	F	183	LYS	3.1
1	A	97	VAL	3.1
1	A	182	VAL	3.1
2	B	181	LYS	3.1
3	H	139	GLY	3.1
4	F	170	ASP	3.1
1	A	419	PHE	3.1
2	B	62	ARG	3.1
4	L	198	HIS	3.1
1	A	21	PHE	3.1
2	B	52	GLU	3.1
3	E	68	ALA	3.1
4	F	188	ARG	3.1
3	E	19	LYS	3.1
2	B	447	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	234	TYR	3.1
2	B	289	TYR	3.1
3	H	210	THR	3.0
1	A	47	GLN	3.0
1	A	354	GLY	3.0
2	B	462	CYS	3.0
4	F	80	SER	3.0
2	D	447	ARG	3.0
3	E	23	THR	3.0
1	C	182	VAL	3.0
2	D	377	ASN	3.0
1	A	417	PHE	3.0
3	H	213	ASP	3.0
1	A	195	LEU	3.0
1	C	248	LEU	3.0
3	E	83	LEU	3.0
3	E	152	PHE	3.0
3	H	17	SER	3.0
3	H	200	THR	3.0
1	A	167	CYS	3.0
2	B	266	VAL	3.0
1	A	248	LEU	3.0
2	B	40	LEU	3.0
2	D	467	LEU	3.0
3	H	130	LEU	3.0
4	F	39	LYS	3.0
2	D	433	CYS	3.0
2	D	439	ALA	3.0
2	D	19	VAL	3.0
2	D	43	ASN	3.0
3	E	77	ASN	3.0
4	F	110	ASP	3.0
4	L	110	ASP	3.0
1	C	1	LEU	2.9
1	C	213	LEU	2.9
1	C	171	PHE	2.9
3	H	207	ALA	2.9
1	A	437	VAL	2.9
1	C	195	LEU	2.9
1	A	439	ALA	2.9
2	B	7	THR	2.9
2	D	177	CYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	457	CYS	2.9
3	E	182	THR	2.9
3	H	18	VAL	2.9
4	L	126	THR	2.9
4	F	104	LEU	2.9
4	L	14	SER	2.9
2	B	256	ILE	2.9
4	F	2	ILE	2.9
1	C	337	PRO	2.9
3	E	179	ASP	2.9
3	E	18	VAL	2.9
2	B	317	LEU	2.9
2	B	382	GLY	2.9
1	A	448	TYR	2.9
1	A	175	VAL	2.9
1	A	186	PRO	2.9
2	D	258	LEU	2.9
2	B	372	ALA	2.9
2	B	27	SER	2.8
2	B	19	VAL	2.8
2	D	10	VAL	2.8
1	A	23	LEU	2.8
2	D	6	THR	2.8
1	A	237	TYR	2.8
1	C	303	ARG	2.8
2	D	57	PRO	2.8
3	E	65	GLN	2.8
4	F	167	ASP	2.8
1	A	146	CYS	2.8
1	A	191	PHE	2.8
1	C	191	PHE	2.8
2	B	223	PHE	2.8
4	L	83	PHE	2.8
3	E	125	PRO	2.8
1	A	193	GLY	2.8
4	F	128	GLY	2.8
1	A	390	LEU	2.8
4	L	170	ASP	2.8
2	D	100	PHE	2.8
4	F	105	GLU	2.8
4	F	198	HIS	2.8
1	A	1	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	378	ALA	2.8
