



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:34 PM UTC

PDB ID : 7UKO / pdb_00007uko
Title : Integrin alpha IIB beta3 complex with sibrifiban (Mn)
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2022-04-01
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

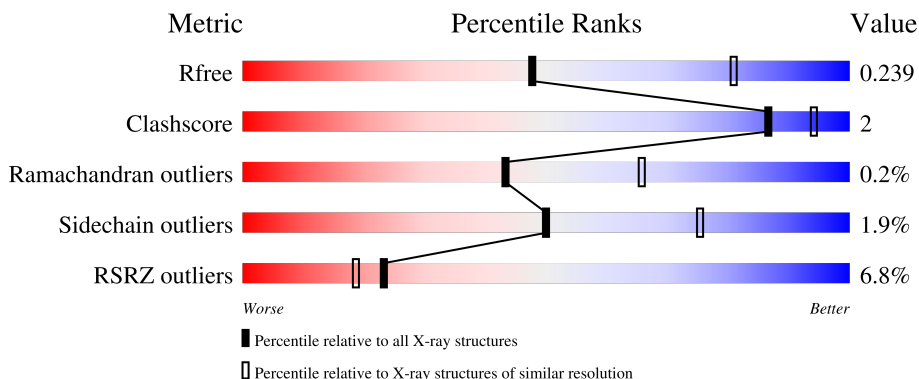
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



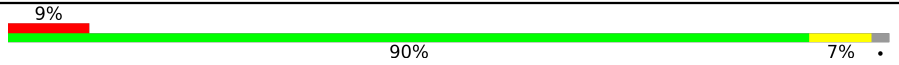
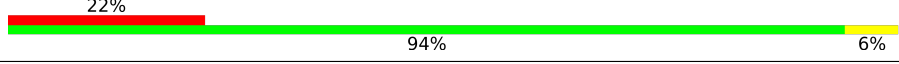
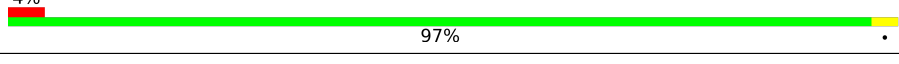
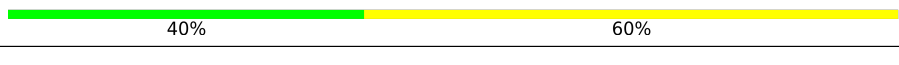
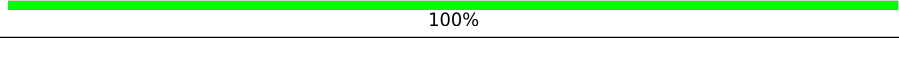

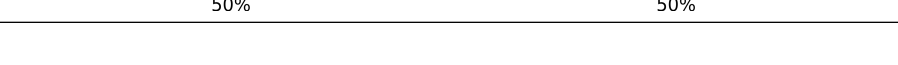
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	 2% 94% 5%
1	C	457	 % 93% 6%
2	B	472	 4% 89% 8%
2	D	472	 6% 92% 8%
3	E	221	 23% 87% 10%

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Mol	Chain	Length	Quality of chain
3	H	221	 <p>9% 90% 7%</p>
4	F	214	 <p>22% 94% 6%</p>
4	L	214	 <p>4% 97%</p>
5	G	5	 <p>40% 60%</p>
6	I	2	 <p>100%</p>
6	K	2	 <p>50% 50%</p>
7	J	4	 <p>50% 50%</p>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 21809 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
			Total	C	N	O	S			
1	A	454	Total	C	N	O	S	0	5	0
			3508	2230	605	665	8			
1	C	453	Total	C	N	O	S	0	3	0
			3495	2219	602	666	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	466	Total	C	N	O	S	4	3	0
			3610	2248	616	713	33			
2	D	471	Total	C	N	O	S	3	1	0
			3631	2260	620	716	35			

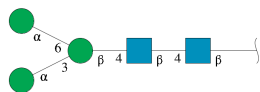
- Molecule 3 is a protein called 10E5 Fab heavy chain.

