Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 11:45 AM EDT

PDB ID	:	7TPD
Title	:	Integrin alaphIIBbeta3 complex with EF5154
Authors	:	Zhu, J.; Lin, F.-Y.; Zhu, J.; Springer, T.A.
Deposited on	:	2022-01-25
Resolution	:	2.60 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:

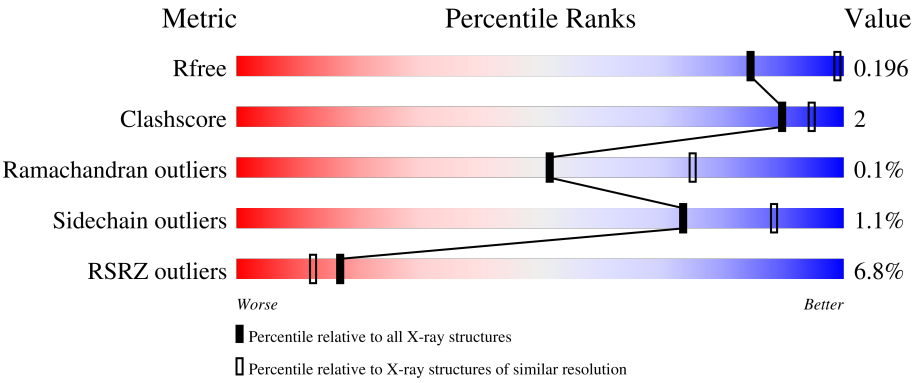
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	94% 6%
1	C	457	92% 7%
2	B	471	8% 94% 5%
2	D	471	5% 94% 6%
3	E	216	17% 97%

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Mol	Chain	Length	Quality of chain
3	H	216	7% 96%
4	F	214	27% 96%
4	L	214	2% 98%
5	G	5	40% 20% 40%
6	I	2	50% 50%
6	K	2	50% 50%
7	J	4	50% 50%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22205 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	457	Total	C	N	O	S	0	7	0
			3542	2251	611	672	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	9	0
			3650	2273	622	721	34			
2	D	471	Total	C	N	O	S	3	6	0
			3666	2285	626	720	35			

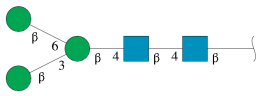
- Molecule 3 is a protein called Fab heavy chain.

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 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 beta-D-mannopyranose-(1-3)-[beta-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
5	G	5	Total C N O 61 34 2 25	0	0	0

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

- Molecule 7 is an oligosaccharide called beta-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
7	J	4	Total C N O 50 28 2 20	0	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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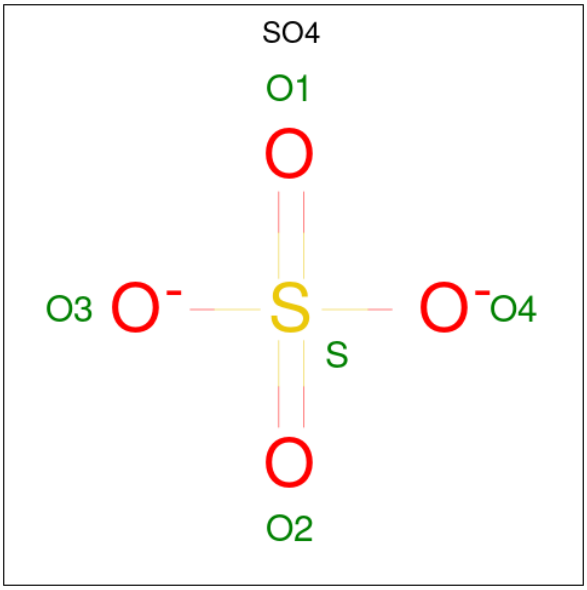
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	2	Total Ca 2 2	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



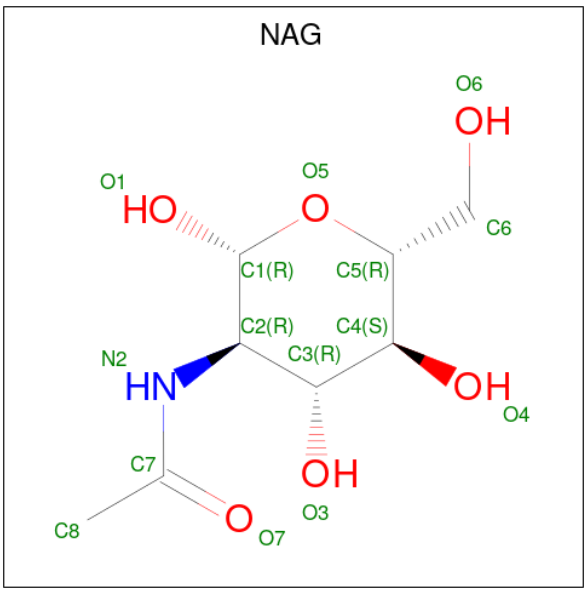
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0

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

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

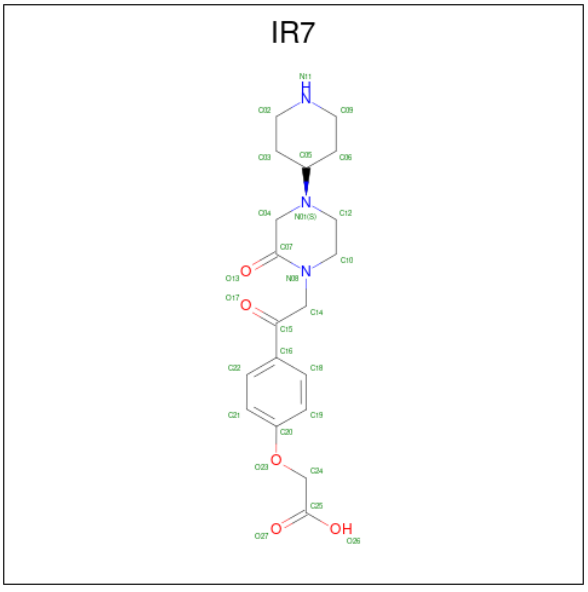
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: $C_8H_{15}NO_6$).



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-{[2-oxo-4-(piperidin-4-yl)piperazin-1-yl]acetyl}phenoxy)acetic acid (three-letter code: IR7) (formula: $C_{19}H_{25}N_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C N O 27 19 3 5	0	0
12	D	1	Total C N O 27 19 3 5	0	0

- Molecule 13 is water.

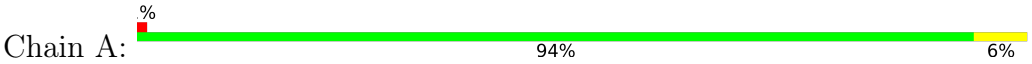
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	374	Total O 374 374	0	0
13	B	190	Total O 190 190	0	0
13	C	233	Total O 233 233	0	0
13	D	132	Total O 132 132	0	0
13	E	13	Total O 13 13	0	0
13	F	6	Total O 6 6	0	0
13	H	21	Total O 21 21	0	0
13	L	41	Total O 41 41	0	0

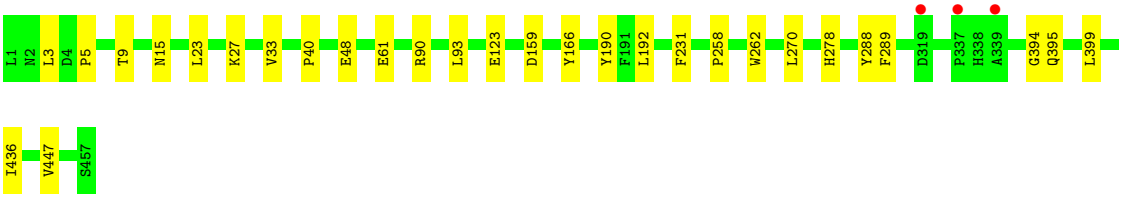
3 Residue-property plots (i)

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 heavy chain

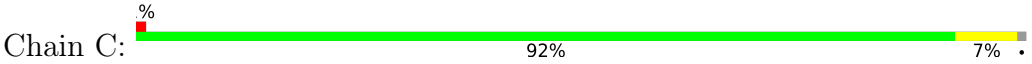
Chain A:

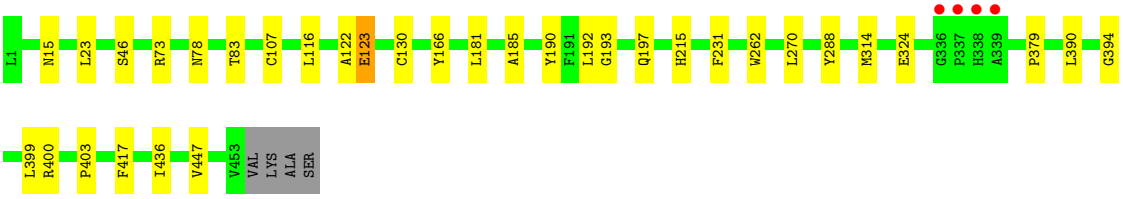




• Molecule 1: Integrin alpha-IIb heavy chain

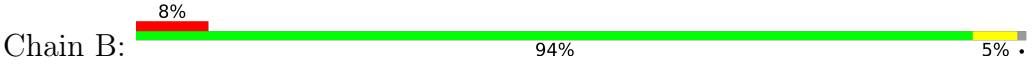
Chain C:

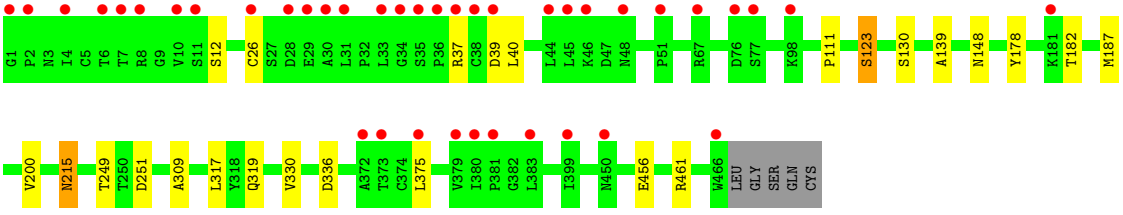




• Molecule 2: Integrin beta-3

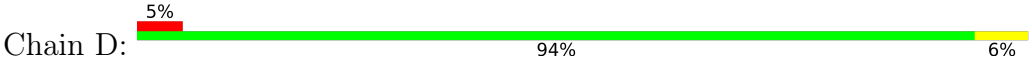
Chain B:

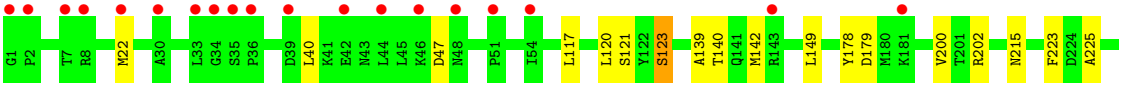




• Molecule 2: Integrin beta-3

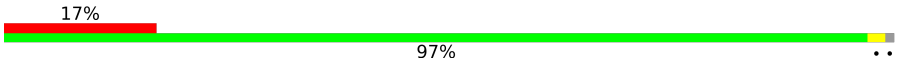
Chain D:

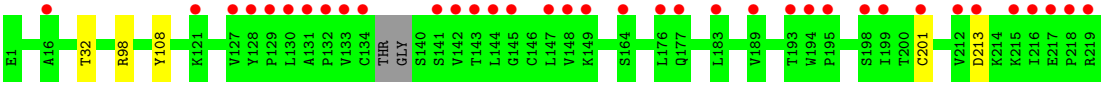




• Molecule 3: Fab heavy chain

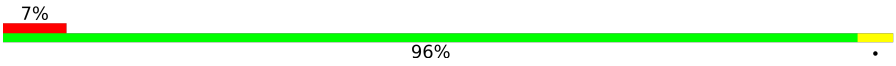
Chain E:





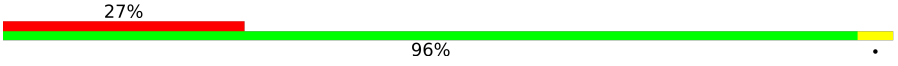
• Molecule 3: Fab heavy chain

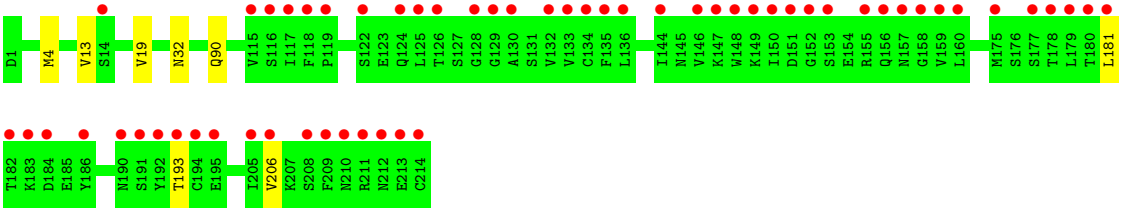
Chain H:



• Molecule 4: Fab light chain

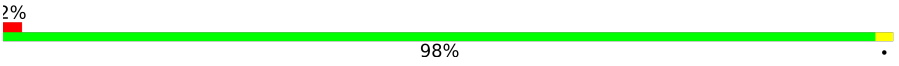
Chain F:

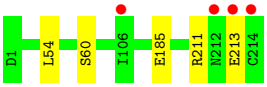




• Molecule 4: Fab light chain

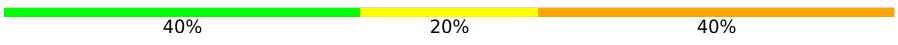
Chain L:





• Molecule 5: beta-D-mannopyranose-(1-3)-[beta-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

Chain G:



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

Chain I:

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

Chain K: 

• Molecule 7: beta-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

Chain J: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	260.18Å 144.34Å 104.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 2.60 48.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.32-2.60) 99.9 (48.32-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.165 , 0.194 0.166 , 0.196	Depositor DCC
R_{free} test set	1022 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22205	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, SO4, MG, BMA, IR7

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	0.27	0/3657	0.55	0/4982
1	C	0.26	0/3605	0.53	0/4912
2	B	0.25	0/3729	0.49	0/5055
2	D	0.25	0/3748	0.49	0/5082
3	E	0.24	0/1673	0.47	0/2290
3	H	0.24	0/1684	0.48	0/2305
4	F	0.25	0/1673	0.46	0/2269
4	L	0.25	0/1673	0.49	0/2269
All	All	0.25	0/21442	0.50	0/29164

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3542	0	3391	15	0
1	C	3502	0	3334	18	0
2	B	3650	0	3572	13	0
2	D	3666	0	3584	16	0
3	E	1631	0	1590	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	4	0
4	F	1637	0	1553	4	0
4	L	1637	0	1553	3	0
5	G	61	0	52	1	0
6	I	28	0	25	0	0
6	K	28	0	25	1	0
7	J	50	0	43	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	2	0	0	0	0
9	A	15	0	0	1	0
9	C	10	0	0	0	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	B	27	0	0	0	0
12	D	27	0	0	1	0
13	A	374	0	0	5	1
13	B	190	0	0	0	0
13	C	233	0	0	3	1
13	D	132	0	0	3	0
13	E	13	0	0	0	0
13	F	6	0	0	0	0
13	H	21	0	0	1	0
13	L	41	0	0	1	0
All	All	22205	0	20348	74	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 (74) 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:B:123[B]:SER:OG	2:B:251:ASP:OD2	2.07	0.71
1:A:15[B]:ASN:ND2	13:A:605:HOH:O	2.26	0.69
1:A:159[A]:ASP:OD2	13:A:602:HOH:O	2.11	0.67
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.31	0.63
1:C:73:ARG:NH1	13:C:604:HOH:O	2.30	0.63
4:L:185:GLU:OE1	13:L:301:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:505:SO4:O4	13:A:601:HOH:O	2.11	0.62
1:C:436:ILE:HG22	1:C:447:VAL:HG22	1.88	0.56
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.88	0.55
2:D:319[A]:GLN:OE1	13:D:2101:HOH:O	2.17	0.55
1:A:192:LEU:HD11	1:A:231:PHE:CD1	2.43	0.54
2:D:123[B]:SER:OG	2:D:251:ASP:OD2	2.17	0.53
1:A:15[B]:ASN:ND2	13:A:612:HOH:O	2.41	0.53
4:F:4:MET:HE1	4:F:90:GLN:HB3	1.91	0.53
2:B:26:CYS:O	2:B:37:ARG:NH1	2.41	0.52
1:C:107:CYS:HA	1:C:130:CYS:HA	1.92	0.51
2:B:111:PRO:HB3	2:B:148:ASN:HB3	1.92	0.51
1:A:48:GLU:OE2	1:A:90[B]:ARG:NH1	2.38	0.50
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.93	0.50
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.94	0.50
1:C:46:SER:OG	13:C:601:HOH:O	2.20	0.49
2:B:130:SER:OG	2:B:336:ASP:O	2.27	0.49
2:B:39:ASP:OD1	2:B:40:LEU:N	2.41	0.49
1:C:192:LEU:HD11	1:C:231:PHE:CD1	2.49	0.48
1:C:390:LEU:HD23	1:C:403:PRO:HG3	1.96	0.48
1:C:400:ARG:HB2	13:C:709:HOH:O	2.14	0.48
2:D:400:GLU:HB2	6:K:1:NAG:H83	1.95	0.47
2:D:409:GLU:OE2	13:D:2102:HOH:O	2.20	0.47
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.96	0.47
2:D:178:TYR:CG	2:D:179:ASP:N	2.83	0.46
1:A:9:THR:HB	1:A:447:VAL:HB	1.96	0.46
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.97	0.46
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.50	0.45
1:A:27:LYS:HG2	1:A:33:VAL:HG22	1.99	0.45
1:A:40:PRO:HA	1:A:93:LEU:O	2.17	0.45
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.98	0.45
1:A:3:LEU:O	1:A:5:PRO:HD3	2.17	0.45
5:G:3:BMA:H62	5:G:5:BMA:H2	1.71	0.44
2:D:117:LEU:HD11	2:D:225:ALA:HB1	2.00	0.44
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.98	0.44
1:C:83:THR:HB	1:C:116:LEU:HB2	1.99	0.44
2:D:121:SER:HB2	12:D:2005:IR7:C25	2.48	0.44
2:D:140:THR:OG1	13:D:2103:HOH:O	2.21	0.44
1:A:278[A]:HIS:NE2	13:A:603:HOH:O	2.24	0.44
1:C:192:LEU:HD11	1:C:231:PHE:HD1	1.83	0.43
1:C:78:ASN:O	4:F:32:ASN:ND2	2.52	0.43
2:B:249:THR:HA	2:B:309:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:GLY:HA2	1:C:399:LEU:HD23	2.00	0.43
4:F:13:VAL:HG11	4:F:19:VAL:HG11	1.99	0.43
3:H:163:GLY:O	13:H:301:HOH:O	2.21	0.43
2:B:187[B]:MET:SD	2:B:215:ASN:HB3	2.58	0.43
2:D:120:LEU:HD23	2:D:120:LEU:HA	1.87	0.43
1:A:192:LEU:HD11	1:A:231:PHE:HD1	1.82	0.43
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.54	0.42
3:E:98:ARG:HG3	3:E:108:TYR:HB2	2.01	0.42
1:C:262:TRP:HB3	2:D:317:LEU:HD13	2.01	0.42
4:L:54:LEU:HD21	4:L:60:SER:HA	2.00	0.42
1:C:181:LEU:O	1:C:197:GLN:HA	2.20	0.42
3:H:98:ARG:HG3	3:H:108:TYR:HB2	2.01	0.42
2:D:139:ALA:HB2	2:D:200:VAL:HG11	2.00	0.42
4:F:193:THR:HG23	4:F:206:VAL:HG13	2.01	0.42
1:A:436:ILE:HG22	1:A:447:VAL:HG22	2.02	0.42
2:B:319[A]:GLN:HA	2:B:330:VAL:HG21	2.00	0.42
1:A:258:PRO:HA	1:A:289:PHE:O	2.19	0.42
2:D:223:PHE:CZ	2:D:254:THR:HG21	2.54	0.42
2:D:142:MET:HB2	2:D:149:LEU:HD22	2.02	0.41
3:E:213:ASP:OD1	3:E:213:ASP:N	2.53	0.41
4:L:211:ARG:O	4:L:213:GLU:N	2.49	0.41
2:B:319[B]:GLN:HA	2:B:330:VAL:HG21	2.01	0.41
1:C:122:ALA:O	1:C:123:GLU:HB2	2.20	0.41
1:C:314:MET:HA	1:C:324:GLU:HA	2.04	0.40
1:C:379:PRO:HA	1:C:417:PHE:O	2.21	0.40
1:C:185:ALA:O	1:C:193:GLY:HA2	2.22	0.40
2:D:22:MET:HG2	2:D:40:LEU:HD22	2.03	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)
13:A:923:HOH:O	13:C:788:HOH:O[1_554]	2.15	0.05