2	B	257	ALA	2.8
3	E	9	ALA	2.8
3	H	199	ILE	2.8
4	F	175	MET	2.8
3	E	151	TYR	2.8
1	A	359	ALA	2.7
3	E	163	GLY	2.7
3	E	155	PRO	2.7
4	F	59	PRO	2.7
2	B	37	ARG	2.7
3	E	166	SER	2.7
4	F	171	SER	2.7
1	A	25	PHE	2.7
4	L	118	PHE	2.7
1	C	143	TYR	2.7
1	A	377	ALA	2.7
3	H	142	VAL	2.7
1	A	221	LEU	2.7
2	D	466	TRP	2.7
1	C	319	ASP	2.7
2	D	382	GLY	2.7
3	E	188	THR	2.7
3	H	131	ALA	2.7
1	C	118	LYS	2.7
4	F	177	SER	2.7
1	A	8	LEU	2.7
1	A	363	LEU	2.7
2	D	90	LEU	2.7
1	A	35	ILE	2.7
2	B	260	GLY	2.7
1	A	185	ALA	2.7
2	B	263	ALA	2.7
4	L	209	PHE	2.7
1	A	166	TYR	2.7
1	A	3	LEU	2.7
2	B	255	HIS	2.7
1	A	172	SER	2.7
2	D	381	PRO	2.7
1	A	257	ALA	2.6
1	A	127	VAL	2.6
3	E	80	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	151	TYR	2.6
3	H	191	SER	2.6
1	C	338	HIS	2.6
2	B	78	SER	2.6
3	E	184	SER	2.6
1	A	435	LEU	2.6
1	A	103	VAL	2.6
1	A	447	VAL	2.6
2	B	157	VAL	2.6
1	A	380	TYR	2.6
4	F	81	GLU	2.6
1	A	312	LEU	2.6
1	A	366	LEU	2.6
2	B	47	ASP	2.6
2	B	79	GLN	2.6
1	C	203	ILE	2.6
4	L	7	SER	2.6
1	C	131	PHE	2.6
1	A	256	GLY	2.6
1	A	381	GLY	2.6
2	D	47	ASP	2.6
2	B	436	ALA	2.6
1	A	410	PRO	2.6
2	B	268	PRO	2.6
4	L	199	LYS	2.6
2	D	449	ASN	2.6
1	C	194	LEU	2.5
3	H	68	ALA	2.5
3	H	144	LEU	2.5
3	E	84	SER	2.5
4	L	171	SER	2.5
1	A	110	TRP	2.5
2	B	5	CYS	2.5
3	E	146	CYS	2.5
1	A	37	VAL	2.5
1	A	420	SER	2.5
1	C	109	PRO	2.5
2	D	450	ASN	2.5
1	C	110	TRP	2.5
4	F	211	ARG	2.5
1	C	47	GLN	2.5
2	B	11	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	CYS	2.5
2	B	16	CYS	2.5
2	B	39	ASP	2.5
1	A	55	LEU	2.5
1	A	170	GLY	2.5
2	D	28	ASP	2.5
3	E	202	ASN	2.5
3	H	208	SER	2.5
1	C	216	VAL	2.5
4	F	19	VAL	2.5
3	H	215	LYS	2.5
4	L	169	LYS	2.5
2	B	3	ASN	2.5
1	C	196	ALA	2.5
3	E	204	ALA	2.5
3	H	169	VAL	2.5
1	C	183	LEU	2.5