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

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

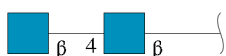
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
			Total	C	N	O			
5	G	5	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
			Total	C	N	O			
6	I	2	28	16	2	10	0	0	0
6	K	2	28	16	2	10	0	0	0

- 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
			Total	C	N	O			
7	J	4	50	28	2	20	0	0	0

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 11 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

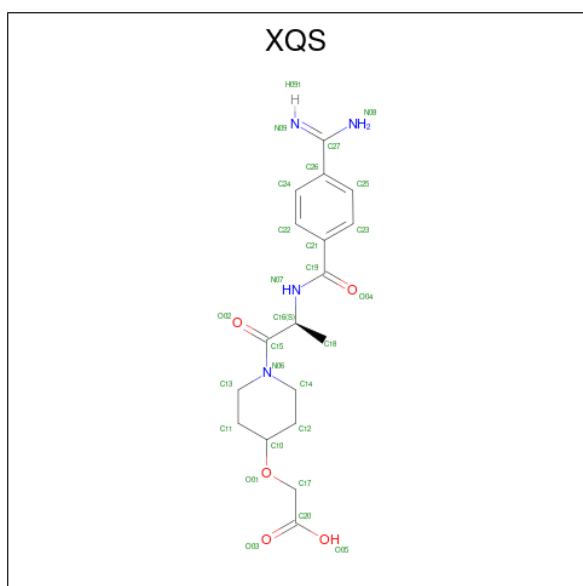
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	3	Total Mn 3 3	0	0
11	D	3	Total Mn 3 3	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 sibralfiban (active form) (CCD ID: XQS) (formula: $C_{18}H_{24}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			27	18	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	D	1	27	18	4	5	0	0

- Molecule 14 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

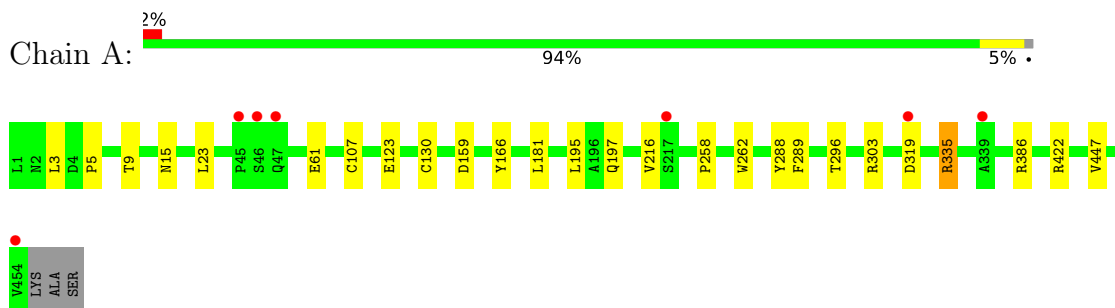
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	299	299	299	0	0
15	B	150	150	150	0	0
15	C	92	92	92	0	0
15	D	85	85	85	0	0
15	E	11	11	11	0	0
15	F	18	18	18	0	0
15	H	24	24	24	0	0
15	L	38	38	38	0	0

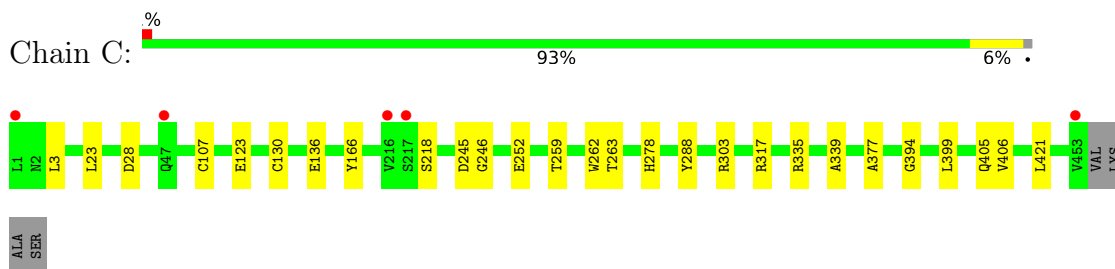
3 Residue-property plots

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.

