



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 12:35 AM EDT

PDB ID : 7UE0
Title : Integrin alpha IIB beta3 complex with fradafiban
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2022-03-20
Resolution : 2.74 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

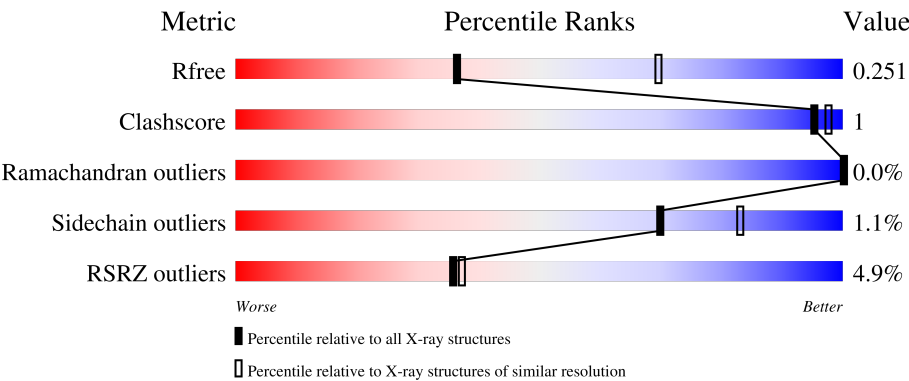
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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.



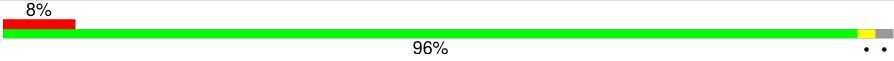
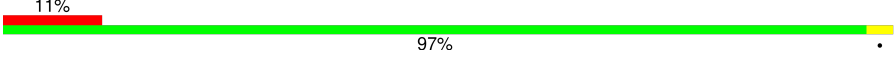
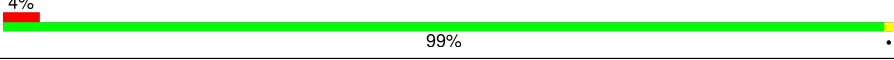

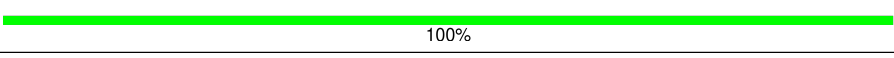
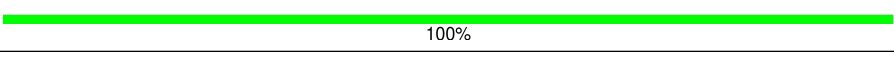

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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>2%</div><div>95%</div><div>5%</div><div></div></div>
1	C	457	<div><div>2%</div><div>96%</div><div></div><div></div></div>
2	B	472	<div><div>4%</div><div>93%</div><div>5%</div><div></div></div>
2	D	472	<div><div>4%</div><div>94%</div><div>5%</div><div></div></div>
3	E	221	<div><div>14%</div><div>93%</div><div></div><div></div></div>

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

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 21373 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	6	0
			3519	2237	607	667	8			
1	C	453	Total	C	N	O	S	0	3	0
			3493	2219	602	664	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	2	0
			3603	2245	615	710	33			
2	D	471	Total	C	N	O	S	0	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)-[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			

- 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)-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	0	0	0
			50	28	2	20			

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



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

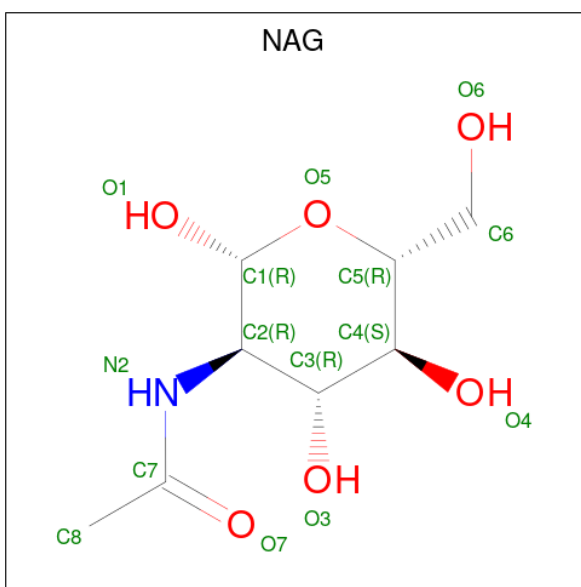
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

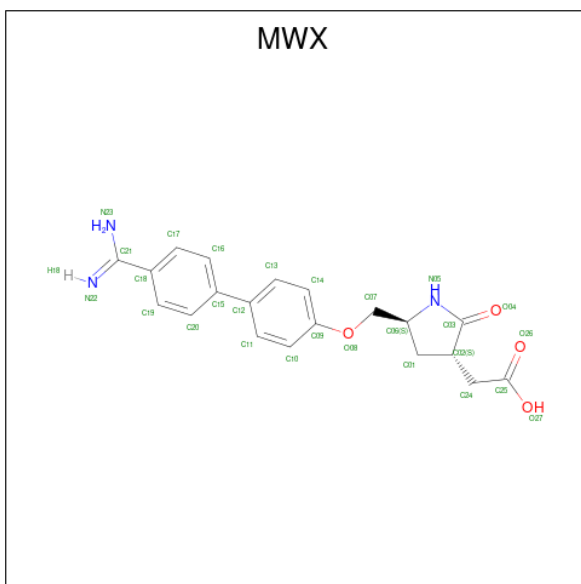
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Mg	0	0
			1	1		
11	D	1	Total	Mg	0	0
			1	1		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 13 is Fradafiban (three-letter code: MWX) (formula: $C_{20}H_{21}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			27	20	3	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	D	1	Total	C	N	O	0	0
			27	20	3	4		

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

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

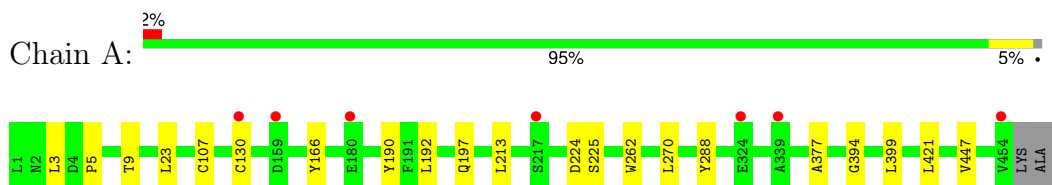
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	97	Total	O	0	0
			97	97		
15	B	75	Total	O	0	0
			75	75		
15	C	47	Total	O	0	0
			47	47		
15	D	27	Total	O	0	0
			27	27		
15	E	8	Total	O	0	0
			8	8		
15	F	4	Total	O	0	0
			4	4		
15	H	9	Total	O	0	0
			9	9		
15	L	18	Total	O	0	0
			18	18		

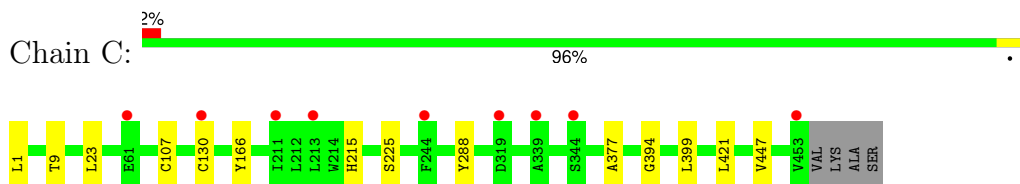
3 Residue-property plots

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.