2	D	164	TYR	2.5
4	L	108	ARG	2.5
1	A	20	GLY	2.4
1	A	94	GLY	2.4
1	A	357	GLY	2.4
4	F	143	ASP	2.4
1	A	239[A]	VAL	2.4
2	B	456	GLU	2.4
1	C	217	SER	2.4
3	H	141	SER	2.4
2	B	156	PHE	2.4
2	D	23	CYS	2.4
3	H	132	PRO	2.4
1	A	216	VAL	2.4
1	A	131	PHE	2.4
1	A	264	LEU	2.4
2	B	57	PRO	2.4
1	C	187	GLY	2.4
4	F	138	ASN	2.4
1	A	106	ALA	2.4
2	D	257	ALA	2.4
1	A	187	GLY	2.4
1	A	233	GLY	2.4
2	D	41	LYS	2.4
1	A	360	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	109	PRO	2.4
1	A	293	VAL	2.4
1	A	93	LEU	2.4
1	A	189	TYR	2.4
1	A	190	TYR	2.4
4	F	10	SER	2.4
4	F	77	SER	2.4
2	D	372	ALA	2.4
3	E	69	THR	2.4
3	E	14	PRO	2.4
2	D	199	GLN	2.4
1	C	376	VAL	2.4
2	D	369	SER	2.3
1	C	435	LEU	2.3
1	A	95	ALA	2.3
1	C	108	ALA	2.3
1	C	273	TYR	2.3
2	B	218	ALA	2.3
3	E	43	GLN	2.3
3	H	65	GLN	2.3
1	A	105	VAL	2.3
2	D	62	ARG	2.3
4	F	142	LYS	2.3
1	A	12	ALA	2.3
1	A	169	ALA	2.3
2	B	22	MET	2.3
1	A	418	GLY	2.3
1	C	389	VAL	2.3
1	A	181	LEU	2.3
3	H	121	LYS	2.3
3	H	206	PRO	2.3
1	A	36	VAL	2.3
1	A	184	GLY	2.3
1	A	188	GLY	2.3
1	A	236	GLY	2.3
1	C	447	VAL	2.3
3	E	89	GLU	2.3
3	H	204	ALA	2.3
1	A	259	THR	2.3
1	C	167	CYS	2.3
4	F	76	SER	2.3
1	A	440	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	417	PHE	2.3
3	E	170	HIS	2.3
1	A	265	GLY	2.3
1	A	228	PRO	2.3
1	A	450	ALA	2.3
3	E	3	GLN	2.3
2	B	74	SER	2.3
3	E	57	TYR	2.2
2	D	370	PHE	2.2
1	A	145	PRO	2.2
2	B	219	PRO	2.2
3	H	148	VAL	2.2
4	L	13	VAL	2.2
1	A	238	SER	2.2
4	F	21	ILE	2.2
1	A	143	TYR	2.2
1	C	207	TYR	2.2
4	L	140	TYR	2.2
1	A	258	PRO	2.2
1	A	263	THR	2.2
1	C	358[A]	SER	2.2
2	B	201	THR	2.2
3	E	159	THR	2.2
1	A	262	TRP	2.2
1	A	118	LYS	2.2
1	A	107	CYS	2.2
1	A	126	PRO	2.2
1	A	358	SER	2.2
2	B	254	THR	2.2
2	D	455	PHE	2.2
3	E	157	THR	2.2
4	L	127	SER	2.2
1	A	266	ALA	2.2