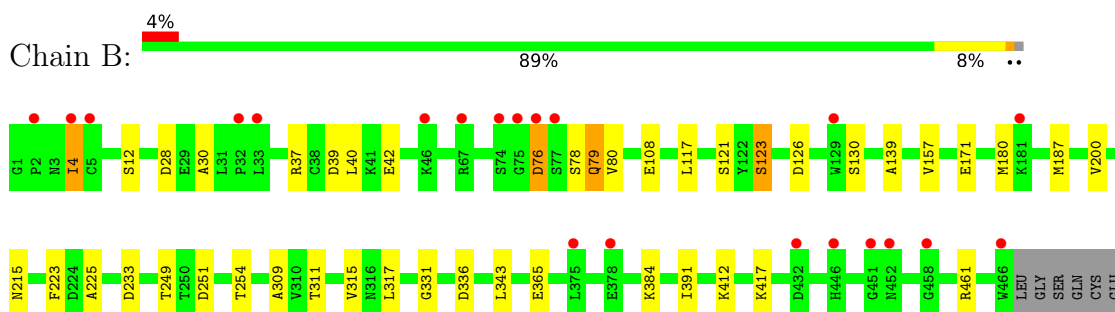
- Molecule 1: Integrin alpha-IIb heavy chain



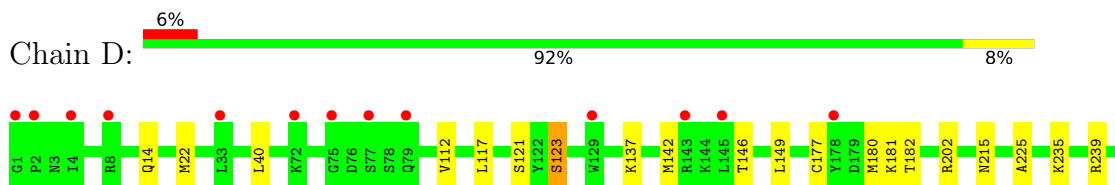
- Molecule 1: Integrin alpha-IIb heavy chain

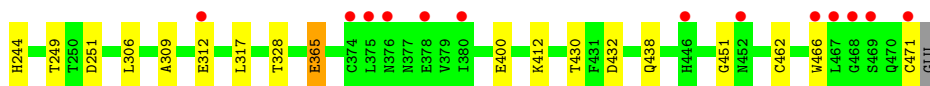


- Molecule 2: Isoform Beta-3C of Integrin beta-3

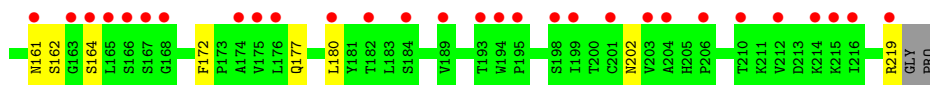
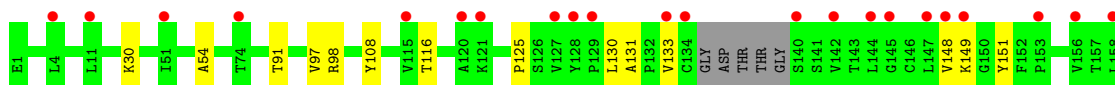
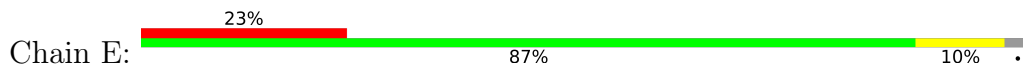


- Molecule 2: Isoform Beta-3C of Integrin beta-3

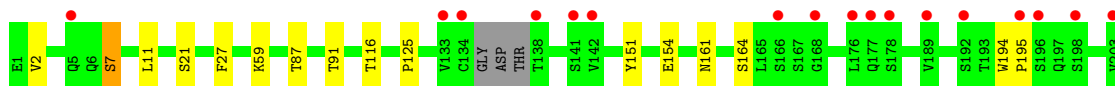
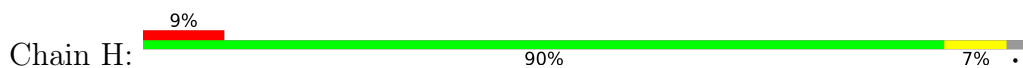




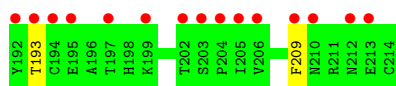
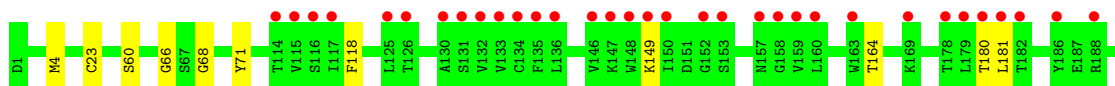
- Molecule 3: 10E5 Fab heavy chain