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	462/457 (101%)	450 (97%)	11 (2%)	1 (0%)	47 71
1	C	455/457 (100%)	442 (97%)	12 (3%)	1 (0%)	47 71
2	B	473/471 (100%)	455 (96%)	17 (4%)	1 (0%)	47 71
2	D	475/471 (101%)	461 (97%)	14 (3%)	0	100 100
3	E	210/216 (97%)	199 (95%)	11 (5%)	0	100 100
3	H	212/216 (98%)	203 (96%)	9 (4%)	0	100 100
4	F	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100 100
All	All	2711/2716 (100%)	2619 (97%)	89 (3%)	3 (0%)	51 75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	375	LEU
1	C	123	GLU

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	371/364 (102%)	364 (98%)	7 (2%)	57 79
1	C	365/364 (100%)	359 (98%)	6 (2%)	62 82
2	B	421/416 (101%)	416 (99%)	5 (1%)	71 87
2	D	422/416 (101%)	416 (99%)	6 (1%)	67 85
3	E	186/187 (100%)	185 (100%)	1 (0%)	88 96
3	H	187/187 (100%)	185 (99%)	2 (1%)	73 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	F	188/188 (100%)	187 (100%)	1 (0%)	88 96
4	L	188/188 (100%)	188 (100%)	0	100 100
All	All	2328/2310 (101%)	2300 (99%)	28 (1%)	73 87

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
1	A	395	GLN
2	B	123[A]	SER
2	B	123[B]	SER
2	B	178	TYR
2	B	182	THR
2	B	215	ASN
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	270	LEU
1	C	288	TYR
2	D	47	ASP
2	D	123[A]	SER
2	D	123[B]	SER
2	D	202	ARG
2	D	215	ASN
2	D	235	LYS
3	E	201	CYS
4	F	181	LEU
3	H	87	THR
3	H	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	438	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	0.35	0	17,19,21	0.57	0
5	NAG	G	2	5	14,14,15	0.37	0	17,19,21	0.52	0
5	BMA	G	3	5	11,11,12	1.72	4 (36%)	15,15,17	2.31	3 (20%)
5	BMA	G	4	5	11,11,12	0.93	0	15,15,17	1.43	3 (20%)
5	BMA	G	5	5	11,11,12	1.17	1 (9%)	15,15,17	1.47	3 (20%)
6	NAG	I	1	2,6	14,14,15	0.90	1 (7%)	17,19,21	0.76	0
6	NAG	I	2	6	14,14,15	0.48	0	17,19,21	0.46	0
7	NAG	J	1	2,7	14,14,15	0.35	0	17,19,21	0.61	0
7	NAG	J	2	7	14,14,15	0.41	0	17,19,21	0.41	0
7	BMA	J	3	7	11,11,12	1.06	1 (9%)	15,15,17	1.28	1 (6%)
7	BMA	J	4	7	11,11,12	1.07	2 (18%)	15,15,17	1.85	3 (20%)
6	NAG	K	1	2,6	14,14,15	0.59	0	17,19,21	0.57	0
6	NAG	K	2	6	14,14,15	0.48	0	17,19,21	0.46	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

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	BMA	C2-C3	3.58	1.57	1.52
5	G	5	BMA	C1-C2	3.10	1.59	1.52
6	I	1	NAG	O5-C1	-2.80	1.39	1.43
7	J	3	BMA	C2-C3	2.77	1.56	1.52
5	G	3	BMA	O5-C1	2.49	1.47	1.43
7	J	4	BMA	C4-C3	2.20	1.57	1.52
7	J	4	BMA	C4-C5	2.19	1.57	1.53
5	G	3	BMA	O5-C5	2.06	1.47	1.43
5	G	3	BMA	C1-C2	2.05	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	3	BMA	O3-C3-C2	5.70	120.91	109.99
5	G	3	BMA	O5-C5-C6	5.13	115.25	107.20
7	J	4	BMA	C1-C2-C3	-4.82	103.74	109.67
7	J	3	BMA	O3-C3-C2	3.67	117.03	109.99
5	G	3	BMA	C1-C2-C3	-3.42	105.46	109.67
7	J	4	BMA	O5-C1-C2	-3.02	106.11	110.77
5	G	4	BMA	C1-C2-C3	-2.84	106.18	109.67
5	G	4	BMA	O5-C1-C2	-2.69	106.61	110.77
5	G	5	BMA	O5-C1-C2	-2.67	106.64	110.77
5	G	5	BMA	C1-C2-C3	-2.63	106.43	109.67
5	G	5	BMA	C1-O5-C5	-2.50	108.81	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	4	BMA	C1-O5-C5	-2.30	109.08	112.19
5	G	4	BMA	C1-O5-C5	-2.13	109.30	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	G	5	BMA	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	4	BMA	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	I	2	NAG	C4-C5-C6-O6
5	G	4	BMA	O5-C5-C6-O6
5	G	5	BMA	C4-C5-C6-O6
7	J	4	BMA	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
7	J	4	BMA	O5-C5-C6-O6

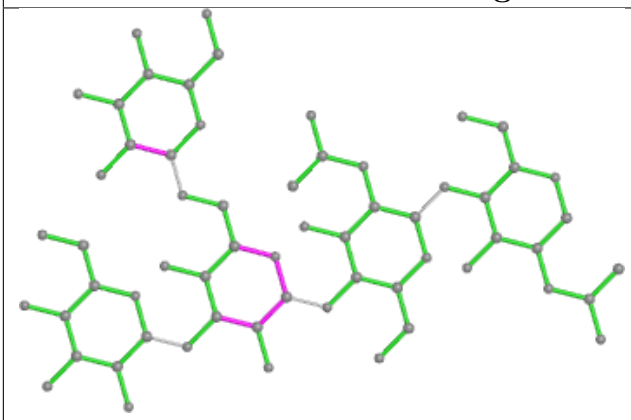
There are no ring outliers.

3 monomers are involved in 2 short contacts:

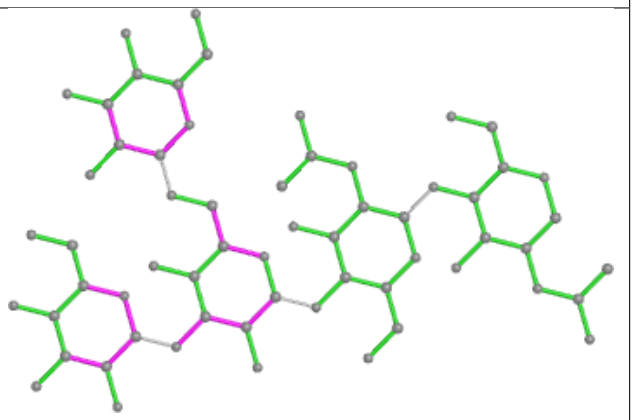
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	3	BMA	1	0
6	K	1	NAG	1	0
5	G	5	BMA	1	0