1	A	446	ALA	2.2
3	H	177	GLN	2.2
1	C	406	VAL	2.2
1	C	437	VAL	2.2
2	D	266	VAL	2.2
1	A	203	ILE	2.2
1	C	68	LEU	2.2
2	B	404	ARG	2.2
2	D	25	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	369	SER	2.2
2	D	55	GLU	2.2
1	C	190	TYR	2.2
1	C	234	TYR	2.2
3	E	150	GLY	2.2
1	A	376	VAL	2.2
2	D	83	VAL	2.2
3	H	218	PRO	2.2
1	A	9	THR	2.2
4	F	164	THR	2.2
3	H	3	GLN	2.2
1	C	186	PRO	2.1
3	E	76	SER	2.1
4	F	162	SER	2.1
4	L	141	PRO	2.1
1	C	360	ILE	2.1
2	B	226	ILE	2.1
1	A	335	ARG	2.1
1	C	23	LEU	2.1
2	D	373	THR	2.1
3	H	123	THR	2.1
2	D	95	ASP	2.1
4	L	109	ALA	2.1
1	C	104	ILE	2.1
1	C	212	LEU	2.1
1	C	359	ALA	2.1
1	C	166	TYR	2.1
1	C	237	TYR	2.1
2	B	321	TYR	2.1
2	D	77	SER	2.1
1	A	387	GLY	2.1
3	H	159	THR	2.1
2	D	265	ILE	2.1
2	B	117	LEU	2.1
1	A	96	SER	2.1
2	B	261	ARG	2.1
2	D	67	ARG	2.1
1	A	379	PRO	2.1
1	A	364	GLY	2.1
1	C	53	VAL	2.1
2	B	314	VAL	2.1
3	E	171	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	107	CYS	2.1
2	B	225	ALA	2.1
2	B	69	LEU	2.1
2	B	66	ASP	2.1
1	A	61	GLU	2.1
4	L	195	GLU	2.1
1	A	38	GLY	2.1
1	A	353	TYR	2.1
2	B	153	PHE	2.1
1	A	225	SER	2.1
2	B	95	ASP	2.1
1	A	213	LEU	2.1
2	D	120	LEU	2.1
1	A	223	PHE	2.0
1	A	231	PHE	2.0
1	A	255	VAL	2.0
2	B	315	VAL	2.0
4	F	58	VAL	2.0
4	L	133	VAL	2.0
3	E	211	LYS	2.0
3	H	195	PRO	2.0
1	C	407	LEU	2.0
2	B	292	LEU	2.0
2	B	325	ILE	2.0
2	D	262	LEU	2.0
2	B	287	MET	2.0
4	F	38	GLN	2.0
1	A	311	PRO	2.0
1	C	38	GLY	2.0
2	B	188	PHE	2.0
2	B	248	PHE	2.0
2	B	264	GLY	2.0
2	D	263	ALA	2.0
1	C	214	TRP	2.0
3	H	196	SER	2.0
2	D	374	CYS	2.0

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

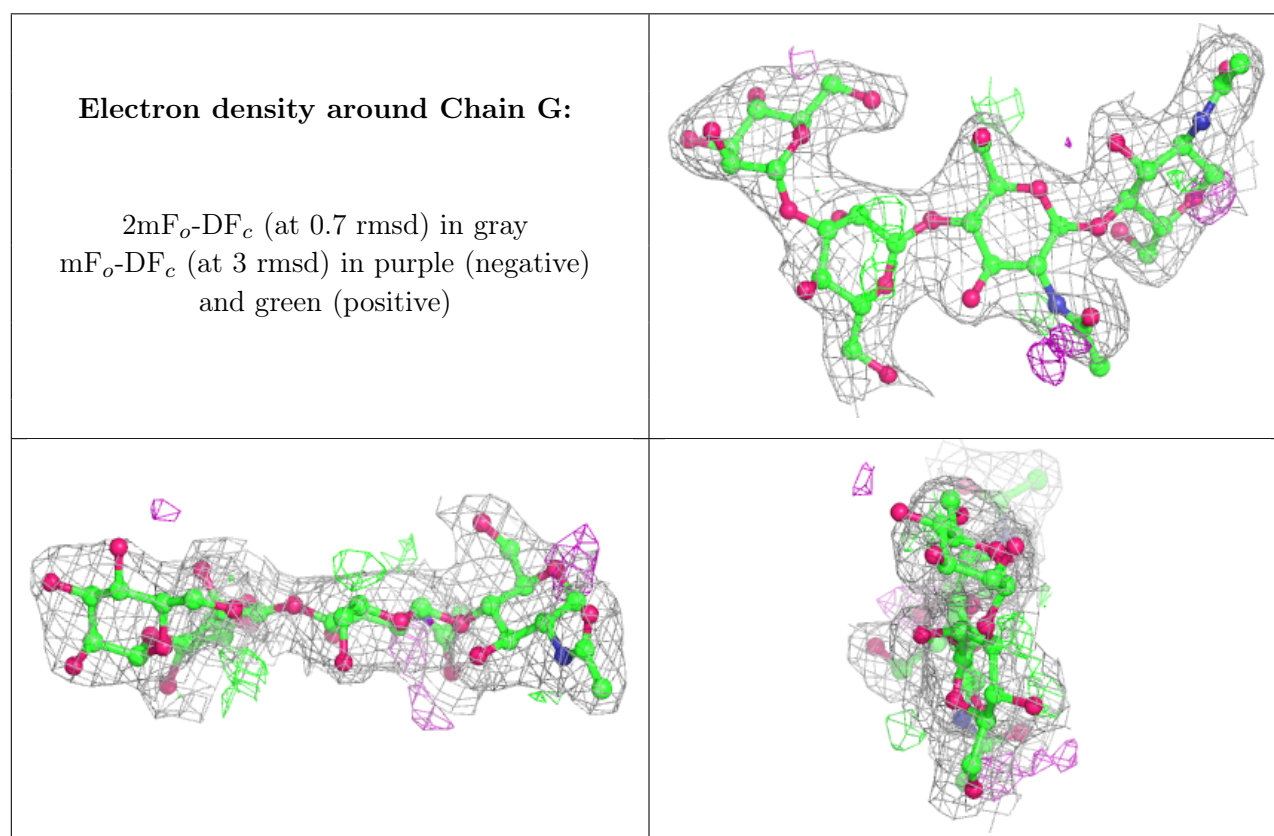
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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.