- 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

Chain I:  100%



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

Chain K:  50% 50%



- 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:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	258.39Å 144.60Å 104.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.60 49.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.29-2.60) 88.8 (49.29-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.214 , 0.239 0.214 , 0.239	Depositor DCC
R_{free} test set	1998 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtrriage
Anisotropy	0.320	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21809	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: XQS, CA, NAG, CL, BMA, MAN, GOL, MN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/3620	0.40	0/4933
1	C	0.14	0/3594	0.38	0/4897
2	B	0.15	0/3680	0.39	1/4991 (0.0%)
2	D	0.13	0/3698	0.35	0/5013
3	E	0.12	0/1673	0.31	0/2290
3	H	0.12	0/1684	0.32	0/2305
4	F	0.13	0/1673	0.34	0/2269
4	L	0.11	0/1673	0.31	0/2269
All	All	0.14	0/21295	0.36	1/28967 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	79	GLN	N-CA-C	-8.54	103.92	112.97

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	3508	0	3355	12	0
1	C	3495	0	3327	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3610	0	3526	23	0
2	D	3631	0	3548	17	0
3	E	1631	0	1590	14	0
3	H	1642	0	1600	7	0
4	F	1637	0	1553	8	0
4	L	1637	0	1553	3	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	1	0
7	J	50	0	43	0	0
8	A	10	0	0	0	0
8	C	10	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	A	12	0	16	2	0
11	B	3	0	0	0	0
11	D	3	0	0	0	0
12	B	14	0	13	0	0
12	D	14	0	13	0	0
13	B	27	0	0	1	0
13	D	27	0	0	1	0
14	C	1	0	0	0	0
15	A	299	0	0	1	0
15	B	150	0	0	0	0
15	C	92	0	0	0	0
15	D	85	0	0	0	0
15	E	11	0	0	0	0
15	F	18	0	0	0	0
15	H	24	0	0	1	0
15	L	38	0	0	0	0
All	All	21809	0	20239	86	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 (86) 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)
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.02	0.74
1:C:245:ASP:OD1	1:C:246:GLY:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:HH11	10:A:507:GOL:H31	1.58	0.67
2:B:121:SER:HB2	13:B:2005:XQS:O03	1.94	0.67
2:B:39:ASP:OD1	2:B:40:LEU:N	2.29	0.64
2:D:121:SER:HB2	13:D:2005:XQS:O03	1.98	0.63
1:A:15[B]:ASN:ND2	15:A:602:HOH:O	2.32	0.61
2:D:123:SER:HB2	2:D:251:ASP:OD2	2.01	0.61
1:A:9:THR:HB	1:A:447:VAL:HB	1.85	0.56
2:B:130:SER:OG	2:B:336:ASP:O	2.19	0.55
2:B:28:ASP:OD1	2:B:30:ALA:N	2.40	0.55
2:D:400:GLU:HB2	6:K:1:NAG:H83	1.90	0.53
3:E:177:GLN:N	3:E:180:LEU:O	2.39	0.53
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.42	0.52
2:B:28:ASP:O	2:B:37:ARG:NH2	2.42	0.52
2:B:123:SER:HB2	2:B:251:ASP:OD2	2.09	0.52
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.92	0.51
4:F:4:MET:HE3	4:F:23:CYS:SG	2.50	0.51
1:A:296:THR:OG1	10:A:508:GOL:H12	2.10	0.51
2:B:76:ASP:HB3	2:B:79:GLN:H	1.75	0.51
2:D:177:CYS:HB3	2:D:182:THR:HG23	1.91	0.51
1:C:107:CYS:HA	1:C:130:CYS:HA	1.93	0.50
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.93	0.50
2:B:331:GLY:HA3	2:B:343:LEU:HD21	1.94	0.50
1:C:3:LEU:O	1:C:405:GLN:NE2	2.36	0.50
1:A:159:ASP:CG	2:D:137:LYS:HG2	2.37	0.49
4:L:4:MET:HE3	4:L:23:CYS:SG	2.52	0.49
2:B:108:GLU:HG3	2:B:391:ILE:HG22	1.95	0.48
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.36	0.48
2:D:117:LEU:HD11	2:D:225:ALA:HB1	1.95	0.48
1:C:377:ALA:HB2	1:C:421:LEU:HD11	1.95	0.48
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.96	0.48