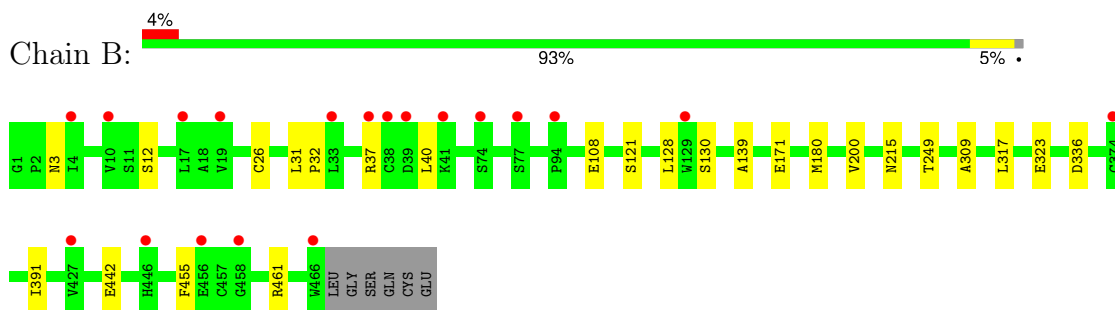
- Molecule 1: Integrin alpha-IIb heavy chain



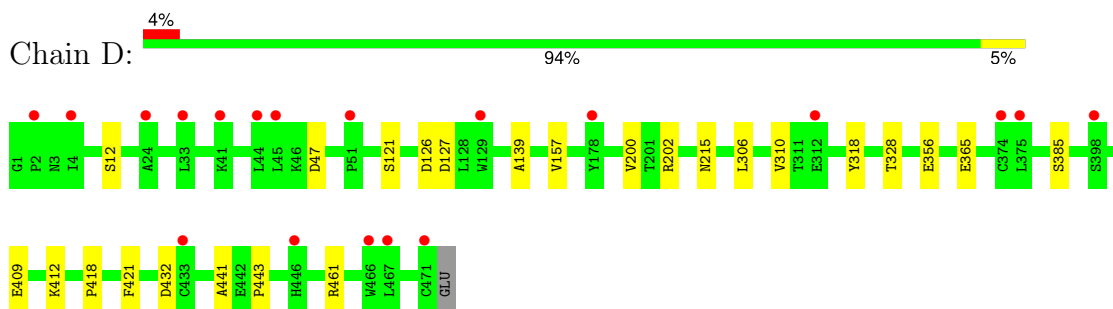
- Molecule 1: Integrin alpha-IIb heavy chain



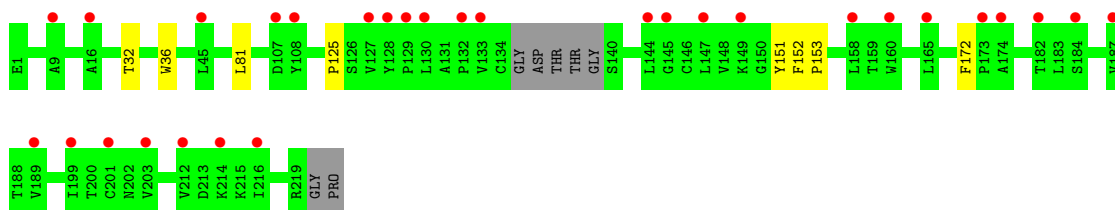
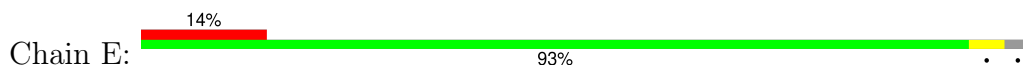
- Molecule 2: Isoform Beta-3C of Integrin beta-3



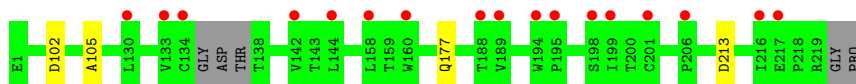
- Molecule 2: Isoform Beta-3C of Integrin beta-3



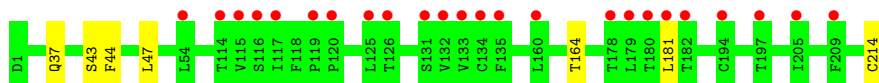
- Molecule 3: 10E5 Fab heavy chain



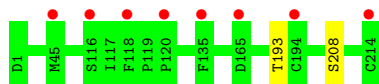
- Molecule 3: 10E5 Fab heavy chain



- Molecule 4: 10E5 Fab light chain



- Molecule 4: 10E5 Fab light chain



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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



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

Chain K:  100%

MAG1
MAG2

- Molecule 7: 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

Chain J:  75% 25%

MAG1
MAG2
EMJ3
MAM4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	258.28Å 145.02Å 104.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.82 – 2.74 42.82 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.82-2.74) 85.5 (42.82-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.225 , 0.253 0.224 , 0.251	Depositor DCC
R_{free} test set	101997 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.9	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	0.93	EDS
Total number of atoms	21373	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: GOL, BMA, SO4, MAN, CA, MWX, CL, MG, NAG

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	0/3628	0.45	0/4944
1	C	0.25	0/3596	0.45	0/4900
2	B	0.24	0/3673	0.43	0/4981
2	D	0.24	0/3690	0.43	0/5003
3	E	0.24	0/1673	0.44	0/2290
3	H	0.24	0/1684	0.45	0/2305
4	F	0.24	0/1673	0.44	0/2269
4	L	0.24	0/1673	0.45	0/2269
All	All	0.25	0/21290	0.44	0/28961

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	3519	0	3364	8	0
1	C	3493	0	3327	6	0
2	B	3603	0	3526	12	0
2	D	3623	0	3540	11	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	2	0
4	F	1637	0	1553	3	0
4	L	1637	0	1553	1	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	0	0
7	J	50	0	43	0	0
8	A	15	0	0	0	0
8	C	10	0	0	0	0
8	L	5	0	0	0	0
9	A	6	0	8	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	14	0	13	0	0
12	D	14	0	13	0	0
13	B	27	0	0	2	0
13	D	27	0	0	3	0
14	B	1	0	0	0	0
14	C	2	0	0	0	0
14	D	1	0	0	0	0
15	A	97	0	0	0	0
15	B	75	0	0	0	0
15	C	47	0	0	0	0
15	D	27	0	0	0	0
15	E	8	0	0	0	0
15	F	4	0	0	0	0
15	H	9	0	0	0	0
15	L	18	0	0	0	0
All	All	21373	0	20232	45	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 1.