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

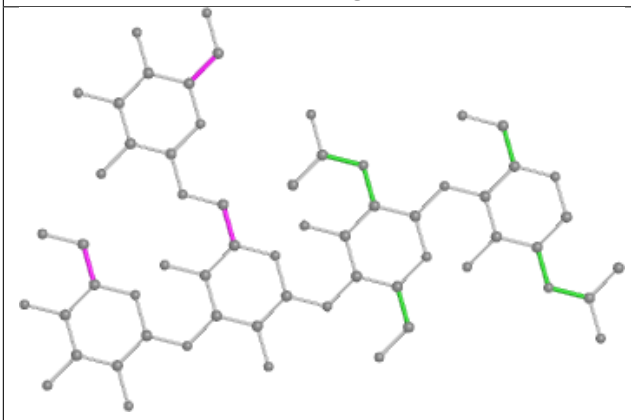
Oligosaccharide Chain G



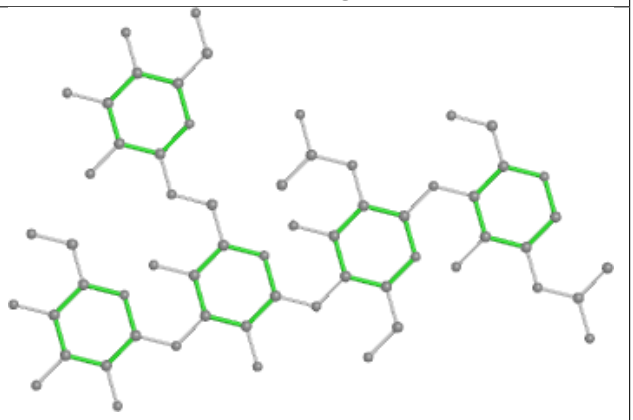
Bond lengths



Bond angles

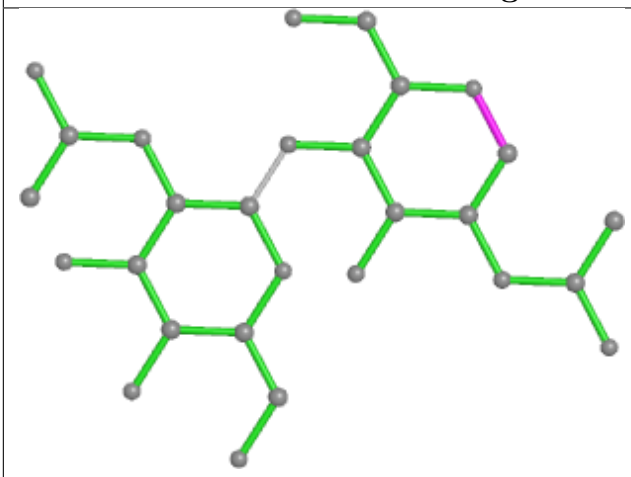


Torsions

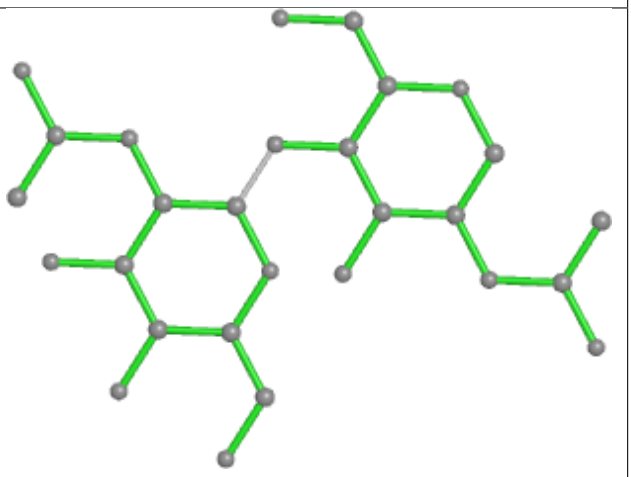


Rings

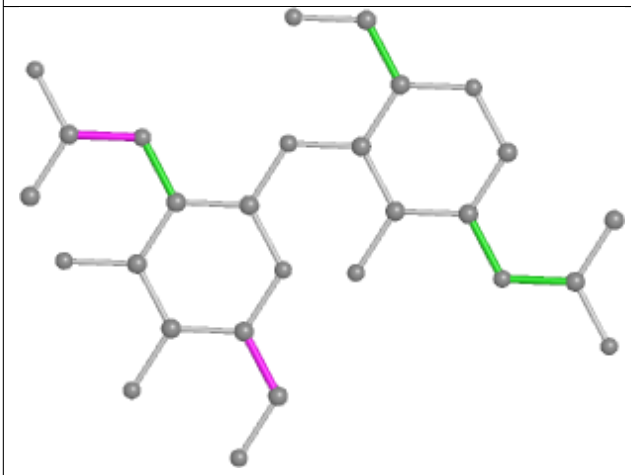
Oligosaccharide Chain I



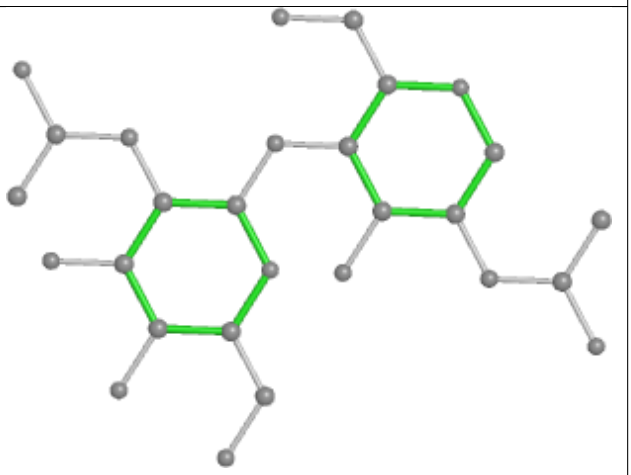
Bond lengths



Bond angles

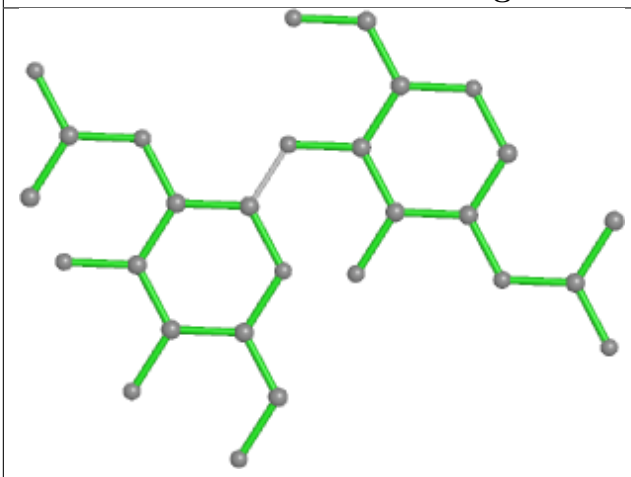


Torsions

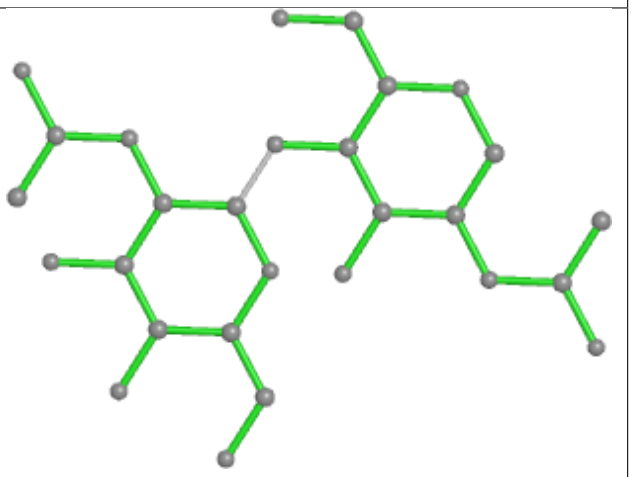


Rings

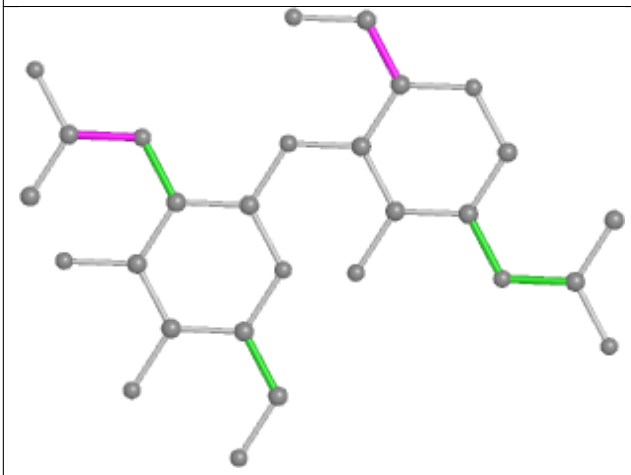
Oligosaccharide Chain K



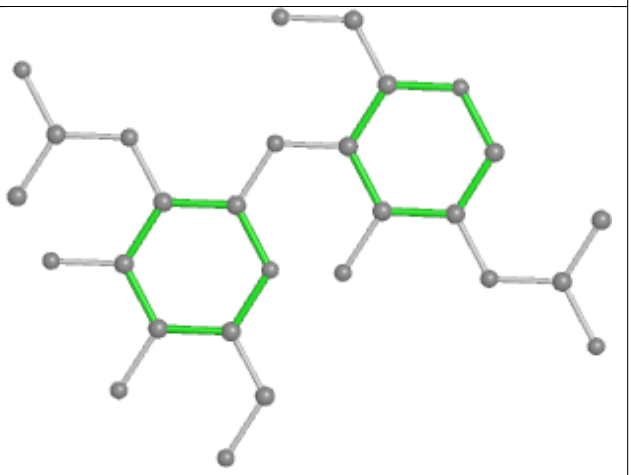
Bond lengths



Bond angles

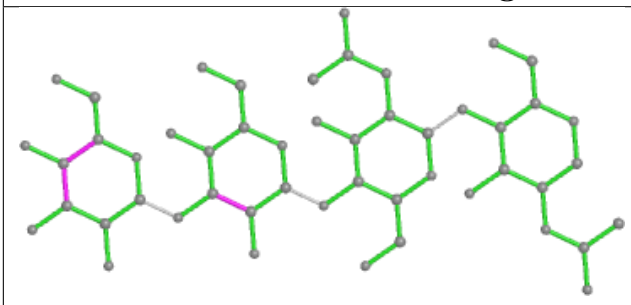


Torsions

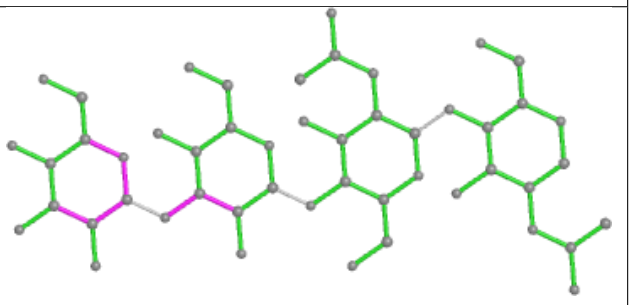


Rings

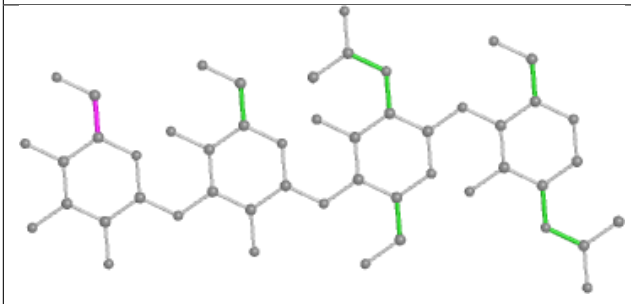
Oligosaccharide Chain J



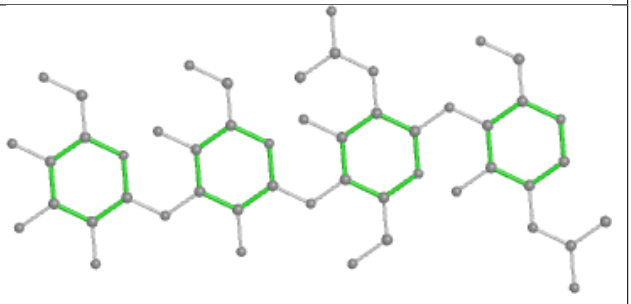
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 14 are monoatomic - leaving 9 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	C	505	-	4,4,4	0.14	0	6,6,6	0.07	0
9	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.09	0
9	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.08	0
11	NAG	D	2004	2	14,14,15	0.37	0	17,19,21	0.53	0
12	IR7	B	2005	10	29,29,29	2.05	9 (31%)	35,39,39	1.57	7 (20%)
9	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.06	0
12	IR7	D	2005	10	29,29,29	1.96	8 (27%)	35,39,39	1.60	6 (17%)
9	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.06	0
11	NAG	B	2004	2	14,14,15	0.41	0	17,19,21	0.52	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
12	IR7	B	2005	10	-	1/17/38/38	0/3/3/3
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	IR7	D	2005	10	-	1/17/38/38	0/3/3/3