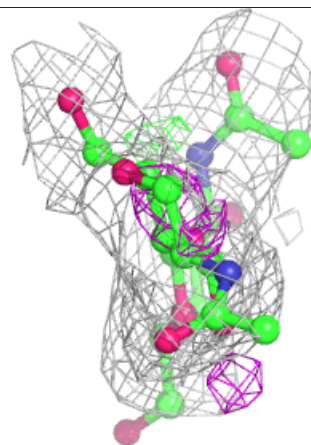
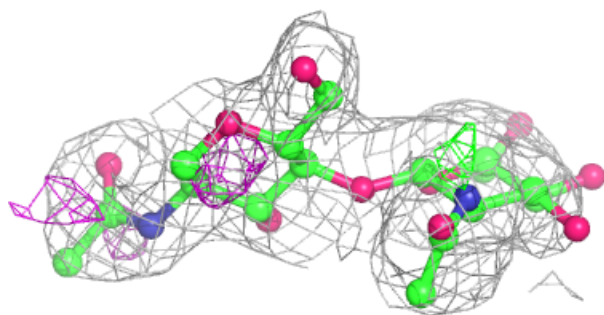
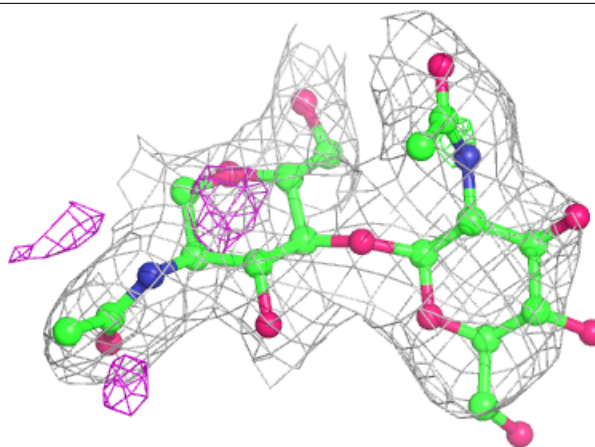
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BMA	J	3	11/12	0.62	0.40	141,145,154,155	0