All (45) 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:121:SER:HB2	13:B:2005:MWX:O27	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASP:OD1	1:A:225:SER:N	2.36	0.58
1:A:9:THR:HB	1:A:447:VAL:HB	1.88	0.55
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.89	0.54
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.92	0.52
2:B:130:SER:OG	2:B:336:ASP:O	2.27	0.50
2:D:139:ALA:HB2	2:D:200:VAL:HG11	1.94	0.50
1:C:107:CYS:HA	1:C:130:CYS:HA	1.95	0.49
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.49	0.48
2:D:121:SER:HB2	13:D:2005:MWX:C25	2.42	0.48
3:H:213:ASP:OD1	3:H:213:ASP:N	2.47	0.48
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.95	0.48
2:B:121:SER:HB2	13:B:2005:MWX:C25	2.43	0.48
1:C:394:GLY:HA2	1:C:399:LEU:HD23	1.96	0.48
1:C:9:THR:HB	1:C:447:VAL:HB	1.96	0.47
2:B:108:GLU:HG3	2:B:391:ILE:HG22	1.97	0.47
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.96	0.47
2:D:356:GLU:HG3	2:D:385:SER:HB3	1.98	0.46
4:L:193:THR:HG23	4:L:208:SER:HB3	1.97	0.46
1:A:107:CYS:HA	1:A:130:CYS:HA	1.97	0.46
2:B:26:CYS:O	2:B:37:ARG:NH1	2.48	0.45
2:D:121:SER:HB2	13:D:2005:MWX:O27	2.16	0.45
1:A:377:ALA:HB2	1:A:421:LEU:HD11	1.99	0.44
3:E:36:TRP:CE2	3:E:81:LEU:HB2	2.52	0.44
2:B:249:THR:HG22	2:B:309:ALA:HB3	2.00	0.43
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.53	0.43
1:A:3:LEU:O	1:A:5:PRO:HD3	2.18	0.43
2:D:126:ASP:OD1	2:D:126:ASP:N	2.49	0.43
2:B:442:GLU:HB3	2:B:455:PHE:HB3	2.00	0.43
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.86	0.42
1:C:377:ALA:HB2	1:C:421:LEU:HD11	2.01	0.42
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.55	0.42
2:D:310:VAL:HG11	2:D:318:TYR:CD2	2.54	0.42
2:D:409:GLU:HB2	2:D:412:LYS:HE3	2.00	0.42
4:F:37:GLN:HB2	4:F:47:LEU:HD11	2.02	0.42
3:E:125:PRO:HB3	3:E:151:TYR:HB3	2.02	0.41
3:E:152:PHE:HA	3:E:153:PRO:HA	1.88	0.41
2:B:3:ASN:ND2	2:B:40:LEU:HG	2.36	0.41
1:A:394:GLY:HA2	1:A:399:LEU:HD23	2.03	0.41
3:H:102:ASP:HB3	3:H:105:ALA:HB2	2.02	0.41
1:C:225:SER:O	13:D:2005:MWX:N23	2.54	0.41
4:F:43:SER:OG	4:F:44:PHE:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TRP:HB3	2:B:317:LEU:HD13	2.03	0.40
2:B:31:LEU:HD23	2:B:32:PRO:O	2.21	0.40
2:D:441:ALA:O	2:D:443:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/457 (100%)	448 (98%)	10 (2%)	0	100	100
1	C	454/457 (99%)	439 (97%)	15 (3%)	0	100	100
2	B	466/472 (99%)	447 (96%)	19 (4%)	0	100	100
2	D	469/472 (99%)	442 (94%)	26 (6%)	1 (0%)	44	63
3	E	210/221 (95%)	195 (93%)	15 (7%)	0	100	100
3	H	212/221 (96%)	199 (94%)	13 (6%)	0	100	100
4	F	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2693/2728 (99%)	2577 (96%)	115 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	157	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/364 (101%)	361 (98%)	7 (2%)	52	71
1	C	364/364 (100%)	360 (99%)	4 (1%)	70	83
2	B	414/417 (99%)	409 (99%)	5 (1%)	67	82
2	D	416/417 (100%)	410 (99%)	6 (1%)	62	78
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	86	92
4	F	188/188 (100%)	186 (99%)	2 (1%)	70	83
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2311/2318 (100%)	2286 (99%)	25 (1%)	70	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	192	LEU
1	A	197	GLN
1	A	270	LEU
1	A	288	TYR
2	B	128	LEU
2	B	171	GLU
2	B	180	MET
2	B	215	ASN
2	B	323	GLU
1	C	1	LEU
1	C	23	LEU
1	C	166	TYR
1	C	288	TYR
2	D	47	ASP
2	D	127	ASP
2	D	202	ARG
2	D	215	ASN
2	D	365	GLU
2	D	432	ASP
4	F	181	LEU
4	F	214	CYS
3	H	177	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	333	GLN
2	D	15	GLN
2	D	301	GLN
4	F	138	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	0.36	0	17,19,21	0.54	0
5	NAG	G	2	5	14,14,15	0.18	0	17,19,21	0.53	0
5	BMA	G	3	5	11,11,12	0.66	0	15,15,17	0.79	0
5	MAN	G	4	5	11,11,12	0.76	0	15,15,17	1.17	2 (13%)
5	MAN	G	5	5	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.29	0	17,19,21	0.50	0
6	NAG	I	2	6	14,14,15	0.16	0	17,19,21	0.52	0
7	NAG	J	1	2,7	14,14,15	0.25	0	17,19,21	0.57	0
7	NAG	J	2	7	14,14,15	0.21	0	17,19,21	0.42	0
7	BMA	J	3	7	11,11,12	0.59	0	15,15,17	0.74	0
7	MAN	J	4	7	11,11,12	0.79	1 (9%)	15,15,17	1.25	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.38	0	17,19,21	0.58	0
6	NAG	K	2	6	14,14,15	0.28	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
5	NAG	G	1	5,2	-	2/6/23/26	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
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	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	MAN	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	4	MAN	C1-C2	2.25	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	4	MAN	C1-O5-C5	3.40	116.74	112.19
5	G	4	MAN	C1-O5-C5	3.34	116.66	112.19
5	G	5	MAN	C1-O5-C5	2.45	115.47	112.19
7	J	4	MAN	O2-C2-C3	-2.29	105.41	110.15
5	G	4	MAN	O2-C2-C3	-2.23	105.52	110.15
5	G	5	MAN	O2-C2-C3	-2.21	105.57	110.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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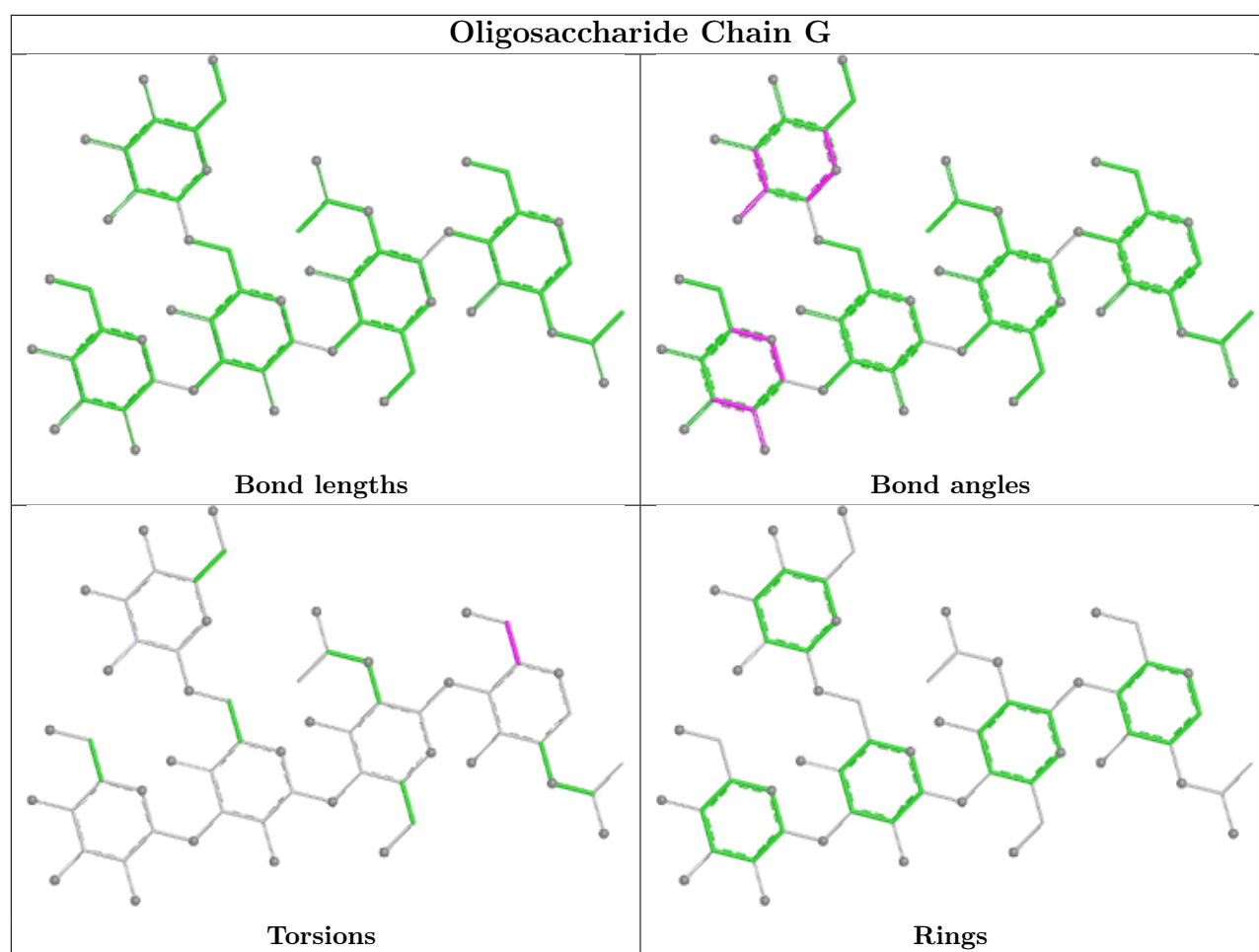
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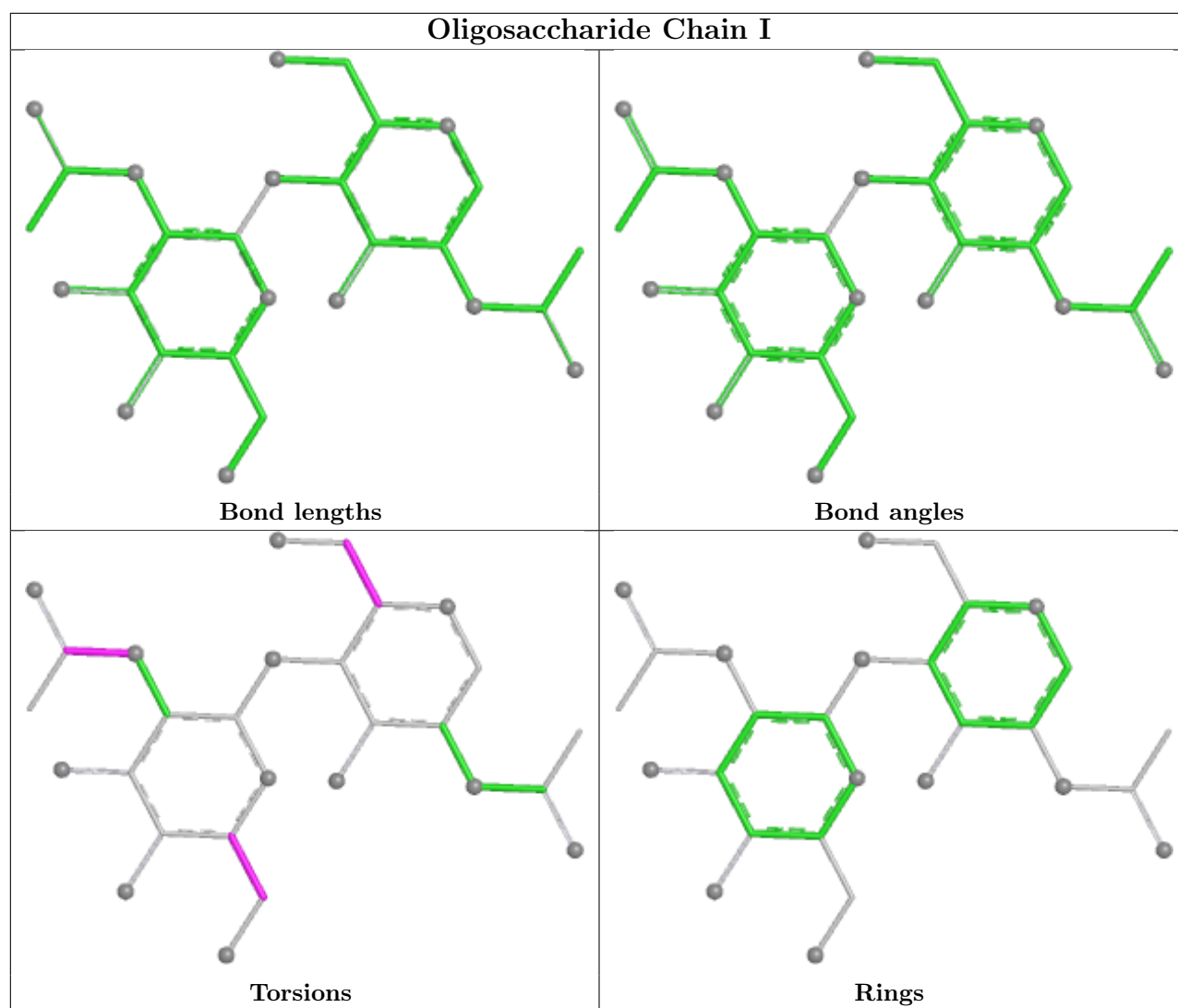
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	I	1	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6

