



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 12:11 AM EDT

PDB ID : 7UJE
Title : Integrin alpha IIB beta3 complex with UR2922 in Mn2+
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2022-03-30
Resolution : 2.50 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

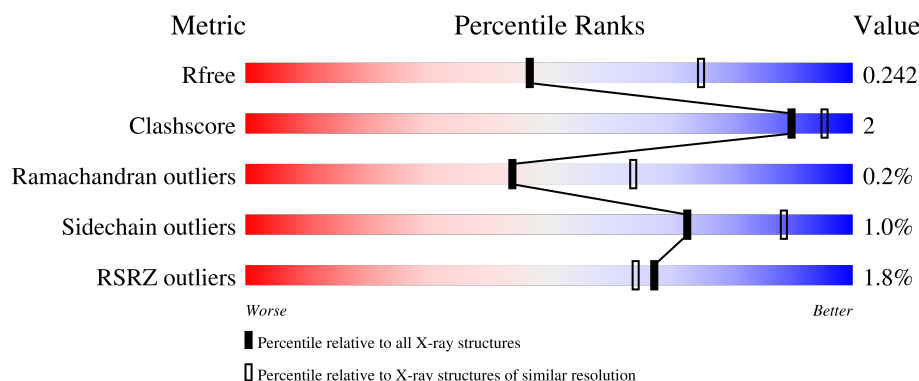
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	454	<div> <div>94%</div> <div>6%</div> </div>
1	C	454	<div> <div>94%</div> <div>5%</div> </div>
2	B	471	<div> <div>92%</div> <div>7%</div> </div>
2	D	471	<div> <div>92%</div> <div>8%</div> </div>
3	E	216	<div> <div>96%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	216	<div><div></div><div>%</div><div>96%</div><div>.</div></div>
4	F	214	<div><div></div><div>3%</div><div>96%</div><div>.</div></div>
4	L	214	<div><div></div><div>98%</div><div>.</div></div>
5	G	5	<div><div></div><div>60%</div><div>40%</div></div>
5	J	5	<div><div></div><div>100%</div></div>
6	I	2	<div><div></div><div>100%</div></div>
6	K	2	<div><div></div><div>100%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22081 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 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 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 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.



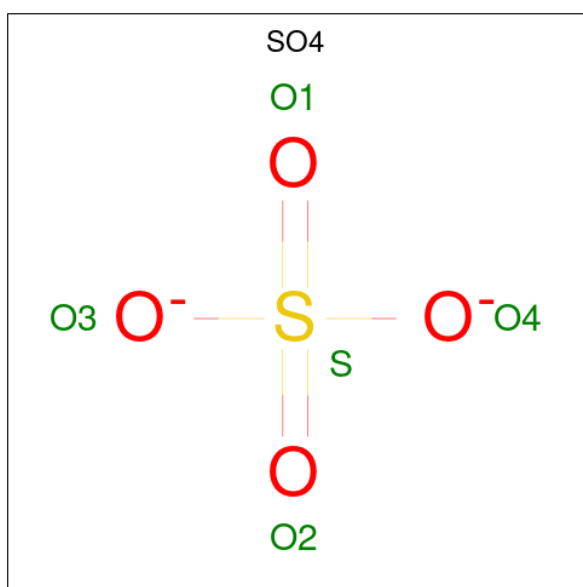
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

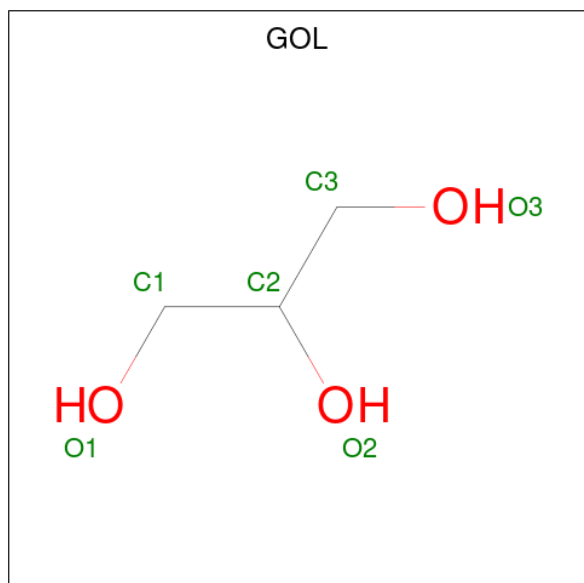


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0

- 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	C	4	Total Ca 4 4	0	0

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

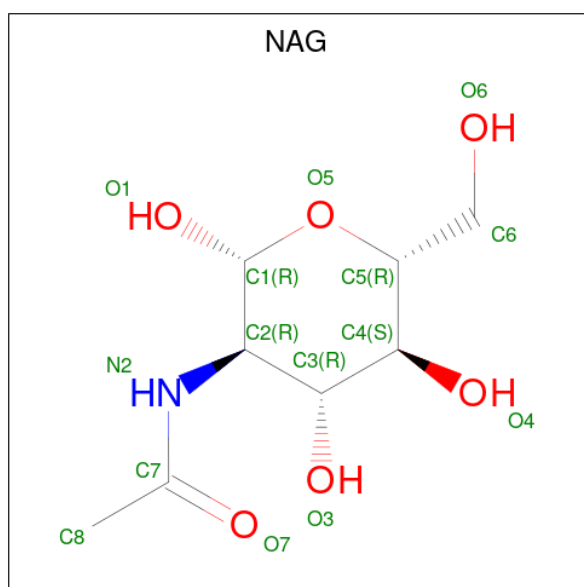


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

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

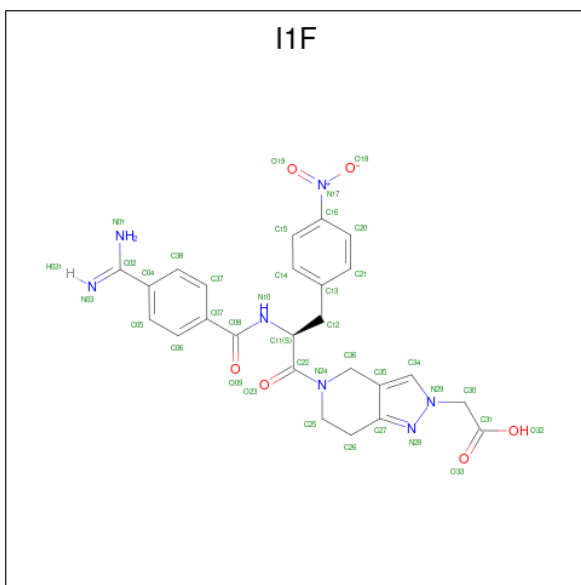
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- 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 {5-[N-(4-carbamimidoylbenzoyl)-4-nitro-L-phenylalanyl]-4,5,6,7-tetrahydro-2H-pyrazolo[4,3-c]pyridin-2-yl}acetic acid (three-letter code: I1F) (formula: C₂₅H₂₅N₇O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			38	25	7	6		
12	D	1	Total	C	N	O	0	0
			38	25	7	6		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	381	Total	O	0	0
			381	381		
14	B	194	Total	O	0	0
			194	194		
14	C	151	Total	O	0	0
			151	151		
14	D	109	Total	O	0	0
			109	109		
14	E	21	Total	O	0	0
			21	21		