5	BMA	G	3	11/12	0.64	0.17	130,136,140,142	0
7	MAN	J	4	11/12	0.67	0.25	131,135,139,141	0
6	NAG	I	1	14/15	0.71	0.30	98,106,112,119	0
6	NAG	K	2	14/15	0.72	0.34	127,152,160,161	0
7	NAG	J	2	14/15	0.73	0.24	98,110,127,139	0
7	MAN	J	5	11/12	0.78	0.33	144,148,151,154	0
6	NAG	I	2	14/15	0.80	0.26	128,134,138,140	0
5	MAN	G	4	11/12	0.80	0.17	113,126,130,131	0
6	NAG	K	1	14/15	0.84	0.24	103,109,127,139	0
7	NAG	J	1	14/15	0.85	0.14	55,64,81,95	0
5	NAG	G	2	14/15	0.91	0.15	71,88,104,119	0
5	NAG	G	1	14/15	0.93	0.12	37,48,65,69	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.



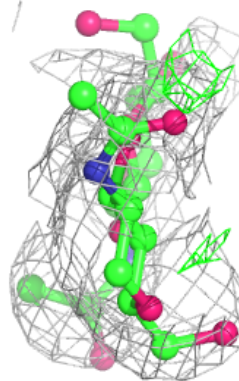
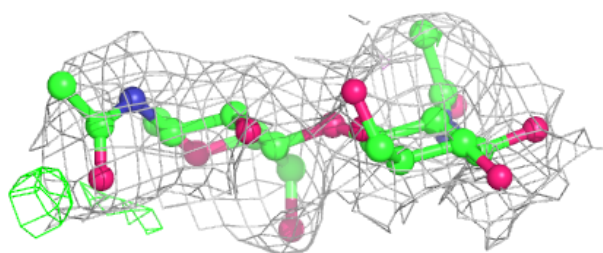
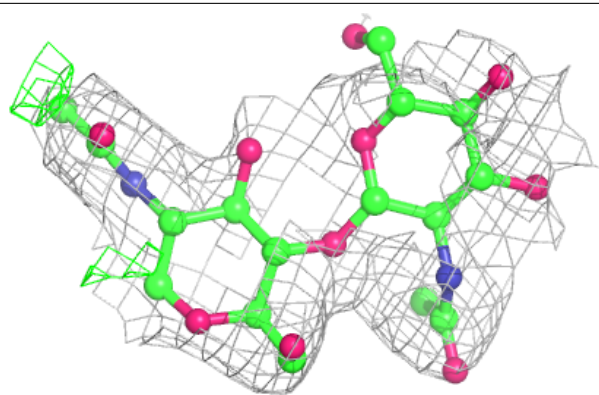
Electron density around Chain I:

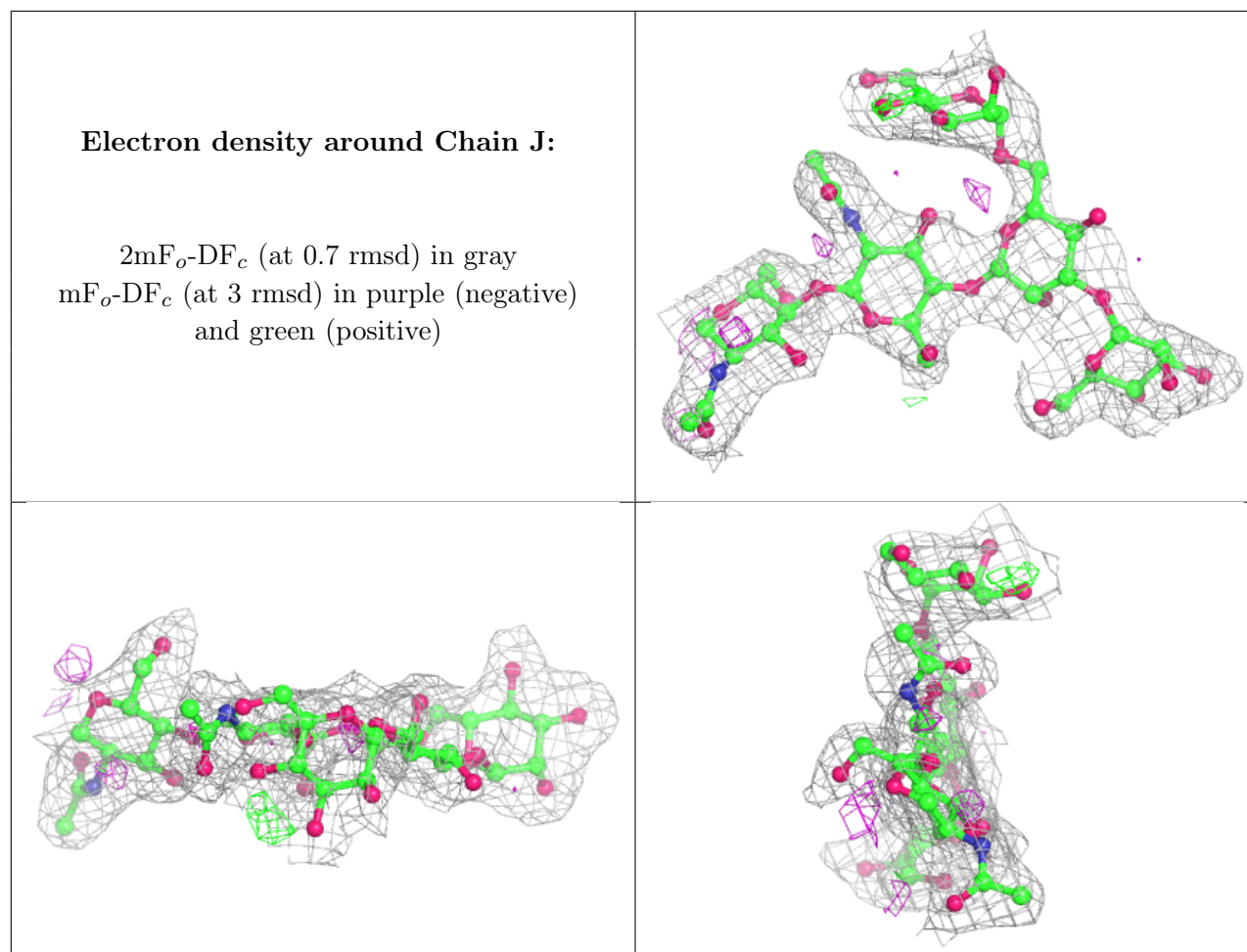
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CL	C	506	1/1	0.46	0.25	129,129,129,129	0
8	SO4	C	503	5/5	0.60	0.34	177,178,178,180	0