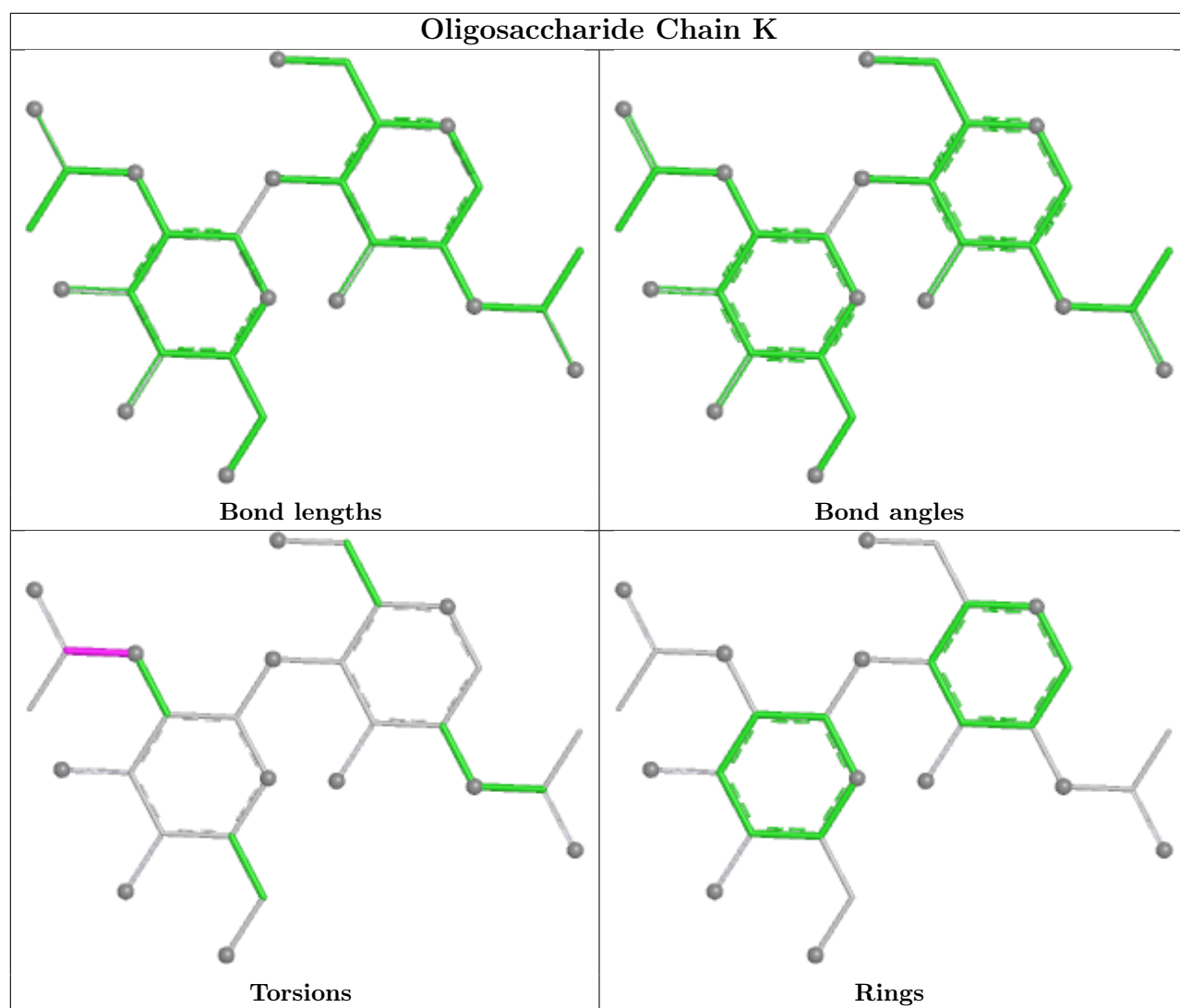
There are no ring outliers.