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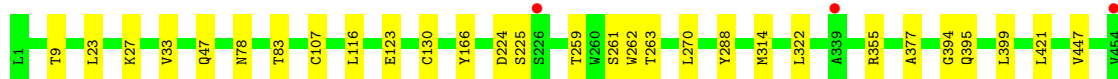
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	F	11	Total 11	O 11	0	0
14	H	34	Total 34	O 34	0	0
14	L	49	Total 49	O 49	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

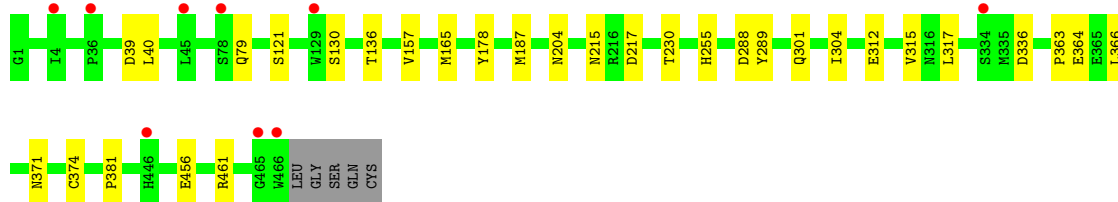
- Molecule 1: Integrin alpha-IIb



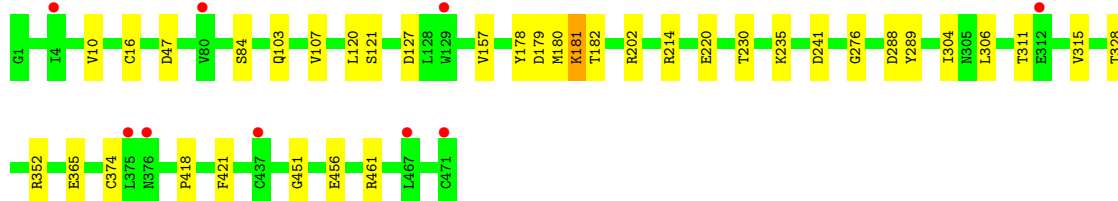
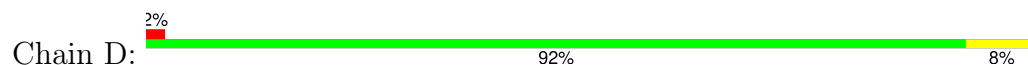
- Molecule 1: Integrin alpha-IIb



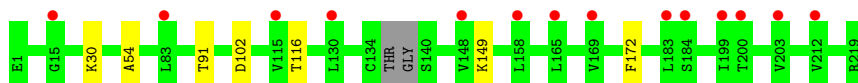
- Molecule 2: Integrin beta-3



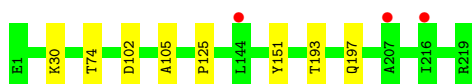
- Molecule 2: Integrin beta-3



- Molecule 3: Fab heavy chain



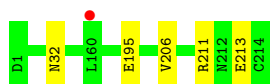
- Molecule 3: Fab heavy chain



- Molecule 4: Fab light chain



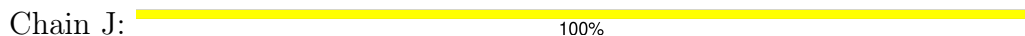
- Molecule 4: Fab light chain



- Molecule 5: 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



- Molecule 5: 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



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



2019
MAG

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

Chain K:

100%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	259.56Å 143.71Å 105.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.50 48.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.74-2.50) 99.4 (48.74-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.209 , 0.239 0.213 , 0.242	Depositor DCC
R_{free} test set	134401 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22081	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: MN, NAG, BMA, SO4, MAN, CA, CL, I1F, GOL