11	NAG	D	2004	2	-	1/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	IR7	C07-N08	6.96	1.43	1.34
12	D	2005	IR7	C07-N08	6.52	1.43	1.34
12	B	2005	IR7	C16-C15	3.77	1.55	1.49
12	D	2005	IR7	C16-C15	3.22	1.54	1.49
12	D	2005	IR7	C12-N01	-3.13	1.41	1.47
12	B	2005	IR7	C12-N01	-3.13	1.41	1.47
12	B	2005	IR7	C18-C19	2.54	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	IR7	C18-C16	2.42	1.43	1.39
12	D	2005	IR7	C18-C19	2.39	1.43	1.38
12	B	2005	IR7	C21-C22	2.39	1.43	1.38
12	D	2005	IR7	C04-N01	-2.37	1.41	1.47
12	D	2005	IR7	C18-C16	2.32	1.43	1.39
12	B	2005	IR7	C04-N01	-2.28	1.42	1.47
12	D	2005	IR7	C21-C22	2.20	1.42	1.38
12	D	2005	IR7	C10-N08	-2.07	1.43	1.47
12	B	2005	IR7	C10-N08	-2.02	1.43	1.47
12	B	2005	IR7	C21-C20	2.01	1.42	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	2005	IR7	C07-C04-N01	-4.87	101.41	112.78
12	B	2005	IR7	C07-C04-N01	-4.13	103.15	112.78
12	D	2005	IR7	O26-C25-O27	4.11	133.55	123.30
12	B	2005	IR7	O26-C25-O27	4.06	133.42	123.30
12	B	2005	IR7	O13-C07-N08	-3.99	118.68	122.82
12	D	2005	IR7	O13-C07-N08	-3.61	119.08	122.82
12	B	2005	IR7	C04-C07-N08	3.11	122.74	118.12
12	B	2005	IR7	C10-N08-C07	-2.58	121.04	123.71
12	D	2005	IR7	C12-N01-C05	-2.40	105.87	112.64
12	D	2005	IR7	C04-C07-N08	2.33	121.58	118.12
12	D	2005	IR7	O23-C24-C25	-2.26	103.52	110.24
12	B	2005	IR7	O27-C25-C24	-2.12	114.50	122.44
12	B	2005	IR7	C12-N01-C05	-2.07	106.80	112.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	IR7	C15-C14-N08-C10
11	D	2004	NAG	O5-C5-C6-O6
12	D	2005	IR7	C15-C14-N08-C10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	505	SO4	1	0

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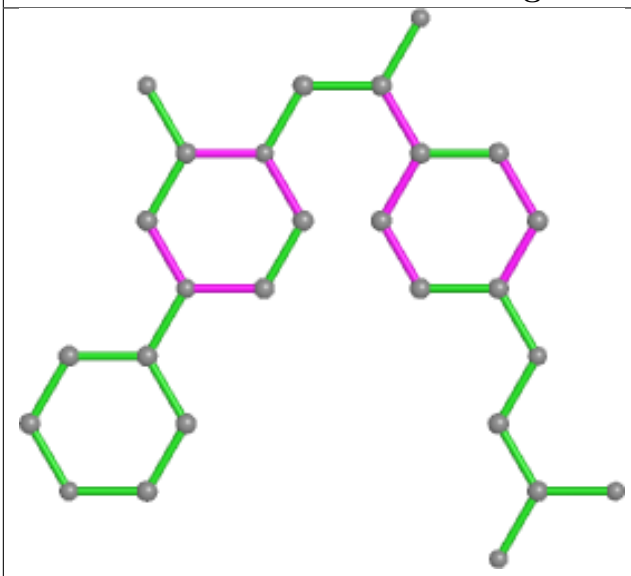
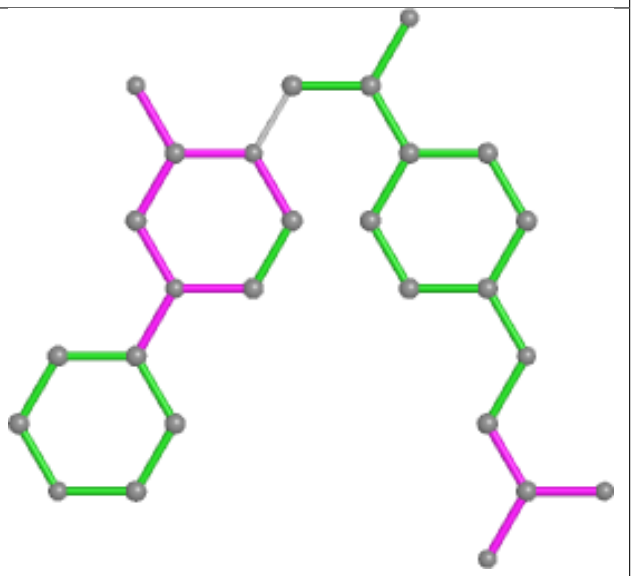
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2005	IR7	1	0