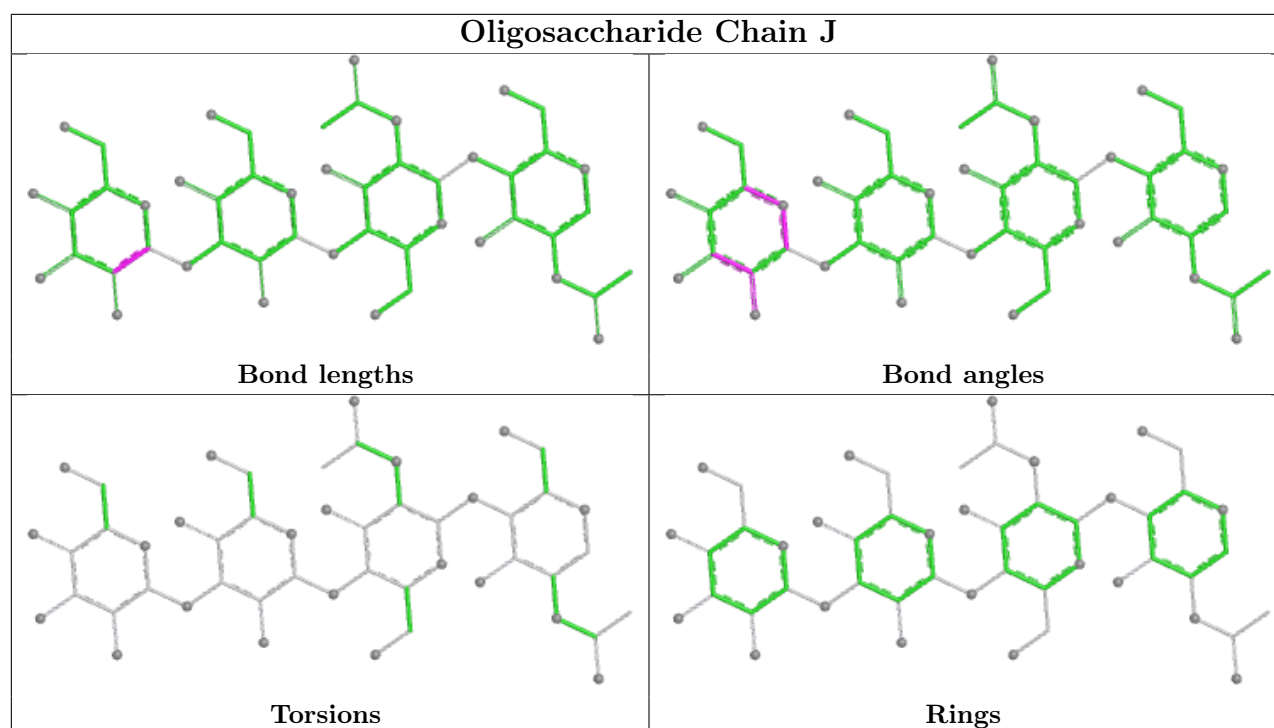
No monomer is involved in short contacts.

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 29 ligands modelled in this entry, 18 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.13	0
12	NAG	D	2004	2	14,14,15	0.58	0	17,19,21	0.64	0
9	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.27	0
13	MWX	B	2005	11	29,29,29	1.85	10 (34%)	32,40,40	2.49	17 (53%)
8	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.13	0
12	NAG	B	2004	2	14,14,15	0.32	0	17,19,21	0.57	0
8	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.09	0
8	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.06	0
8	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.11	0
8	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.08	0
13	MWX	D	2005	11	29,29,29	1.79	8 (27%)	32,40,40	2.49	16 (50%)