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	0.25	0/3608	0.45	0/4918
1	C	0.24	0/3605	0.44	0/4912
2	B	0.24	0/3680	0.43	0/4989
2	D	0.24	0/3690	0.42	0/5003
3	E	0.24	0/1673	0.44	0/2290
3	H	0.24	0/1684	0.44	0/2305
4	F	0.24	0/1673	0.43	0/2269
4	L	0.24	0/1673	0.44	0/2269
All	All	0.24	0/21286	0.44	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	14	0
1	C	3502	0	3334	9	0
2	B	3610	0	3530	15	0
2	D	3623	0	3540	18	0
3	E	1631	0	1590	5	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	4	0
5	G	61	0	52	0	0
5	J	61	0	52	1	0
6	I	28	0	25	0	0
6	K	28	0	25	0	0
7	A	25	0	0	0	0
7	C	15	0	0	0	0
7	L	5	0	0	0	0
8	A	4	0	0	0	0
8	C	4	0	0	0	0
9	A	6	0	8	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	0	0
12	B	38	0	0	2	0
12	D	38	0	0	3	0
13	C	2	0	0	0	0
13	D	1	0	0	0	0
14	A	381	0	0	3	0
14	B	194	0	0	1	0
14	C	151	0	0	0	0
14	D	109	0	0	1	0
14	E	21	0	0	0	0
14	F	11	0	0	0	0
14	H	34	0	0	0	0
14	L	49	0	0	1	0
All	All	22081	0	20233	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (69) 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)
1:C:107:CYS:HA	1:C:130:CYS:HA	1.88	0.55
2:B:121:SER:HB2	12:B:2005:I1F:O32	2.06	0.55
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.89	0.55
4:L:213:GLU:O	14:L:401:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:GLN:NE2	14:B:2104:HOH:O	2.39	0.53
2:D:121:SER:HB2	12:D:2006:I1F:O32	2.09	0.53
1:A:47:GLN:NE2	14:A:613:HOH:O	2.42	0.53
1:A:355:ARG:NH1	14:A:604:HOH:O	2.32	0.53
1:C:83:THR:HB	1:C:116:LEU:HB2	1.90	0.53
1:A:107:CYS:HA	1:A:130:CYS:HA	1.90	0.52
2:D:107:VAL:O	2:D:352:ARG:NH2	2.39	0.52
1:C:77:ARG:NH2	3:E:102:ASP:OD2	2.37	0.51
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.92	0.51
3:H:102:ASP:HB3	3:H:105:ALA:HB2	1.94	0.50
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.46	0.48
1:A:27:LYS:HG2	1:A:33:VAL:HG22	1.94	0.48
2:D:180:MET:O	2:D:182:THR:N	2.46	0.48
1:C:377:ALA:HB2	1:C:421:LEU:HD11	1.96	0.48
2:B:121:SER:HB2	12:B:2005:I1F:C31	2.44	0.47
1:A:9:THR:HB	1:A:447:VAL:HB	1.95	0.47
1:A:261:SER:O	14:A:601:HOH:O	2.21	0.47
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.97	0.47
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.30	0.47
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.97	0.46
2:B:39:ASP:OD1	2:B:40:LEU:N	2.40	0.46
4:F:201:SER:OG	4:F:203:SER:O	2.24	0.45
2:D:230:THR:HG23	2:D:304:ILE:HG13	1.98	0.45
2:B:288:ASP:OD1	2:B:289:TYR:N	2.50	0.45
3:H:30:LYS:HD3	3:H:74:THR:HG21	1.97	0.45
1:C:224:ASP:OD1	1:C:225:SER:N	2.44	0.45
2:B:217:ASP:OD2	2:B:255:HIS:NE2	2.49	0.45
1:A:224:ASP:OD1	1:A:225:SER:N	2.45	0.45
2:D:456:GLU:OE2	2:D:461:ARG:NH1	2.49	0.44
3:H:193:THR:O	3:H:197:GLN:N	2.48	0.44
2:B:136:THR:HG23	2:B:204:ASN:HD21	1.83	0.44
2:D:214:ARG:NE	12:D:2006:I1F:O18	2.44	0.43
1:C:180:GLU:HB3	1:C:197:GLN:HE21	1.83	0.43
2:D:10:VAL:HG21	2:D:16:CYS:HB2	2.00	0.43
1:A:83:THR:HB	1:A:116:LEU:HB2	2.00	0.43
2:D:288:ASP:OD1	2:D:289:TYR:N	2.50	0.43
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.00	0.43
2:D:121:SER:HB2	12:D:2006:I1F:C31	2.47	0.43
1:A:377:ALA:HB2	1:A:421:LEU:HD11	2.01	0.43
2:B:165:MET:HG3	2:B:187[B]:MET:HG3	2.01	0.43
1:A:314:MET:HB3	1:A:322:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:SER:OG	2:B:336:ASP:O	2.33	0.42
3:E:91:THR:HG23	3:E:116:THR:HA	2.02	0.42
2:B:230:THR:HG23	2:B:304:ILE:HG13	2.01	0.42
5:J:1:NAG:H61	5:J:2:NAG:HN2	1.85	0.42
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.55	0.42
2:B:363:PRO:HD2	2:B:366:LEU:HD12	2.01	0.42
1:C:192:LEU:HD11	1:C:231:PHE:CD1	2.55	0.41
1:C:276:ARG:HD2	1:C:279:ARG:HB2	2.02	0.41
2:B:371:ASN:OD1	2:B:381:PRO:HA	2.19	0.41
2:D:178:TYR:CG	2:D:179:ASP:N	2.88	0.41
2:D:181:LYS:NZ	14:D:2107:HOH:O	2.53	0.41
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.55	0.41
1:C:432:TYR:CZ	1:C:452:PRO:HA	2.55	0.41
2:D:311:THR:O	2:D:315:VAL:HG23	2.20	0.41
4:F:149:LYS:HB2	4:F:193:THR:HB	2.03	0.41
2:D:235:LYS:HE3	2:D:276:GLY:O	2.20	0.41
3:E:30:LYS:HG3	3:E:54:ALA:HA	2.02	0.41
2:D:120:LEU:HD23	2:D:120:LEU:HA	1.86	0.41
1:A:78:ASN:O	4:L:32:ASN:ND2	2.54	0.40
1:A:259:THR:HA	1:A:263:THR:HA	2.02	0.40
2:D:157:VAL:O	2:D:220:GLU:HB3	2.21	0.40
2:B:312:GLU:HA	2:B:315:VAL:HG23	2.04	0.40
2:D:84:SER:O	2:D:103:GLN:N	2.41	0.40
4:L:211:ARG:O	4:L:213:GLU:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	456/454 (100%)	442 (97%)	13 (3%)	1 (0%)	44 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	455/454 (100%)	440 (97%)	14 (3%)	1 (0%)	44	64
2	B	467/471 (99%)	452 (97%)	14 (3%)	1 (0%)	44	64
2	D	469/471 (100%)	448 (96%)	18 (4%)	3 (1%)	22	39
3	E	210/216 (97%)	198 (94%)	12 (6%)	0	100	100
3	H	212/216 (98%)	200 (94%)	12 (6%)	0	100	100
4	F	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	2693/2710 (99%)	2584 (96%)	103 (4%)	6 (0%)	44	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	D	181	LYS
2	D	374	CYS
1	C	123	GLU
2	B	157	VAL
2	D	451	GLY

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	366/362 (101%)	361 (99%)	5 (1%)	62	83
1	C	365/362 (101%)	359 (98%)	6 (2%)	58	80
2	B	415/416 (100%)	410 (99%)	5 (1%)	67	86
2	D	416/416 (100%)	411 (99%)	5 (1%)	67	86
3	E	186/187 (100%)	186 (100%)	0	100	100
3	H	187/187 (100%)	187 (100%)	0	100	100
4	F	188/188 (100%)	186 (99%)	2 (1%)	70	87
4	L	188/188 (100%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2311/2306 (100%)	2288 (99%)	23 (1%)	73	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	270	LEU
1	A	288	TYR
1	A	395	GLN
2	B	79	GLN
2	B	178	TYR
2	B	215	ASN
2	B	364	GLU
2	B	374	CYS
1	C	1	LEU
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	270	LEU
1	C	288	TYR
2	D	47	ASP
2	D	127	ASP
2	D	202	ARG
2	D	241	ASP
2	D	365	GLU
4	F	181	LEU
4	F	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	197	GLN
2	B	301	GLN
2	D	15	GLN
2	D	280	HIS
3	H	170	HIS

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 ⓘ

14 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	0.37	0	17,19,21	0.45	0
5	NAG	G	2	5	14,14,15	0.17	0	17,19,21	0.55	0
5	BMA	G	3	5	11,11,12	0.70	0	15,15,17	0.99	0
5	MAN	G	4	5	11,11,12	0.59	0	15,15,17	0.95	2 (13%)
5	MAN	G	5	5	11,11,12	0.55	0	15,15,17	0.95	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	I	2	6	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	J	1	5,2	14,14,15	0.36	0	17,19,21	0.57	0
5	NAG	J	2	5	14,14,15	0.20	0	17,19,21	0.48	0
5	BMA	J	3	5	11,11,12	0.67	0	15,15,17	1.05	1 (6%)
5	MAN	J	4	5	11,11,12	0.98	1 (9%)	15,15,17	1.16	2 (13%)
5	MAN	J	5	5	11,11,12	0.97	0	15,15,17	1.29	2 (13%)
6	NAG	K	1	2,6	14,14,15	0.34	0	17,19,21	0.50	0
6	NAG	K	2	6	14,14,15	0.27	0	17,19,21	0.41	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	-	2/6/23/26	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
5	MAN	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	-	3/6/23/26	0/1/1/1
5	NAG	J	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	1/2/19/22	0/1/1/1
5	MAN	J	5	5	-	1/2/19/22	1/1/1/1
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	MAN	O5-C5	2.24	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	5	MAN	C1-O5-C5	3.91	117.43	112.19
5	J	4	MAN	C1-O5-C5	2.92	116.11	112.19
5	G	5	MAN	C1-O5-C5	2.51	115.55	112.19
5	G	4	MAN	C1-O5-C5	2.43	115.44	112.19
5	J	3	BMA	C1-O5-C5	2.42	115.43	112.19
5	J	5	MAN	O2-C2-C3	-2.30	105.38	110.15
5	G	4	MAN	O2-C2-C3	-2.13	105.73	110.15
5	G	5	MAN	O2-C2-C3	-2.07	105.86	110.15
5	J	4	MAN	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