3:E:131:ALA:HB3	3:E:219:ARG:HG3	1.96	0.48
1:C:394:GLY:HA2	1:C:399:LEU:HD23	1.96	0.47
3:E:30:LYS:HG3	3:E:54:ALA:HA	1.96	0.47
2:B:233:ASP:N	2:B:233:ASP:OD1	2.43	0.47
2:D:112:VAL:HG23	2:D:146:THR:HG21	1.95	0.47
2:D:239:ARG:O	2:D:244:HIS:NE2	2.44	0.47
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.98	0.47
1:A:303:ARG:NH1	1:A:335:ARG:HG3	2.29	0.46
4:L:193:THR:HG23	4:L:208:SER:HB3	1.97	0.46
3:E:149:LYS:HZ3	4:F:180:THR:HG21	1.78	0.46
3:E:125:PRO:HB3	3:E:151:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ARG:NH1	1:C:335:ARG:HD3	2.30	0.46
3:E:91:THR:HG23	3:E:116:THR:HA	1.97	0.46
3:E:161:ASN:O	3:E:164:SER:OG	2.27	0.46
1:A:258:PRO:HA	1:A:289:PHE:O	2.16	0.46
2:D:14:GLN:HB2	2:D:438:GLN:HE22	1.80	0.46
2:B:4:ILE:H	2:B:4:ILE:HD13	1.81	0.45
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.98	0.45
3:E:162:SER:N	3:E:202:ASN:OD1	2.50	0.45
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.45
3:H:161:ASN:HB2	3:H:164:SER:HB3	1.99	0.44
2:D:142:MET:HB2	2:D:149:LEU:HD22	1.99	0.44
3:H:59:LYS:NZ	15:H:303:HOH:O	2.51	0.43
1:A:181:LEU:O	1:A:197:GLN:HA	2.19	0.43
1:C:28:ASP:HB2	1:C:136:GLU:OE2	2.19	0.43
1:C:278:HIS:CE1	1:C:339:ALA:HB1	2.54	0.42
3:E:133:VAL:HG21	4:F:209:PHE:HB3	2.00	0.42
3:E:98:ARG:HG3	3:E:108:TYR:HB2	2.02	0.42
1:A:319:ASP:OD1	2:B:384:LYS:NZ	2.43	0.42
3:H:194:TRP:CG	3:H:195:PRO:HA	2.54	0.42
2:D:365:GLU:CD	2:D:365:GLU:H	2.27	0.42
1:A:3:LEU:O	1:A:5:PRO:HD3	2.20	0.42
4:F:66:GLY:HA3	4:F:71:TYR:HA	2.00	0.42
2:B:42:GLU:H	2:B:42:GLU:CD	2.28	0.42
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.02	0.42
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.55	0.42
2:B:78:SER:C	2:B:80:VAL:H	2.28	0.41
2:B:249:THR:HA	2:B:309:ALA:O	2.20	0.41
3:E:130:LEU:HB3	4:F:118:PHE:HB3	2.01	0.41
3:H:2:VAL:HG13	3:H:27:PHE:CE1	2.54	0.41
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.02	0.41
2:D:22:MET:HG2	2:D:40:LEU:HD22	2.03	0.41
2:D:306:LEU:HB3	2:D:328:THR:HG22	2.02	0.41
4:F:149:LYS:HB2	4:F:193:THR:HB	2.03	0.41
2:D:249:THR:HG22	2:D:309:ALA:HB3	2.02	0.41
4:L:195:GLU:HG2	4:L:206:VAL:HG22	2.03	0.41
1:C:259:THR:HA	1:C:263:THR:HA	2.02	0.41
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.02	0.41
1:A:107:CYS:HA	1:A:130:CYS:HA	2.02	0.41
1:C:303:ARG:HH12	1:C:335:ARG:NE	2.19	0.40
2:B:311:THR:O	2:B:315[B]:VAL:HG23	2.21	0.40
2:D:466:TRP:HB3	2:D:471:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:7:SER:HG	3:H:21:SER:H	1.64	0.40
3:H:91:THR:HG23	3:H:116:THR:HA	2.04	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	457/457 (100%)	443 (97%)	13 (3%)	1 (0%)	43	66
1	C	454/457 (99%)	443 (98%)	10 (2%)	1 (0%)	43	66
2	B	467/472 (99%)	445 (95%)	20 (4%)	2 (0%)	30	51
2	D	470/472 (100%)	448 (95%)	21 (4%)	1 (0%)	43	66
3	E	210/221 (95%)	191 (91%)	19 (9%)	0	100	100
3	H	212/221 (96%)	201 (95%)	11 (5%)	0	100	100
4	F	212/214 (99%)	198 (93%)	13 (6%)	1 (0%)	24	46
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2694/2728 (99%)	2574 (96%)	114 (4%)	6 (0%)	43	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	76	ASP
1	C	123	GLU
2	D	451	GLY
2	B	157	VAL
4	F	68	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	367/364 (101%)	359 (98%)	8 (2%)	45	72
1	C	364/364 (100%)	357 (98%)	7 (2%)	50	75
2	B	415/417 (100%)	406 (98%)	9 (2%)	45	72
2	D	417/417 (100%)	406 (97%)	11 (3%)	40	68
3	E	186/190 (98%)	185 (100%)	1 (0%)	81	92
3	H	187/190 (98%)	182 (97%)	5 (3%)	39	67
4	F	188/188 (100%)	186 (99%)	2 (1%)	65	84
4	L	188/188 (100%)	187 (100%)	1 (0%)	81	92
All	All	2312/2318 (100%)	2268 (98%)	44 (2%)	50	75