11	NAG	D	2004	14/15	0.62	0.29	99,110,119,120	0
8	SO4	A	507	5/5	0.63	0.30	167,169,171,171	0
13	MAN	C	501	11/12	0.67	0.32	134,136,140,140	0
11	NAG	B	2004	14/15	0.75	0.29	114,130,138,139	0
8	SO4	C	502	5/5	0.78	0.28	156,157,159,160	0
8	SO4	A	508	5/5	0.84	0.26	137,140,144,144	0
8	SO4	C	511	5/5	0.87	0.30	170,170,171,171	0
14	CL	C	505	1/1	0.87	0.56	108,108,108,108	0
12	MWO	D	2006	22/22	0.87	0.20	52,77,103,106	0

Continued on next page...

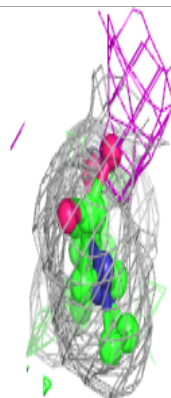
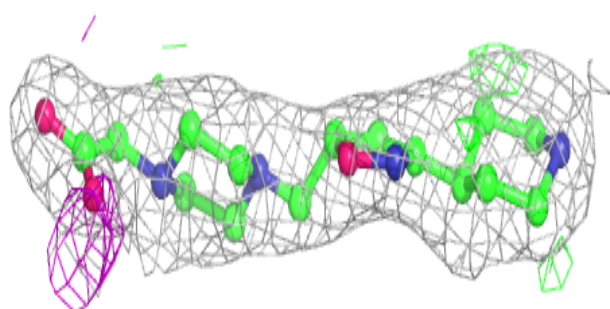
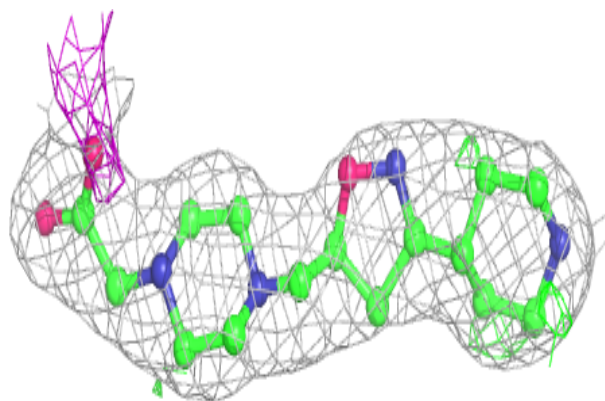
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	MWO	B	2005	22/22	0.88	0.23	36,66,85,88	0
8	SO4	L	301	5/5	0.89	0.19	144,145,145,146	0
8	SO4	A	501	5/5	0.90	0.22	117,118,120,123	0
14	CL	D	2005	1/1	0.90	0.27	110,110,110,110	0
9	CA	C	507	1/1	0.92	0.05	73,73,73,73	0
8	SO4	C	504	5/5	0.93	0.15	132,133,133,141	0