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

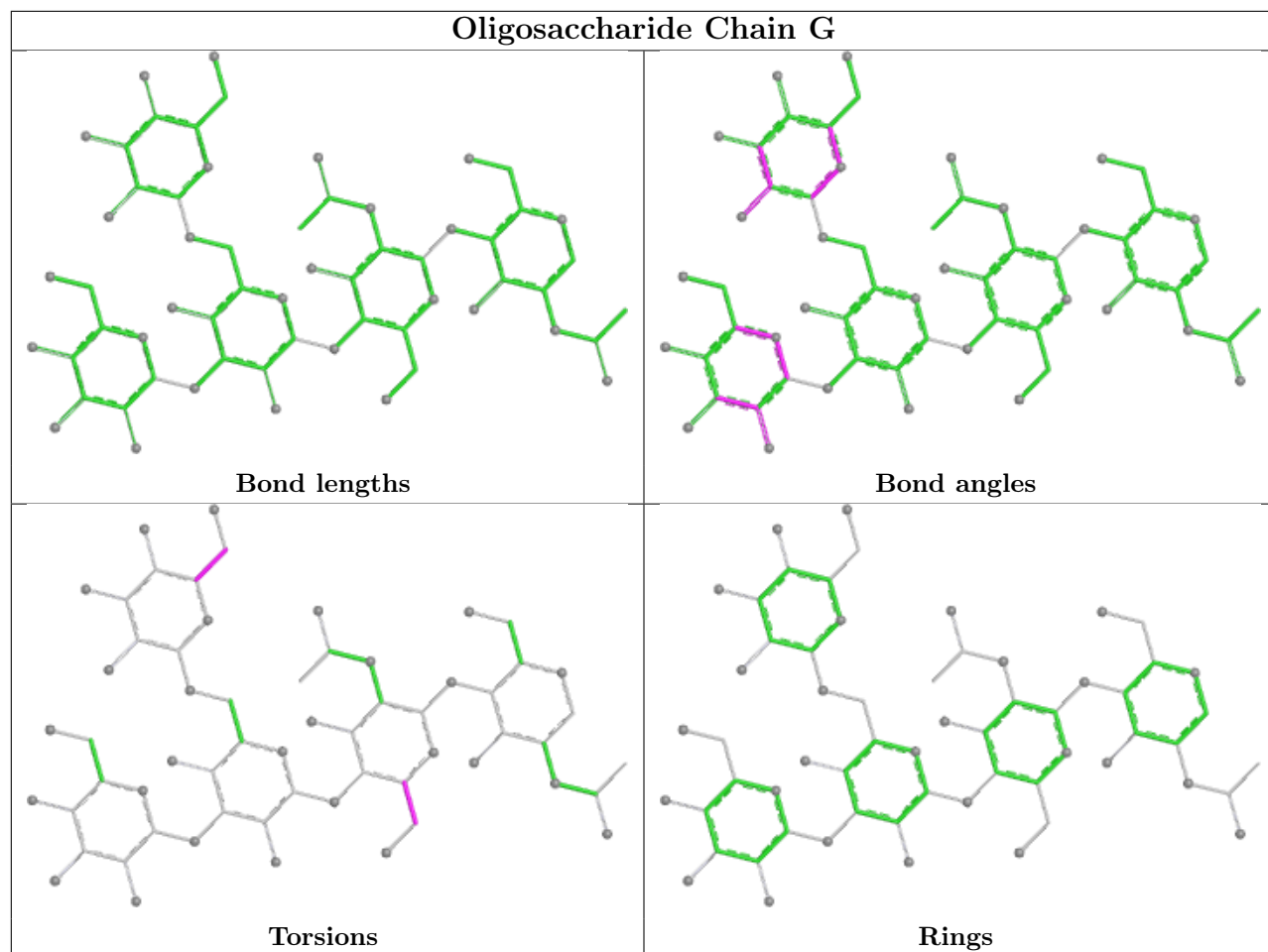
All (1) ring outliers are listed below:

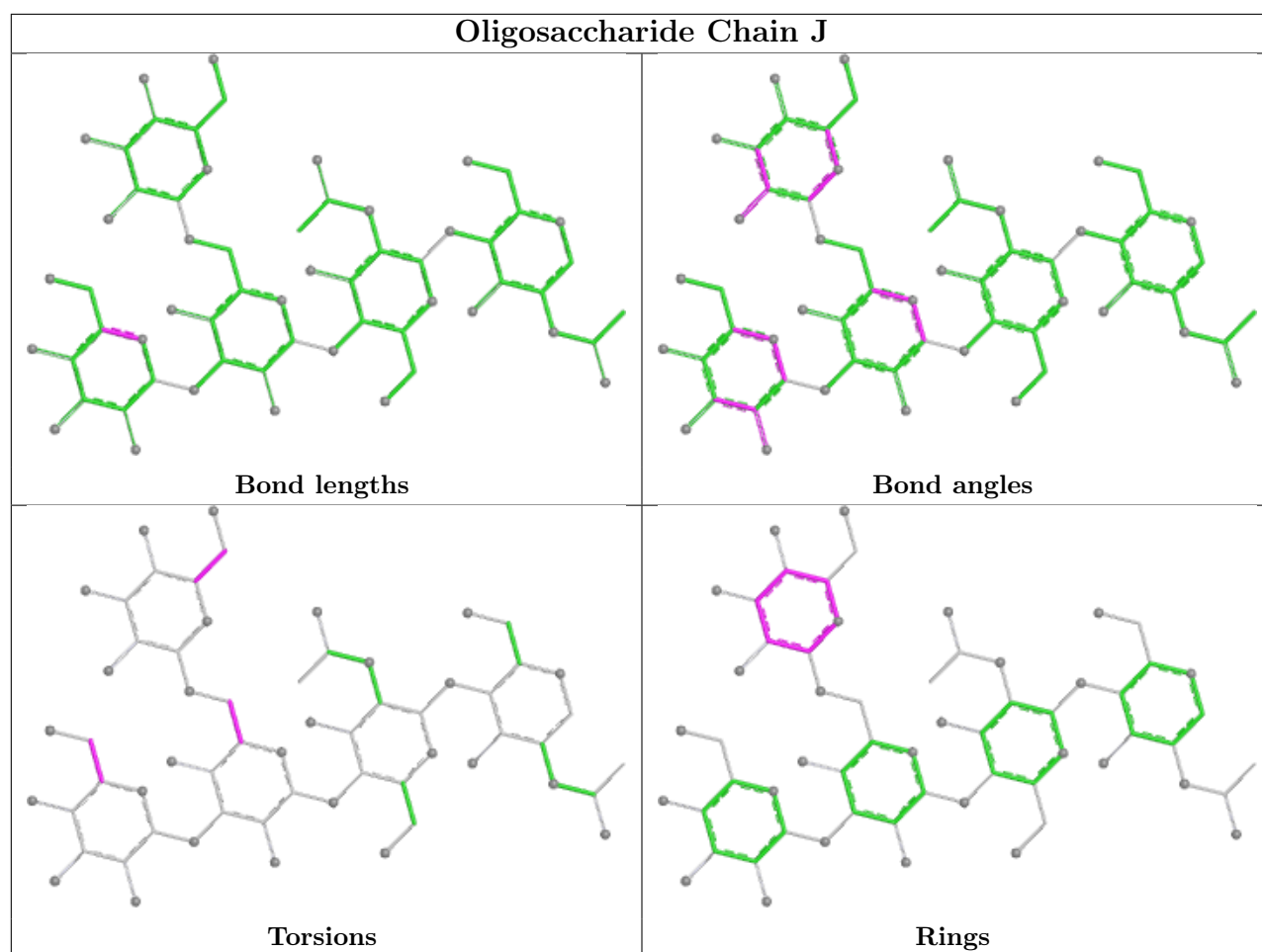
Mol	Chain	Res	Type	Atoms
5	J	5	MAN	C1-C2-C3-C4-C5-O5