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	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
9	GOL	A	504	-	-	2/4/4/4	-
12	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
13	MWX	B	2005	11	-	8/17/29/29	0/3/3/3
13	MWX	D	2005	11	-	8/17/29/29	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	2005	MWX	C07-C06	4.02	1.59	1.52
13	D	2005	MWX	C07-C06	3.96	1.59	1.52
13	B	2005	MWX	C24-C25	3.60	1.60	1.51
13	B	2005	MWX	C03-N05	3.28	1.40	1.33
13	D	2005	MWX	C24-C25	3.17	1.59	1.51
13	D	2005	MWX	C03-N05	3.12	1.39	1.33
13	B	2005	MWX	C18-C21	2.74	1.52	1.47
13	D	2005	MWX	C18-C21	2.74	1.52	1.47
13	B	2005	MWX	C21-N23	2.72	1.41	1.33
13	D	2005	MWX	C21-N23	2.59	1.40	1.33
13	D	2005	MWX	C14-C13	2.58	1.43	1.38
13	B	2005	MWX	C14-C13	2.53	1.42	1.38
13	B	2005	MWX	C15-C12	2.46	1.54	1.49
13	D	2005	MWX	C20-C19	2.36	1.42	1.38
13	B	2005	MWX	C11-C10	2.21	1.42	1.38
13	D	2005	MWX	C11-C10	2.19	1.42	1.38
13	B	2005	MWX	C20-C19	2.16	1.42	1.38
13	B	2005	MWX	C17-C16	2.13	1.42	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	2005	MWX	C14-C09-C10	-4.88	113.04	120.16
13	D	2005	MWX	C14-C09-C10	-4.86	113.07	120.16
13	B	2005	MWX	C13-C12-C11	-4.01	110.50	117.68
13	D	2005	MWX	C13-C12-C11	-3.93	110.65	117.68
13	D	2005	MWX	O04-C03-N05	-3.75	121.32	126.57
13	B	2005	MWX	O04-C03-N05	-3.70	121.38	126.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	2005	MWX	C14-C13-C12	3.60	125.74	121.12
13	B	2005	MWX	C02-C03-N05	3.60	113.61	107.28
13	D	2005	MWX	C17-C16-C15	3.59	125.73	121.12
13	B	2005	MWX	C11-C10-C09	3.58	123.82	119.73
13	D	2005	MWX	C02-C03-N05	3.58	113.58	107.28
13	D	2005	MWX	C11-C10-C09	3.56	123.80	119.73
13	D	2005	MWX	C14-C13-C12	3.56	125.69	121.12
13	B	2005	MWX	C01-C02-C24	3.56	121.60	116.23
13	B	2005	MWX	C17-C16-C15	3.46	125.56	121.12
13	D	2005	MWX	C01-C02-C24	3.45	121.44	116.23
13	D	2005	MWX	C19-C18-C17	-3.22	114.47	118.57
13	D	2005	MWX	O08-C07-C06	3.19	116.66	108.73
13	B	2005	MWX	C19-C18-C17	-3.16	114.55	118.57
13	B	2005	MWX	C20-C19-C18	2.98	123.99	120.80
13	B	2005	MWX	C20-C15-C16	-2.98	112.34	117.68
13	D	2005	MWX	C20-C15-C16	-2.95	112.40	117.68
13	B	2005	MWX	O08-C07-C06	2.93	116.03	108.73
13	D	2005	MWX	C20-C19-C18	2.83	123.82	120.80
13	B	2005	MWX	C10-C11-C12	2.70	124.59	121.12
13	D	2005	MWX	C10-C11-C12	2.64	124.51	121.12
13	B	2005	MWX	C13-C12-C15	2.48	125.54	121.25
13	D	2005	MWX	C13-C12-C15	2.47	125.52	121.25
13	D	2005	MWX	C18-C21-N23	2.41	121.67	118.01
13	B	2005	MWX	C18-C21-N23	2.31	121.52	118.01
13	B	2005	MWX	C13-C14-C09	2.25	122.30	119.73
13	D	2005	MWX	C13-C14-C09	2.24	122.28	119.73
13	B	2005	MWX	C01-C02-C03	-2.16	100.13	102.88

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	504	GOL	O1-C1-C2-C3
13	B	2005	MWX	C01-C02-C24-C25
13	B	2005	MWX	C03-C02-C24-C25
13	B	2005	MWX	N05-C06-C07-O08
13	B	2005	MWX	C17-C18-C21-N23
13	B	2005	MWX	C19-C18-C21-N23
13	D	2005	MWX	C01-C06-C07-O08
13	D	2005	MWX	N05-C06-C07-O08
12	B	2004	NAG	O5-C5-C6-O6
13	B	2005	MWX	C14-C09-O08-C07

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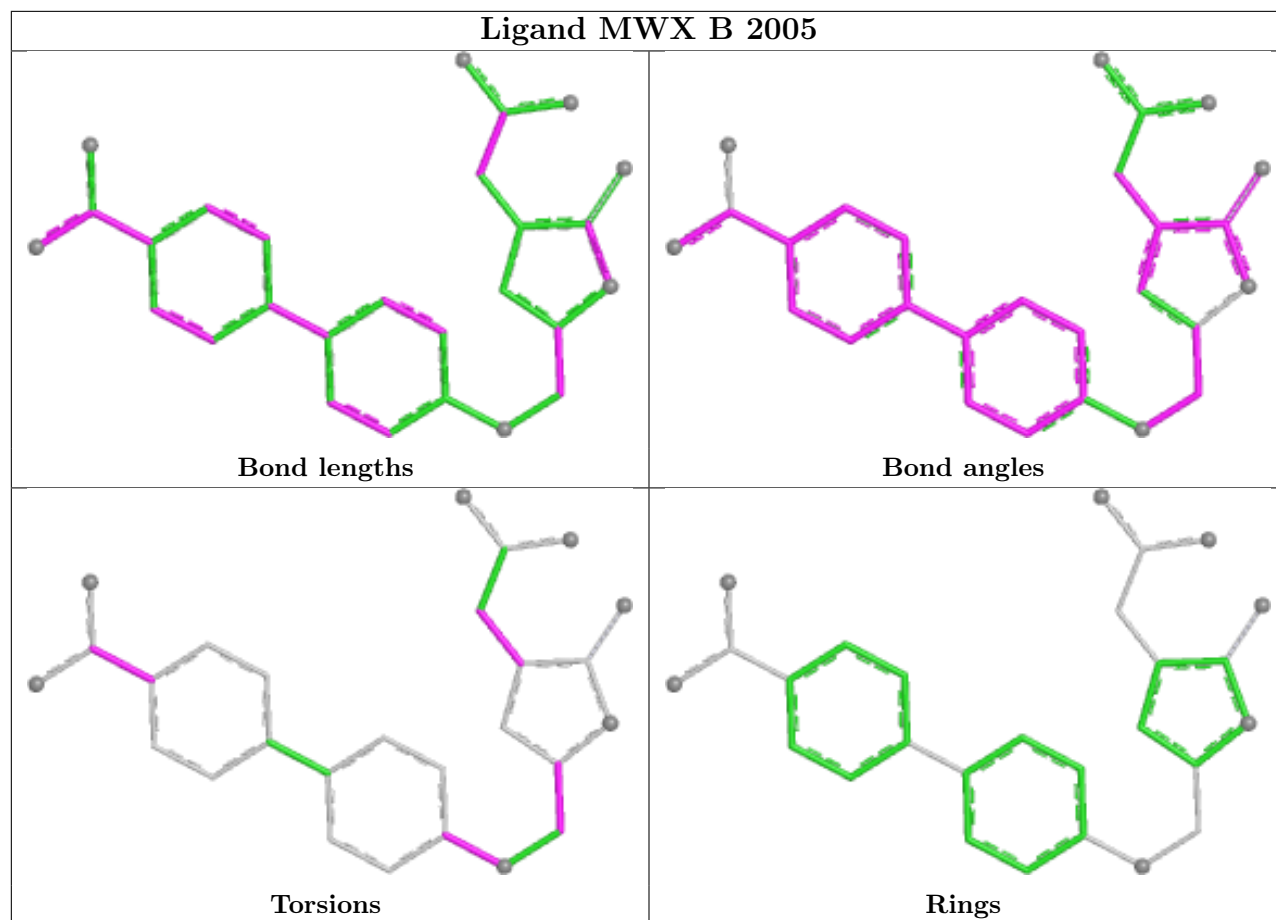
Mol	Chain	Res	Type	Atoms
13	B	2005	MWX	C10-C09-O08-C07
12	B	2004	NAG	C4-C5-C6-O6
12	D	2004	NAG	O5-C5-C6-O6
12	D	2004	NAG	C4-C5-C6-O6
13	D	2005	MWX	C14-C09-O08-C07
9	A	504	GOL	O1-C1-C2-O2
13	D	2005	MWX	C10-C09-O08-C07
13	D	2005	MWX	C17-C18-C21-N23
13	D	2005	MWX	C19-C18-C21-N23
13	B	2005	MWX	C19-C18-C21-N22
13	D	2005	MWX	C17-C18-C21-N22
13	D	2005	MWX	C19-C18-C21-N22