9	CA	C	510	1/1	0.94	0.11	51,51,51,51	0
10	MN	D	2002	1/1	0.95	0.06	61,61,61,61	0
8	SO4	A	502	5/5	0.97	0.13	72,73,75,77	0
9	CA	A	503	1/1	0.97	0.06	47,47,47,47	0
10	MN	B	2002	1/1	0.97	0.06	74,74,74,74	0
9	CA	C	509	1/1	0.98	0.10	57,57,57,57	0
10	MN	D	2003	1/1	0.98	0.10	50,50,50,50	0
10	MN	B	2003	1/1	0.99	0.13	37,37,37,37	0
10	MN	D	2001	1/1	0.99	0.12	48,48,48,48	0
9	CA	C	508	1/1	0.99	0.08	60,60,60,60	0
9	CA	A	505	1/1	0.99	0.17	37,37,37,37	0
9	CA	A	506	1/1	0.99	0.19	39,39,39,39	0
9	CA	A	504	1/1	0.99	0.15	39,39,39,39	0
10	MN	B	2001	1/1	1.00	0.19	36,36,36,36	0

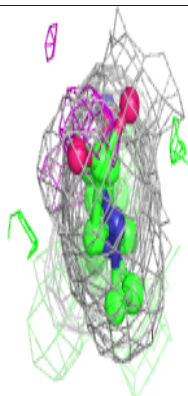
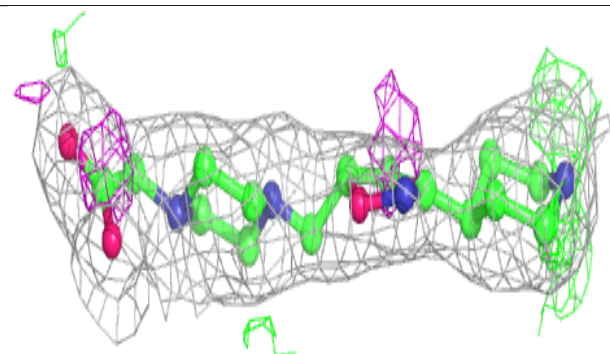
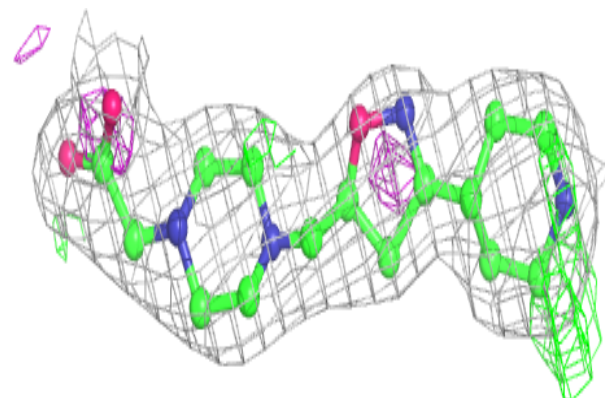
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MWO D 2006:

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

**Electron density around MWO B 2005:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.