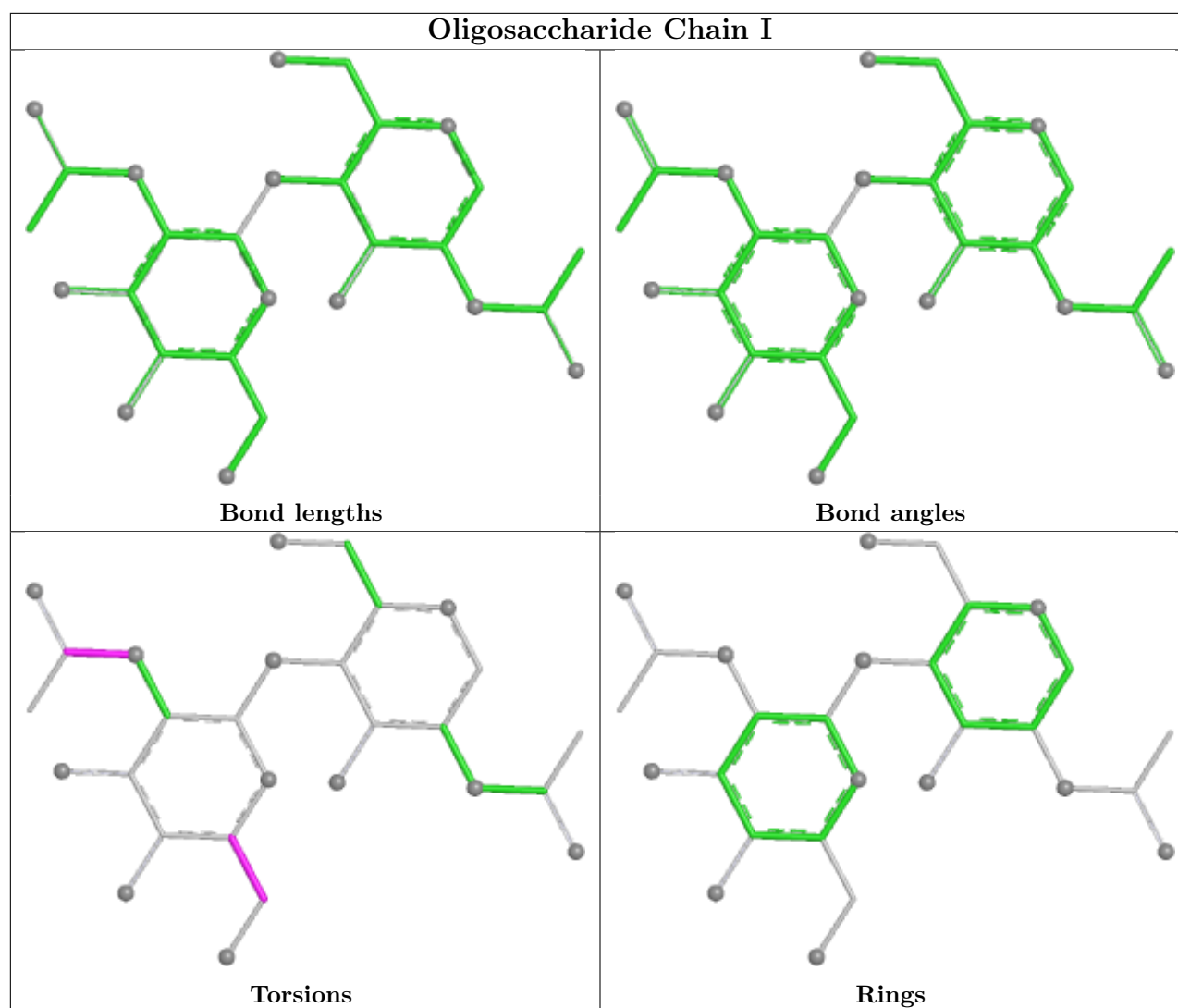
2 monomers are involved in 1 short contact:

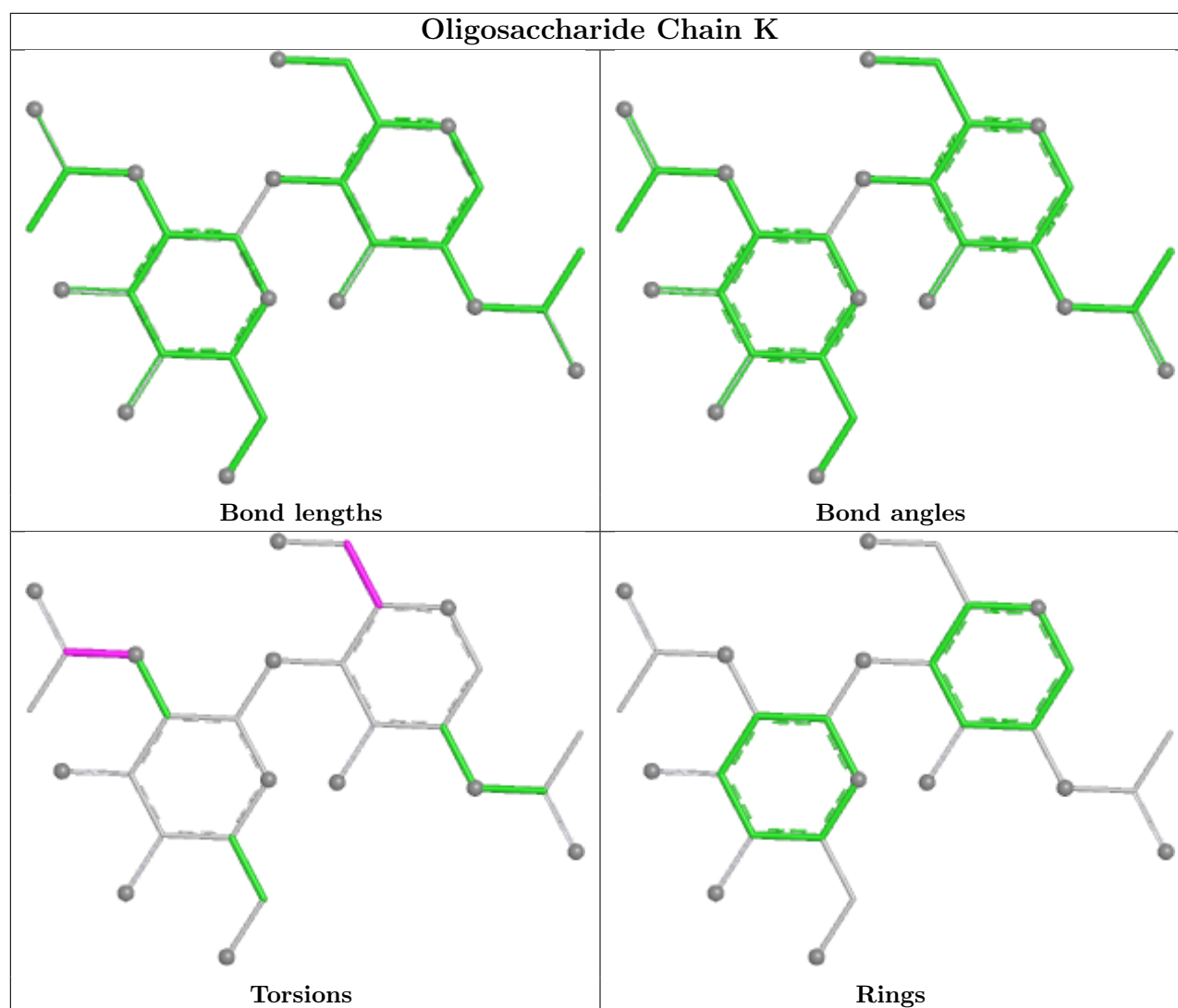
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	1	0
5	J	2	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
7	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.08	0
12	I1F	D	2006	10	39,41,41	2.34	14 (35%)	45,58,58	2.01	12 (26%)
7	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	I1F	B	2005	10	39,41,41	2.24	13 (33%)	45,58,58	1.89	10 (22%)
7	SO4	A	507	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	A	509	-	4,4,4	0.25	0	6,6,6	0.17	0
7	SO4	C	503	-	4,4,4	0.27	0	6,6,6	0.07	0
11	NAG	D	2004	2	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
9	GOL	A	510	-	5,5,5	0.37	0	5,5,5	0.25	0
7	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.11	0
7	SO4	A	508	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.09	0
11	NAG	B	2004	2	14,14,15	0.39	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	I1F	D	2006	10	-	4/30/41/41	0/4/4/4
12	I1F	B	2005	10	-	4/30/41/41	0/4/4/4
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
9	GOL	A	510	-	-	2/4/4/4	-
11	NAG	B	2004	2	-	2/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2006	I1F	C30-C31	7.57	1.60	1.51
12	B	2005	I1F	C30-C31	7.01	1.59	1.51
12	D	2006	I1F	O19-N17	6.35	1.33	1.22
12	B	2005	I1F	O19-N17	6.32	1.33	1.22
12	D	2006	I1F	C02-N03	4.49	1.46	1.27
12	B	2005	I1F	C02-N03	4.46	1.46	1.27
12	B	2005	I1F	C11-C22	3.30	1.59	1.53
12	D	2006	I1F	C08-N10	3.16	1.41	1.34
12	D	2006	I1F	C11-C22	3.13	1.59	1.53
12	D	2006	I1F	C27-N28	3.01	1.38	1.34
12	B	2005	I1F	C27-N28	2.82	1.37	1.34
12	D	2006	I1F	C22-N24	2.75	1.39	1.35
12	B	2005	I1F	C08-N10	2.73	1.40	1.34
12	B	2005	I1F	C22-N24	2.67	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2006	I1F	O18-N17	-2.50	1.18	1.35
12	B	2005	I1F	O18-N17	-2.50	1.18	1.35
12	D	2006	I1F	C34-C35	2.50	1.40	1.37
12	B	2005	I1F	C02-N01	-2.49	1.27	1.33
12	D	2006	I1F	C12-C11	2.43	1.59	1.54
12	B	2005	I1F	C34-C35	2.42	1.40	1.37
12	B	2005	I1F	C20-C16	2.29	1.43	1.38
12	D	2006	I1F	C20-C16	2.26	1.43	1.38
12	D	2006	I1F	C02-N01	-2.16	1.28	1.33
12	D	2006	I1F	C25-C26	2.14	1.55	1.51
12	D	2006	I1F	C21-C13	2.07	1.43	1.38
12	B	2005	I1F	C12-C11	2.06	1.59	1.54
12	B	2005	I1F	C21-C13	2.01	1.42	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2006	I1F	C04-C02-N01	6.15	127.34	118.01
12	B	2005	I1F	C04-C02-N01	5.20	125.91	118.01
12	D	2006	I1F	C30-N29-C34	-5.20	122.93	129.38
12	B	2005	I1F	C30-N29-C34	-5.05	123.11	129.38
12	D	2006	I1F	C15-C16-N17	4.46	123.23	119.34
12	B	2005	I1F	C15-C16-N17	4.30	123.09	119.34
12	D	2006	I1F	C07-C08-N10	3.56	123.63	117.04
12	B	2005	I1F	C07-C08-N10	3.43	123.41	117.04
12	D	2006	I1F	C30-N29-N28	3.13	125.78	120.87
12	B	2005	I1F	C30-N29-N28	2.94	125.48	120.87
12	B	2005	I1F	O19-N17-C16	-2.89	114.84	118.82
12	D	2006	I1F	O19-N17-C16	-2.85	114.90	118.82
11	D	2004	NAG	C1-O5-C5	2.46	115.49	112.19
12	B	2005	I1F	C11-C22-N24	2.43	122.50	118.85
12	D	2006	I1F	O09-C08-N10	-2.40	117.90	122.47
12	B	2005	I1F	O09-C08-N10	-2.33	118.04	122.47
12	D	2006	I1F	C11-C22-N24	2.28	122.28	118.85
12	D	2006	I1F	C37-C07-C06	-2.27	115.67	118.57
12	D	2006	I1F	O32-C31-O33	2.23	129.07	123.33
12	B	2005	I1F	O32-C31-O33	2.23	129.06	123.33
12	D	2006	I1F	C13-C12-C11	2.14	119.06	113.36
12	D	2006	I1F	C15-C14-C13	2.07	123.72	121.00
12	B	2005	I1F	C15-C14-C13	2.04	123.69	121.00

There are no chirality outliers.

All (14) torsion outliers are listed below:

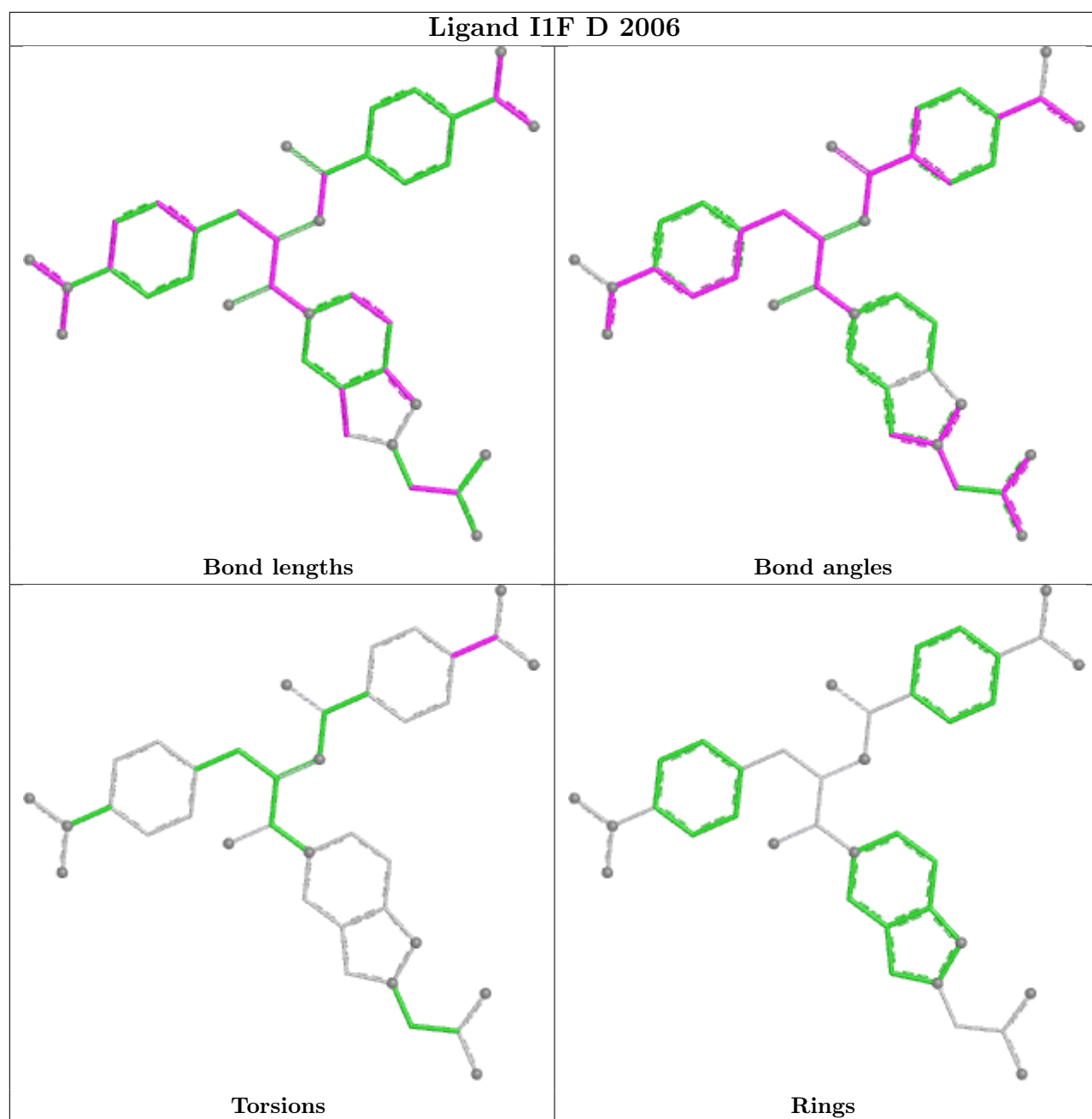
Mol	Chain	Res	Type	Atoms
9	A	510	GOL	O1-C1-C2-O2
9	A	510	GOL	O1-C1-C2-C3
12	B	2005	I1F	N29-C30-C31-O32
12	B	2005	I1F	N29-C30-C31-O33
12	B	2005	I1F	N01-C02-C04-C05
12	B	2005	I1F	N01-C02-C04-C38
12	D	2006	I1F	N01-C02-C04-C05
12	D	2006	I1F	N01-C02-C04-C38
11	D	2004	NAG	O5-C5-C6-O6
11	B	2004	NAG	O5-C5-C6-O6
11	D	2004	NAG	C4-C5-C6-O6
11	B	2004	NAG	C4-C5-C6-O6
12	D	2006	I1F	N03-C02-C04-C05
12	D	2006	I1F	N03-C02-C04-C38

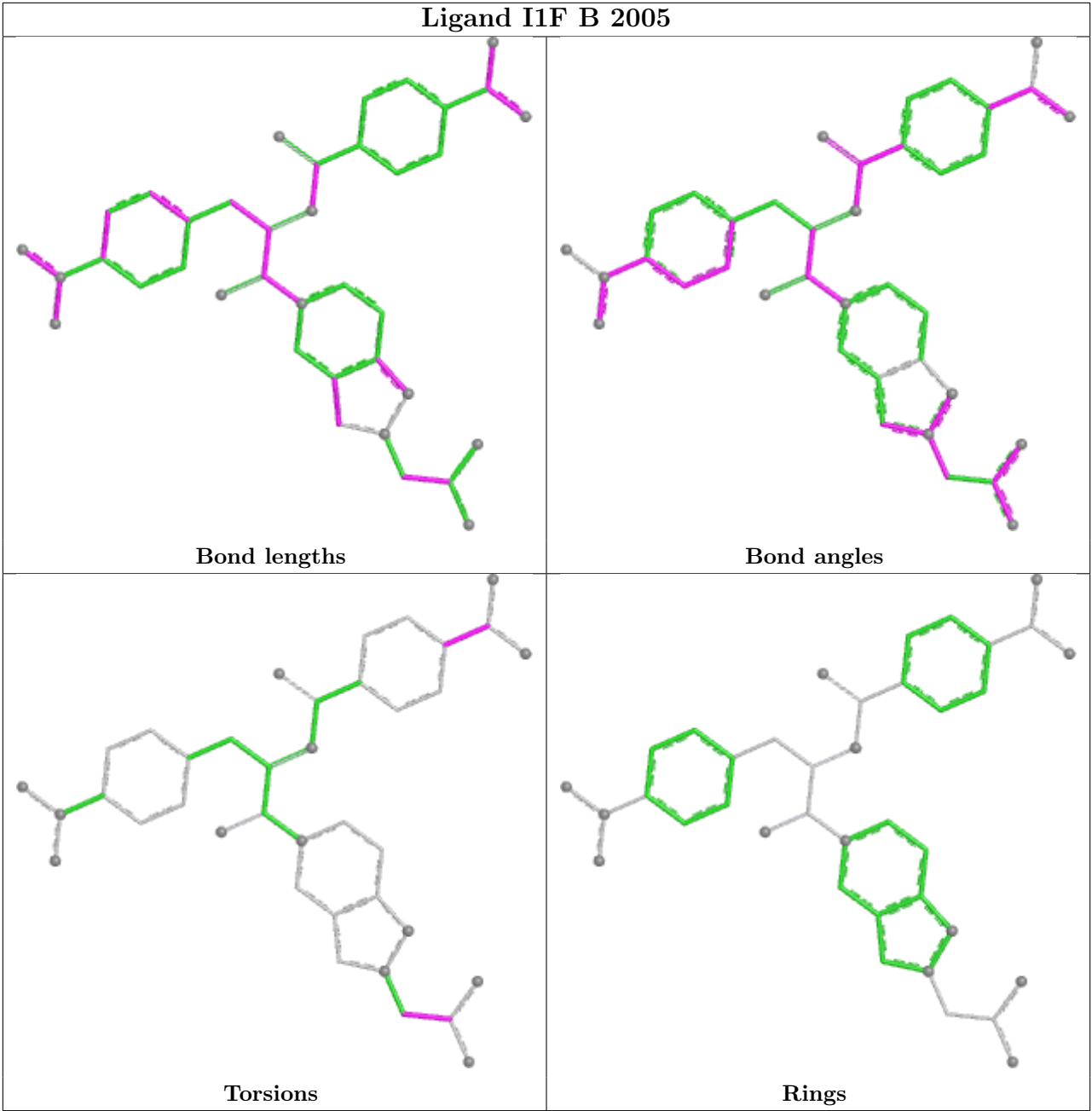
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2006	I1F	3	0
12	B	2005	I1F	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	7.04