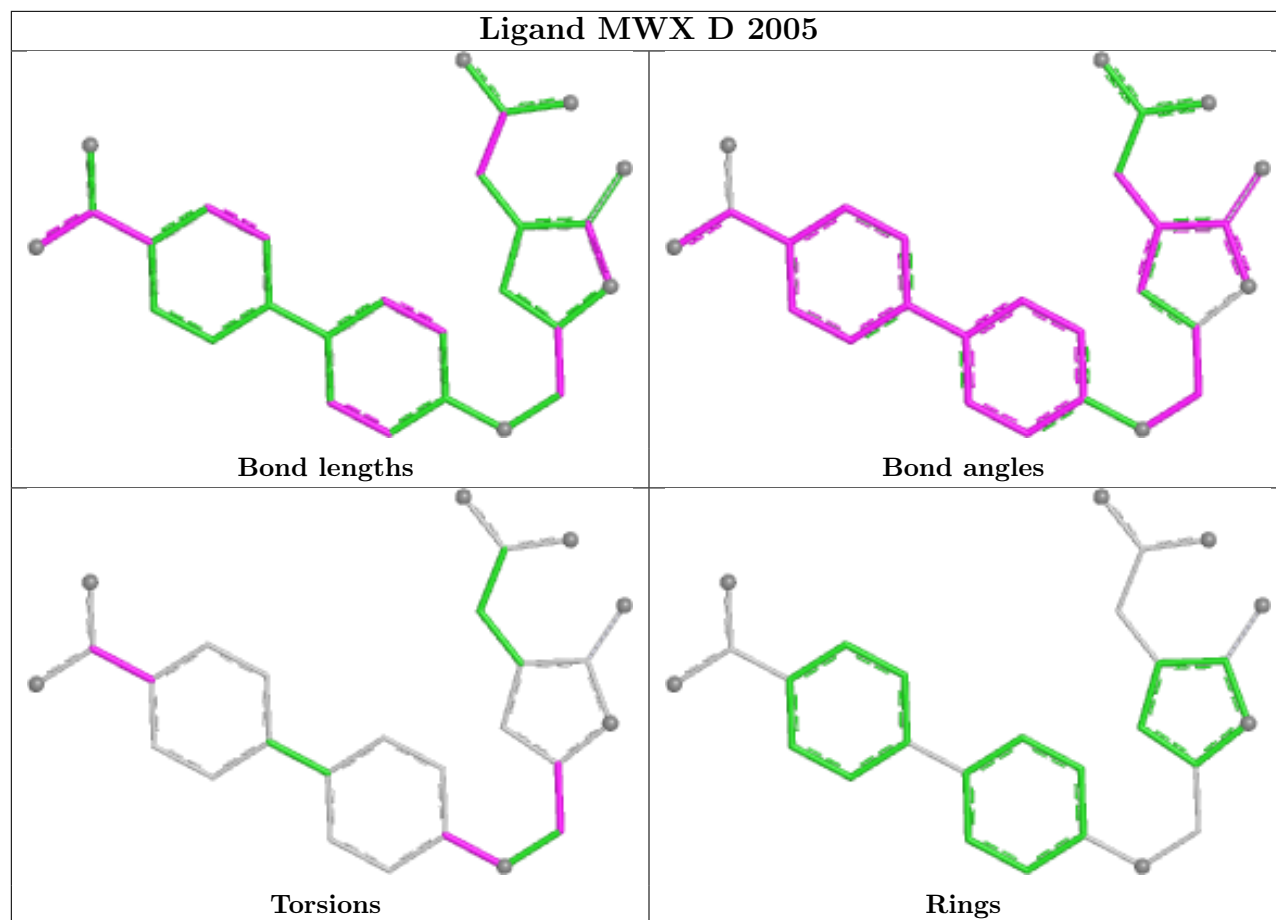
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2005	MWX	2	0
13	D	2005	MWX	3	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%)	0.01	7 (1%) 71 72	34, 59, 81, 102	6 (1%)
1	C	453/457 (99%)	0.23	9 (1%) 64 64	40, 75, 95, 113	3 (0%)
2	B	466/472 (98%)	0.44	19 (4%) 42 43	32, 82, 147, 163	3 (0%)
2	D	471/472 (99%)	0.55	19 (4%) 43 44	60, 95, 138, 156	0
3	E	214/221 (96%)	1.10	30 (14%) 7 10	91, 131, 195, 206	0
3	H	216/221 (97%)	0.73	17 (7%) 20 23	71, 105, 144, 153	0
4	F	214/214 (100%)	0.92	24 (11%) 11 13	93, 132, 195, 206	0
4	L	214/214 (100%)	0.69	8 (3%) 45 46	73, 98, 117, 140	0
All	All	2702/2728 (99%)	0.48	133 (4%) 36 37	32, 89, 170, 206	12 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	135	PHE	5.3
1	A	454	VAL	5.3
3	E	147	LEU	4.9
1	C	453	VAL	4.3
3	E	212	VAL	4.1
3	E	144	LEU	4.1
3	H	216	ILE	4.0
3	E	203	VAL	3.9
3	E	133	VAL	3.9
4	F	134	CYS	3.9
2	D	375	LEU	3.9
3	E	130	LEU	3.8
1	A	217	SER	3.8
2	B	39	ASP	3.7
4	F	133	VAL	3.6
3	E	128	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	178	THR	3.6
4	F	115	VAL	3.5
2	B	4	ILE	3.5
3	H	217	GLU	3.4
2	B	458	GLY	3.4
3	E	214	LYS	3.4
3	H	158	LEU	3.3
4	L	135	PHE	3.3
3	E	201	CYS	3.3
4	F	131	SER	3.2
3	E	189	VAL	3.2
4	F	117	ILE	3.2
4	F	132	VAL	3.1
3	E	107	ASP	3.1
2	B	33	LEU	3.1
3	E	184	SER	3.1
3	H	194	TRP	3.1
3	H	189	VAL	3.1
1	A	130	CYS	3.0
2	D	433	CYS	3.0
2	B	17	LEU	2.9
1	C	130	CYS	2.9
2	D	33	LEU	2.9
3	E	165	LEU	2.8
3	H	144	LEU	2.8
2	D	4	ILE	2.8
2	B	10	VAL	2.8
3	E	149	LYS	2.8
2	B	94	PRO	2.8
3	E	129	PRO	2.8
2	B	77	SER	2.7
2	D	44	LEU	2.6
2	D	471	CYS	2.6
4	F	205	ILE	2.6
3	E	132	PRO	2.6
2	B	38	CYS	2.6
1	C	61	GLU	2.6
4	F	180	THR	2.6
2	B	466	TRP	2.5
2	D	41	LYS	2.5
4	F	116	SER	2.5
1	C	319	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	201	CYS	2.5
4	F	125	LEU	2.5
4	L	120	PRO	2.5
3	E	174	ALA	2.5
2	D	45	LEU	2.4
3	H	130	LEU	2.4
4	L	118	PHE	2.4
4	F	54	LEU	2.4
3	E	160	TRP	2.4
4	F	209	PHE	2.4
2	D	398	SER	2.4
1	A	339	ALA	2.4
3	E	182	THR	2.4
1	A	159	ASP	2.4
2	B	374	CYS	2.4
4	F	119	PRO	2.3
4	L	45	MET	2.3
4	F	182	THR	2.3
2	D	2	PRO	2.3
2	B	446	HIS	2.3
3	H	199	ILE	2.3
3	E	45	LEU	2.3
4	F	179	LEU	2.3
2	B	456	GLU	2.3
4	F	197	THR	2.3
2	B	427	VAL	2.3
2	D	129	TRP	2.3
3	E	158	LEU	2.3
1	A	180	GLU	2.2
4	F	114	THR	2.2
4	F	194	CYS	2.2
3	E	127	VAL	2.2
3	E	187	VAL	2.2
3	E	9	ALA	2.2
1	C	213	LEU	2.2
4	F	181	LEU	2.2
2	B	74	SER	2.2
3	E	108	TYR	2.2
4	L	214	CYS	2.2
3	H	198	SER	2.2
2	D	51	PRO	2.2
3	H	142	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	160	TRP	2.2
3	E	216	ILE	2.2
2	D	466	TRP	2.1
2	D	446	HIS	2.1
4	L	165	ASP	2.1
1	C	244	PHE	2.1
3	E	199	ILE	2.1
4	F	160	LEU	2.1
2	D	24	ALA	2.1
2	D	374	CYS	2.1
3	E	16	ALA	2.1
2	D	178	TYR	2.1
2	B	37	ARG	2.1
2	B	129	TRP	2.1
4	L	116	SER	2.1
3	E	145	GLY	2.1
4	L	194	CYS	2.1
3	H	206	PRO	2.1
3	H	188	THR	2.1
1	C	344	SER	2.1
2	B	19	VAL	2.1
3	E	173	PRO	2.0
4	F	120	PRO	2.0
1	A	324	GLU	2.0
4	F	126	THR	2.0
2	D	467	LEU	2.0
3	H	195	PRO	2.0
2	B	41	LYS	2.0
2	D	312	GLU	2.0
3	H	134	CYS	2.0
1	C	211	ILE	2.0
3	H	133	VAL	2.0
1	C	339	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands ⓘ