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

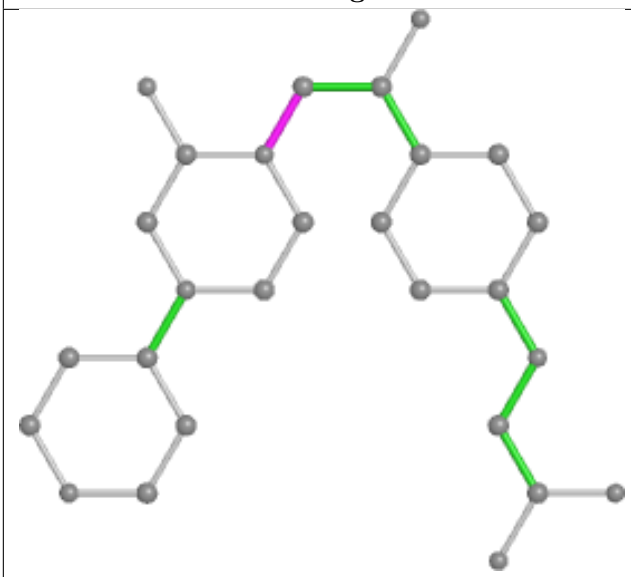
Ligand IR7 B 2005



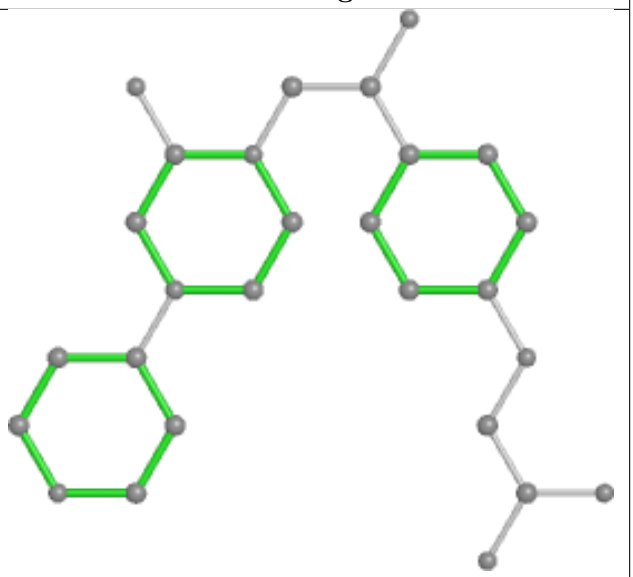
Bond lengths



Bond angles

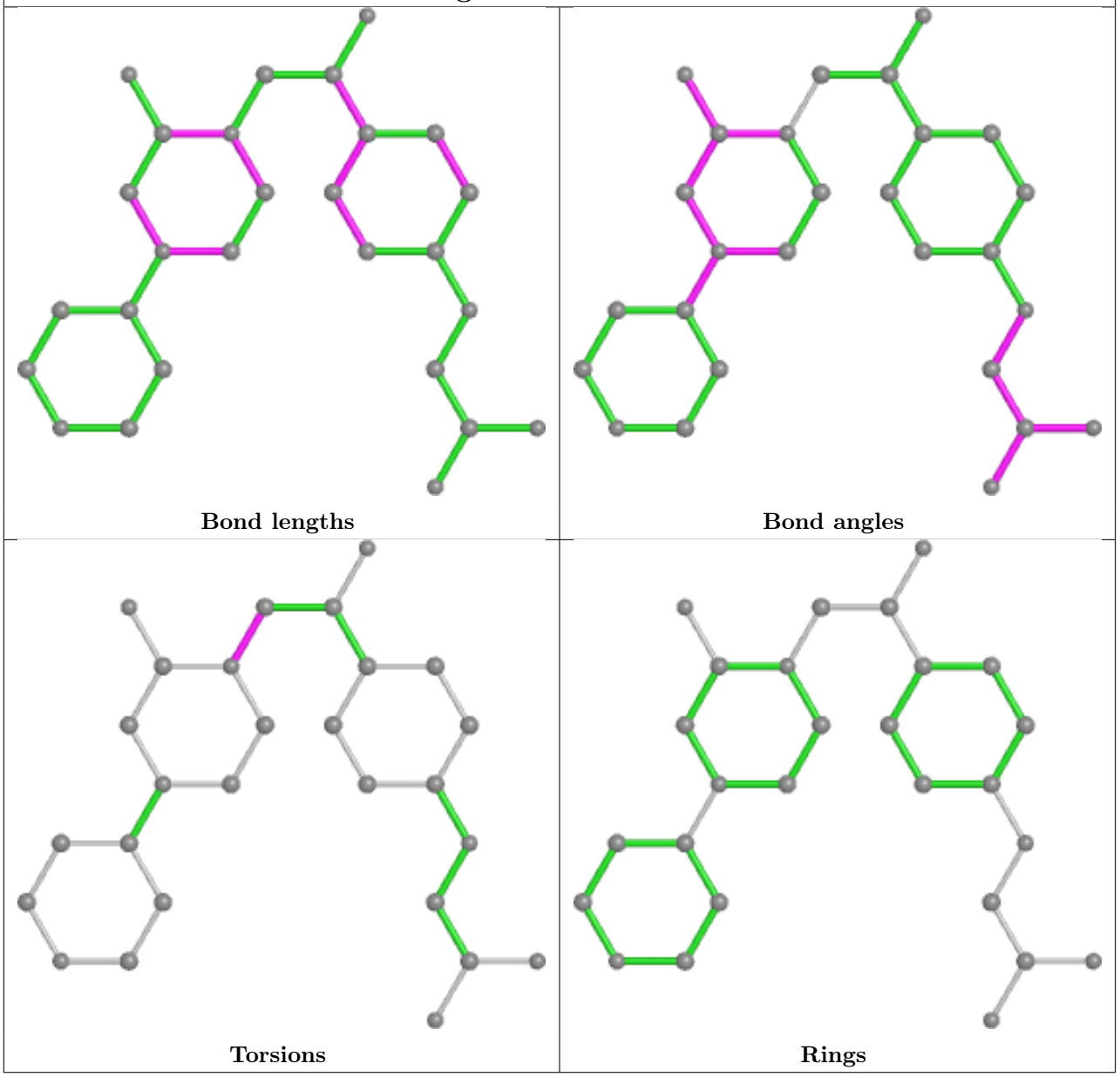


Torsions



Rings

Ligand IR7 D 2005



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:CYS	C	138:THR	N	6.87

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, 95^{th} 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%)	-0.23	3 (0%) 87 86	19, 28, 53, 113	3 (0%)
1	C	453/457 (99%)	-0.24	4 (0%) 84 82	22, 44, 74, 115	0
2	B	466/471 (98%)	0.36	40 (8%) 10 7	17, 55, 142, 187	1 (0%)
2	D	471/471 (100%)	0.07	24 (5%) 28 22	25, 60, 120, 166	2 (0%)
3	E	214/216 (99%)	0.81	36 (16%) 1 1	52, 100, 151, 179	0
3	H	216/216 (100%)	0.22	16 (7%) 14 10	34, 82, 136, 153	0
4	F	214/214 (100%)	1.34	58 (27%) 0 0	56, 100, 180, 208	0
4	L	214/214 (100%)	0.00	4 (1%) 66 62	40, 71, 97, 161	0
All	All	2705/2716 (99%)	0.18	185 (6%) 17 12	17, 58, 139, 208	6 (0%)

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	214	CYS	9.6
4	F	193	THR	9.0
2	B	10	VAL	6.9
3	E	134	CYS	6.8
2	D	469	SER	6.7
4	F	179	LEU	6.7
4	F	117	ILE	6.5
2	B	33	LEU	6.4
4	F	130	ALA	6.3
4	F	209	PHE	6.2
2	B	36	PRO	6.2
2	B	375	LEU	6.2
2	B	77	SER	6.1
4	F	181	LEU	6.1
3	E	132	PRO	5.8
3	E	219	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
4	F	132	VAL	5.7
3	E	131	ALA	5.7
3	E	133	VAL	5.6
4	F	149	LYS	5.6
3	E	216	ILE	5.6
4	F	152	GLY	5.3
4	F	182	THR	5.3
3	E	142	VAL	5.3
4	L	214	CYS	5.2
4	F	129	GLY	5.1
2	D	34	GLY	5.1
4	F	192	TYR	5.1
4	F	158	GLY	5.1
3	E	144	LEU	5.0
4	F	157	ASN	4.8
4	L	212	ASN	4.8
2	B	39	ASP	4.8
2	B	2	PRO	4.7
4	F	148	TRP	4.7
4	F	125	LEU	4.6
4	F	159	VAL	4.5
4	F	115	VAL	4.5
4	F	213	GLU	4.5
3	E	130	LEU	4.4
4	F	186	TYR	4.3
4	F	178	THR	4.2
4	F	180	THR	4.1
2	B	1	GLY	4.1
2	D	33	LEU	4.1
4	F	118	PHE	4.1
4	F	153	SER	4.1
4	F	212	ASN	4.0
2	B	34	GLY	4.0
4	F	194	CYS	3.9
4	F	191	SER	3.9
2	B	28	ASP	3.9
3	E	199	ILE	3.9
4	F	151	ASP	3.9
2	B	466	TRP	3.9
2	D	470	GLN	3.9
4	F	119	PRO	3.7
4	F	150	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
3	E	176	LEU	3.6
4	F	184	ASP	3.6
2	B	6	THR	3.6
3	E	147	LEU	3.6
4	F	205	ILE	3.6
2	D	44	LEU	3.6
3	H	217	GLU	3.5
3	E	215	LYS	3.5
2	B	181	LYS	3.5
3	E	217	GLU	3.5
2	B	46	LYS	3.4
4	F	133	VAL	3.4
4	F	147	LYS	3.4
3	E	141	SER	3.4
3	E	194	TRP	3.4
2	B	44	LEU	3.4
4	F	206	VAL	3.3
2	B	31	LEU	3.3
4	F	144	ILE	3.3
2	B	11	SER	3.3
4	F	211	ARG	3.2
3	E	148	VAL	3.2
3	E	128	TYR	3.2
4	F	128	GLY	3.2
2	B	51	PRO	3.2
2	B	37	ARG	3.2
3	E	198	SER	3.2
3	E	183	LEU	3.1
2	B	48	ASN	3.1
2	B	381	PRO	3.0
3	H	216	ILE	3.0
3	E	218	PRO	3.0
2	B	38	CYS	3.0
2	D	2	PRO	3.0
4	F	208	SER	3.0
2	B	30	ALA	3.0
1	A	337	PRO	3.0
4	F	126	THR	2.9
3	E	201	CYS	2.9
2	B	35	SER	2.9
2	D	1	GLY	2.9
4	F	183	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	134	CYS	2.9
4	F	210	ASN	2.9
3	E	143	THR	2.9
3	E	212	VAL	2.9
2	B	4	ILE	2.9
2	D	35	SER	2.9
2	B	45	LEU	2.9
4	F	195	GLU	2.9
2	B	372	ALA	2.9
3	E	195	PRO	2.9
4	F	156	GLN	2.8
2	D	36	PRO	2.8
1	C	336	GLY	2.8
3	H	215	LYS	2.8
3	H	144	LEU	2.7
3	E	213	ASP	2.7
4	F	135	PHE	2.7
4	F	160	LEU	2.7
2	B	26	CYS	2.7
3	H	138	THR	2.7
2	B	450	ASN	2.7
3	H	142	VAL	2.7
3	E	193	THR	2.7
4	F	122	SER	2.7
3	E	149	LYS	2.6
2	D	30	ALA	2.6
1	A	319	ASP	2.6
3	H	200	THR	2.6
2	D	8	ARG	2.6
4	F	190	ASN	2.6
2	D	54	ILE	2.6
2	D	42	GLU	2.5
4	F	146	VAL	2.5
4	F	116	SER	2.5
2	B	7	THR	2.5
2	D	46	LYS	2.5
4	F	155	ARG	2.5
3	E	129	PRO	2.5
3	H	211	LYS	2.5
1	A	339	ALA	2.5
4	F	136	LEU	2.5
2	B	379	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	29	GLU	2.4
3	H	189	VAL	2.4
2	D	380	ILE	2.4
3	H	208	SER	2.4
2	B	76	ASP	2.4
2	B	98	LYS	2.4
2	B	399	ILE	2.4
3	H	199	ILE	2.4
4	F	14	SER	2.4
2	D	39	ASP	2.4
2	D	22	MET	2.4
3	H	201	CYS	2.4
3	E	127	VAL	2.3
3	E	189	VAL	2.3
3	E	177	GLN	2.3
3	H	133	VAL	2.3
2	B	8	ARG	2.3
2	D	51	PRO	2.3
4	F	124	GLN	2.3
2	B	67	ARG	2.3
3	H	188	THR	2.3
3	H	207	ALA	2.2
3	H	160	TRP	2.2
2	D	378	GLU	2.2
2	B	380	ILE	2.2
2	D	375	LEU	2.2
3	E	121	LYS	2.2
1	C	339	ALA	2.2
4	L	213	GLU	2.1
2	B	373	THR	2.1
4	F	177	SER	2.1
2	D	7	THR	2.1
4	F	175	MET	2.1
2	B	383	LEU	2.1
3	E	145	GLY	2.1
3	E	16	ALA	2.1
2	D	181	LYS	2.1
2	D	143	ARG	2.1
1	C	337	PRO	2.0
4	L	106	ILE	2.0
3	E	164	SER	2.0
2	D	48	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	338	HIS	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)