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	454/454 (100%)	-0.07	3 (0%) 84 81	33, 56, 85, 124	4 (0%)
1	C	453/454 (99%)	0.17	3 (0%) 84 81	34, 69, 101, 132	4 (0%)
2	B	466/471 (98%)	0.27	9 (1%) 66 63	28, 84, 160, 177	4 (0%)
2	D	471/471 (100%)	0.46	9 (1%) 66 63	50, 86, 137, 178	1 (0%)
3	E	214/216 (99%)	0.90	14 (6%) 26 24	72, 116, 152, 173	0
3	H	216/216 (100%)	0.57	3 (1%) 73 70	61, 98, 147, 164	0
4	F	214/214 (100%)	0.72	7 (3%) 49 46	81, 113, 171, 191	0
4	L	214/214 (100%)	0.30	1 (0%) 87 85	67, 91, 119, 187	0
All	All	2702/2710 (99%)	0.34	49 (1%) 67 64	28, 82, 148, 191	13 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	129	TRP	5.5
1	A	454	VAL	5.1
2	B	4	ILE	3.7
3	E	199	ILE	3.4
4	F	160	LEU	3.2
2	B	465	GLY	3.2
4	F	133	VAL	3.2
3	E	165	LEU	3.1
1	C	453	VAL	3.0
3	E	212	VAL	2.9
2	B	466	TRP	2.9
1	A	226	SER	2.8
4	F	146	VAL	2.8
3	E	169	VAL	2.7
2	D	471	CYS	2.7
4	L	160	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	130	LEU	2.6
3	E	200	THR	2.6
4	F	135	PHE	2.6
2	D	437	CYS	2.6
2	B	78	SER	2.6
3	H	207	ALA	2.6
2	B	129	TRP	2.5
3	E	115	VAL	2.5
2	D	467	LEU	2.5
2	B	334[A]	SER	2.4
4	F	115	VAL	2.4
3	E	184	SER	2.3
2	B	446	HIS	2.3
2	D	312	GLU	2.3
1	C	192	LEU	2.2
2	D	80	VAL	2.2
1	C	161	SER	2.2
3	E	203	VAL	2.2
3	H	144	LEU	2.2
3	H	216	ILE	2.2
3	E	183	LEU	2.2
1	A	339	ALA	2.2
4	F	193	THR	2.1
2	D	376	ASN	2.1
3	E	15	GLY	2.1
4	F	118	PHE	2.1
2	B	45	LEU	2.1
2	D	375	LEU	2.1
3	E	83	LEU	2.1
2	D	4	ILE	2.1
3	E	148	VAL	2.0
3	E	158	LEU	2.0
2	B	36	PRO	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 ⓘ

SUGAR-RSR INFOmissingINFO

6.4 Ligands ⓘ

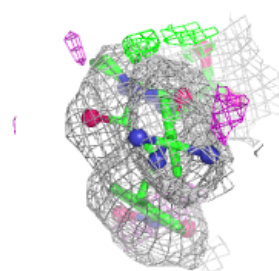
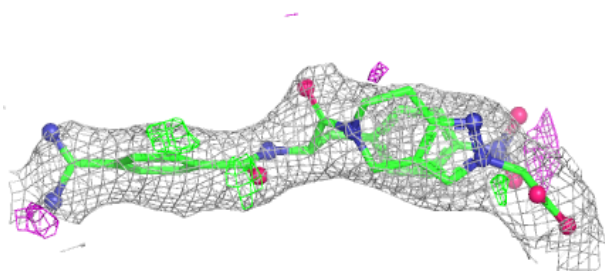
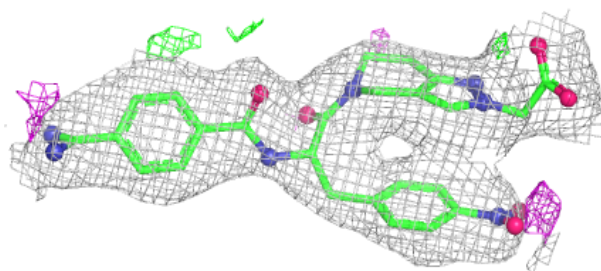
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	NAG	D	2004	14/15	0.49	0.15	112,132,141,142	0
13	CL	C	505	1/1	0.68	0.16	115,115,115,115	0
7	SO4	C	502	5/5	0.76	0.12	108,110,117,120	0
9	GOL	A	510	6/6	0.76	0.31	75,94,100,100	0
11	NAG	B	2004	14/15	0.79	0.12	105,122,135,140	0
7	SO4	C	501	5/5	0.80	0.15	90,104,109,122	0
7	SO4	C	503	5/5	0.80	0.08	90,96,113,119	0
7	SO4	A	507	5/5	0.83	0.10	72,88,107,108	0
7	SO4	A	509	5/5	0.86	0.14	49,69,92,98	0
7	SO4	A	502	5/5	0.87	0.09	77,85,88,92	0
7	SO4	A	508	5/5	0.88	0.10	89,93,101,103	0
7	SO4	L	301	5/5	0.88	0.07	94,94,104,107	0
13	CL	D	2005	1/1	0.88	0.19	90,90,90,90	0
7	SO4	A	501	5/5	0.90	0.10	80,80,96,108	0
12	IIF	B	2005	38/38	0.93	0.11	40,63,100,111	0
12	IIF	D	2006	38/38	0.94	0.11	50,64,114,118	0
10	MN	D	2002	1/1	0.97	0.07	90,90,90,90	0
10	MN	D	2003	1/1	0.97	0.06	66,66,66,66	0
13	CL	C	504	1/1	0.97	0.06	71,71,71,71	0
8	CA	A	505	1/1	0.97	0.04	46,46,46,46	0
8	CA	A	503	1/1	0.97	0.04	61,61,61,61	0
10	MN	B	2003	1/1	0.98	0.03	55,55,55,55	0
8	CA	C	507	1/1	0.98	0.04	80,80,80,80	0
8	CA	C	508	1/1	0.98	0.04	75,75,75,75	0
8	CA	C	509	1/1	0.98	0.04	65,65,65,65	0
8	CA	A	506	1/1	0.98	0.04	53,53,53,53	0
10	MN	D	2001	1/1	0.99	0.04	59,59,59,59	0
8	CA	C	506	1/1	0.99	0.04	98,98,98,98	0
10	MN	B	2001	1/1	0.99	0.03	53,53,53,53	0
10	MN	B	2002	1/1	0.99	0.07	100,100,100,100	0
8	CA	A	504	1/1	0.99	0.03	46,46,46,46	0

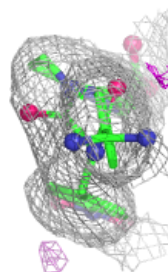
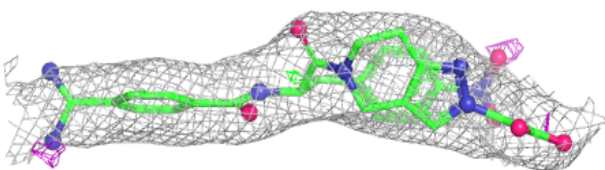
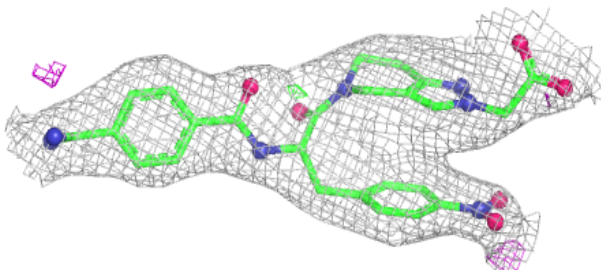
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I1F 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 I1F 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.