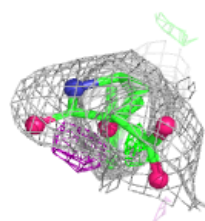
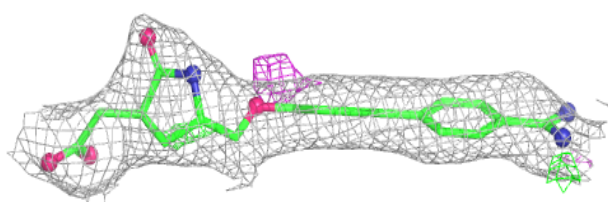
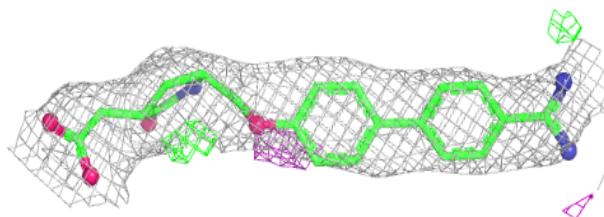
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	NAG	D	2004	14/15	0.45	0.15	110,110,110,110	0
12	NAG	B	2004	14/15	0.65	0.12	112,112,112,112	0
8	SO4	C	501	5/5	0.70	0.20	97,97,97,97	0
8	SO4	L	301	5/5	0.73	0.22	102,102,102,102	0
9	GOL	A	504	6/6	0.80	0.12	76,76,76,76	0
8	SO4	A	501	5/5	0.84	0.26	96,96,96,96	0
14	CL	D	2006	1/1	0.84	0.23	103,103,103,103	0
8	SO4	A	503	5/5	0.85	0.13	76,76,76,76	0
8	SO4	C	502	5/5	0.86	0.13	96,96,96,96	0
13	MWX	D	2005	27/27	0.87	0.13	78,78,78,78	0
8	SO4	A	502	5/5	0.87	0.31	75,75,75,75	0
14	CL	C	508	1/1	0.88	0.15	87,87,87,87	0
14	CL	B	2006	1/1	0.88	0.16	88,88,88,88	0
13	MWX	B	2005	27/27	0.89	0.12	64,64,64,64	0
10	CA	D	2002	1/1	0.95	0.09	77,77,77,77	0
10	CA	C	504	1/1	0.96	0.07	97,97,97,97	0
14	CL	C	503	1/1	0.96	0.07	79,79,79,79	0
10	CA	A	507	1/1	0.98	0.04	51,51,51,51	0
10	CA	D	2003	1/1	0.98	0.04	66,66,66,66	0
11	MG	B	2001	1/1	0.98	0.05	54,54,54,54	0
11	MG	D	2001	1/1	0.98	0.05	71,71,71,71	0
10	CA	B	2002	1/1	0.98	0.09	71,71,71,71	0
10	CA	A	505	1/1	0.98	0.05	73,73,73,73	0
10	CA	A	506	1/1	0.99	0.03	54,54,54,54	0
10	CA	B	2003	1/1	0.99	0.03	56,56,56,56	0
10	CA	A	508	1/1	0.99	0.03	52,52,52,52	0
10	CA	C	505	1/1	0.99	0.05	83,83,83,83	0
10	CA	C	506	1/1	0.99	0.03	77,77,77,77	0
10	CA	C	507	1/1	0.99	0.03	77,77,77,77	0

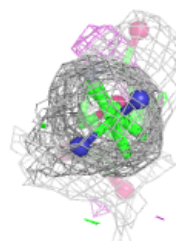
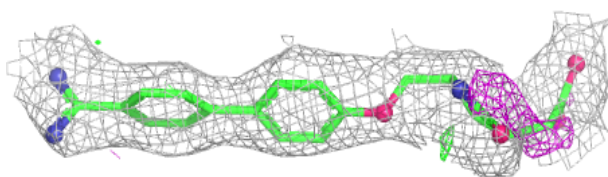
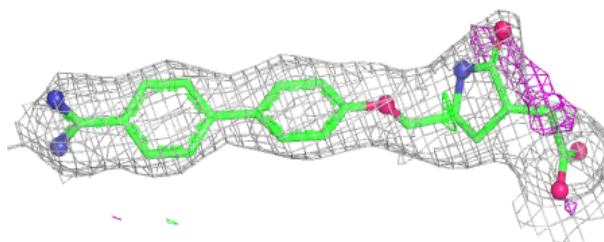
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MWX 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)

**Electron density around MWX 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 ⓘ

There are no such residues in this entry.