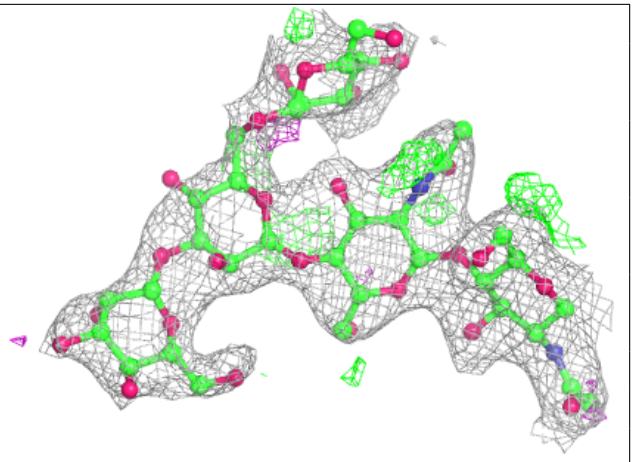
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

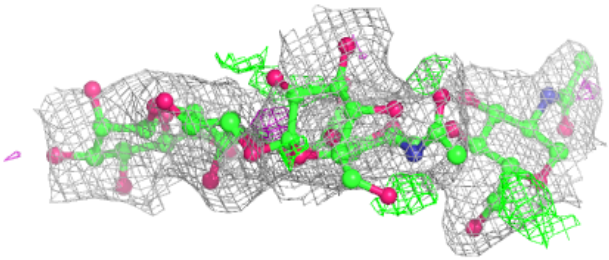
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	G	5	11/12	0.62	0.29	120,123,125,125	0
6	NAG	K	2	14/15	0.76	0.33	115,119,123,123	0
7	BMA	J	3	11/12	0.76	0.25	110,115,120,122	0
6	NAG	K	1	14/15	0.81	0.31	79,92,103,110	0
7	BMA	J	4	11/12	0.83	0.26	118,123,135,135	0
5	BMA	G	4	11/12	0.84	0.27	103,107,111,112	0
5	BMA	G	3	11/12	0.85	0.23	92,114,121,123	0
6	NAG	I	1	14/15	0.86	0.27	77,87,98,106	0
6	NAG	I	2	14/15	0.88	0.34	109,115,121,122	0
5	NAG	G	2	14/15	0.91	0.15	56,63,77,90	0
7	NAG	J	2	14/15	0.92	0.23	74,87,95,104	0
7	NAG	J	1	14/15	0.98	0.14	47,53,62,72	0
5	NAG	G	1	14/15	0.98	0.12	25,33,44,46	0

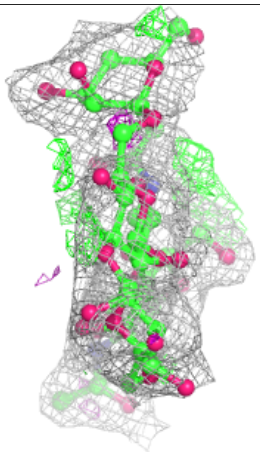
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

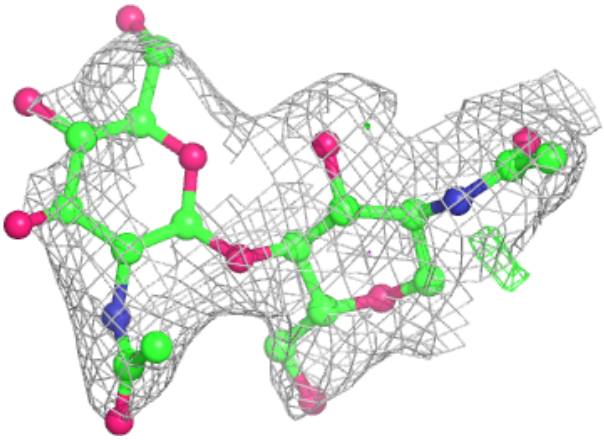


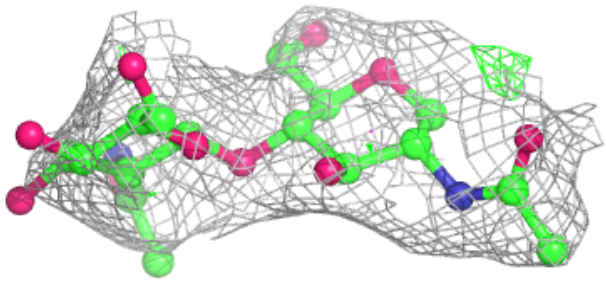


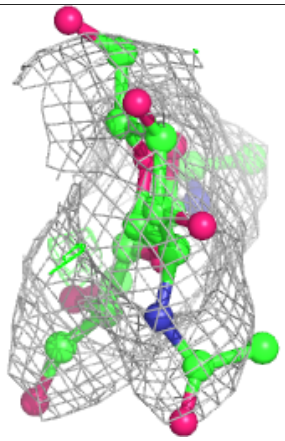


Electron density around Chain I:

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

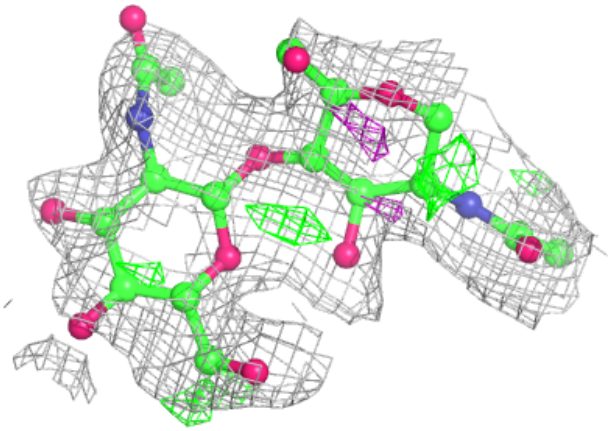


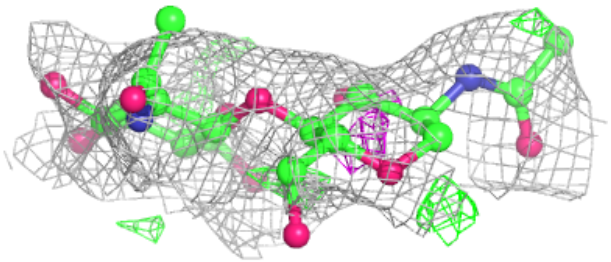


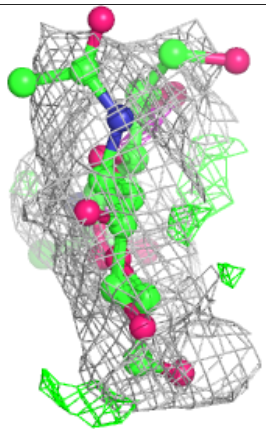


Electron density around Chain K:

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

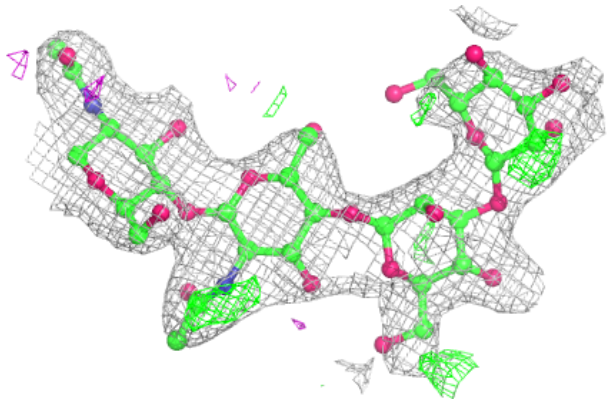


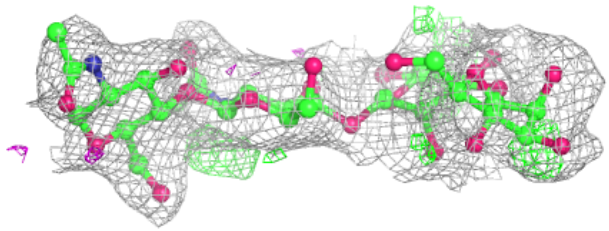


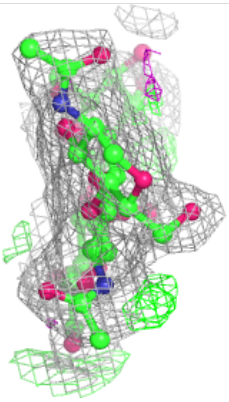


Electron density around Chain J:

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







6.4 Ligands (i)

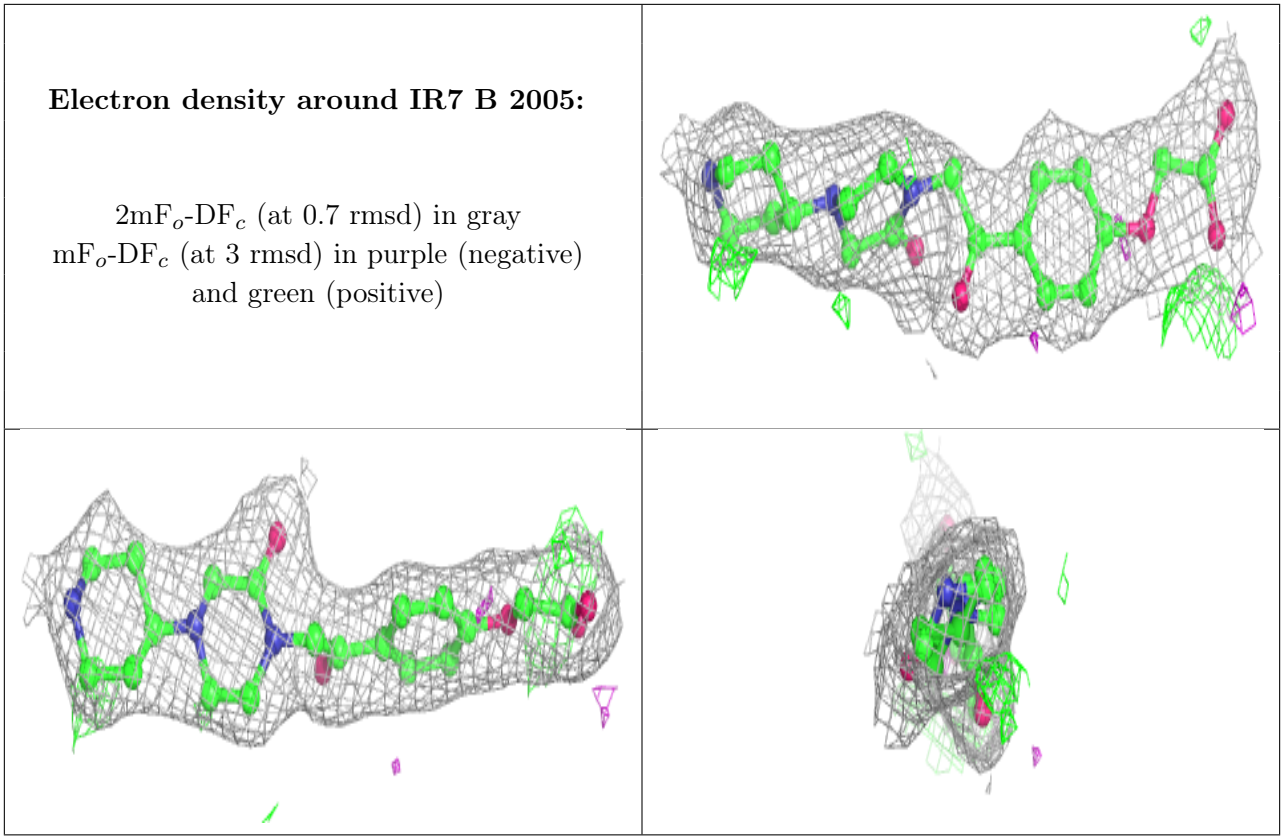
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
9	SO4	C	506	5/5	0.78	0.21	126,127,128,128	0
9	SO4	A	505	5/5	0.79	0.28	113,114,115,117	0
11	NAG	D	2004	14/15	0.81	0.37	85,95,102,104	0
9	SO4	C	505	5/5	0.82	0.26	111,114,116,118	0
11	NAG	B	2004	14/15	0.90	0.41	89,100,104,105	0
8	CA	C	501	1/1	0.92	0.04	70,70,70,70	0
9	SO4	A	506	5/5	0.93	0.20	93,98,100,101	0
9	SO4	A	507	5/5	0.94	0.13	89,91,95,96	0
8	CA	B	2002	1/1	0.95	0.06	70,70,70,70	0
10	MG	D	2001	1/1	0.95	0.22	33,33,33,33	0
10	MG	B	2001	1/1	0.97	0.26	21,21,21,21	0
12	IR7	B	2005	27/27	0.97	0.14	19,30,42,46	0
12	IR7	D	2005	27/27	0.97	0.16	23,42,50,52	0
8	CA	D	2002	1/1	0.98	0.08	57,57,57,57	0
8	CA	C	503	1/1	0.98	0.09	44,44,44,44	0
8	CA	C	504	1/1	0.99	0.09	51,51,51,51	0
8	CA	A	501	1/1	0.99	0.05	37,37,37,37	0
8	CA	D	2003	1/1	0.99	0.16	34,34,34,34	0
8	CA	B	2003	1/1	0.99	0.15	19,19,19,19	0
8	CA	A	502	1/1	0.99	0.11	29,29,29,29	0
8	CA	C	502	1/1	0.99	0.04	54,54,54,54	0
8	CA	A	504	1/1	0.99	0.13	24,24,24,24	0
8	CA	A	503	1/1	1.00	0.17	24,24,24,24	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.

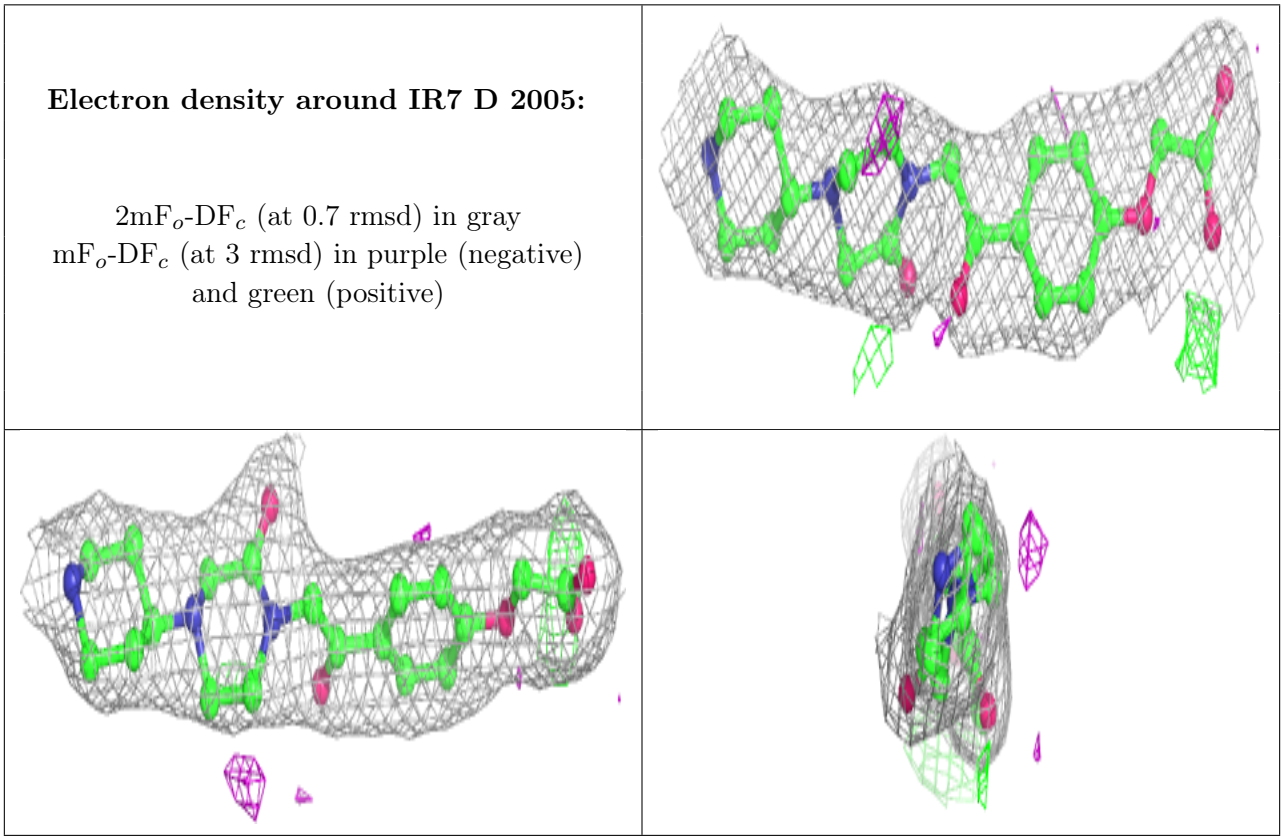
Electron density around IR7 B 2005:

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



Electron density around IR7 D 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.