All (44) 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	195	LEU
1	A	216	VAL
1	A	288	TYR
1	A	335	ARG
1	A	422	ARG
2	B	4	ILE
2	B	123	SER
2	B	126[A]	ASP
2	B	126[B]	ASP
2	B	171	GLU
2	B	180	MET
2	B	187	MET
2	B	215	ASN
2	B	417	LYS
1	C	23	LEU
1	C	166	TYR

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Mol	Chain	Res	Type
1	C	218	SER
1	C	252	GLU
1	C	288	TYR
1	C	317	ARG
1	C	406	VAL
2	D	123	SER
2	D	180	MET
2	D	181	LYS
2	D	202	ARG
2	D	215	ASN
2	D	235	LYS
2	D	312	GLU
2	D	365	GLU
2	D	430	THR
2	D	432	ASP
2	D	462	CYS
3	E	97	VAL
4	F	60	SER
4	F	181	LEU
3	H	7	SER
3	H	11	LEU
3	H	87	THR
3	H	154	GLU
3	H	213	ASP
4	L	54	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	215	HIS
1	A	372	ASN
1	A	444	GLN
2	B	141	GLN
2	B	272	GLN
2	B	305	ASN
1	C	134	GLN
1	C	158	ASN
1	C	333	GLN
2	D	141	GLN
2	D	210	GLN
2	D	438	GLN

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Mol	Chain	Res	Type
2	D	440	GLN
2	D	452	ASN
4	F	24	HIS
4	F	137	ASN
4	F	156	GLN
4	L	189	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.49	0	17,19,21	0.41	0
5	NAG	G	2	5	14,14,15	0.41	0	17,19,21	0.51	0
5	BMA	G	3	5	11,11,12	1.24	2 (18%)	15,15,17	0.92	1 (6%)
5	MAN	G	4	5	11,11,12	0.76	0	15,15,17	0.89	1 (6%)
5	MAN	G	5	5	11,11,12	1.15	1 (9%)	15,15,17	1.07	1 (6%)
6	NAG	I	1	6,2	14,14,15	0.36	0	17,19,21	0.45	0
6	NAG	I	2	6	14,14,15	0.50	0	17,19,21	0.41	0
7	NAG	J	1	2,7	14,14,15	0.51	0	17,19,21	0.52	0
7	NAG	J	2	7	14,14,15	0.42	0	17,19,21	0.38	0
7	BMA	J	3	7	11,11,12	0.88	0	15,15,17	0.84	1 (6%)
7	MAN	J	4	7	11,11,12	0.75	0	15,15,17	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	K	1	6,2	14,14,15	0.47	0	17,19,21	0.38	0
6	NAG	K	2	6	14,14,15	0.37	0	17,19,21	0.42	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. '2' 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	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	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	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	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	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	MAN	C1-C2	2.25	1.57	1.52
5	G	3	BMA	C2-C3	2.16	1.55	1.52
5	G	3	BMA	C4-C5	2.13	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	MAN	C1-C2-C3	2.92	113.90	109.64
7	J	4	MAN	O2-C2-C3	-2.28	105.44	110.15
5	G	4	MAN	O2-C2-C3	-2.25	105.48	110.15
5	G	3	BMA	C2-C3-C4	2.20	114.73	110.86
7	J	3	BMA	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

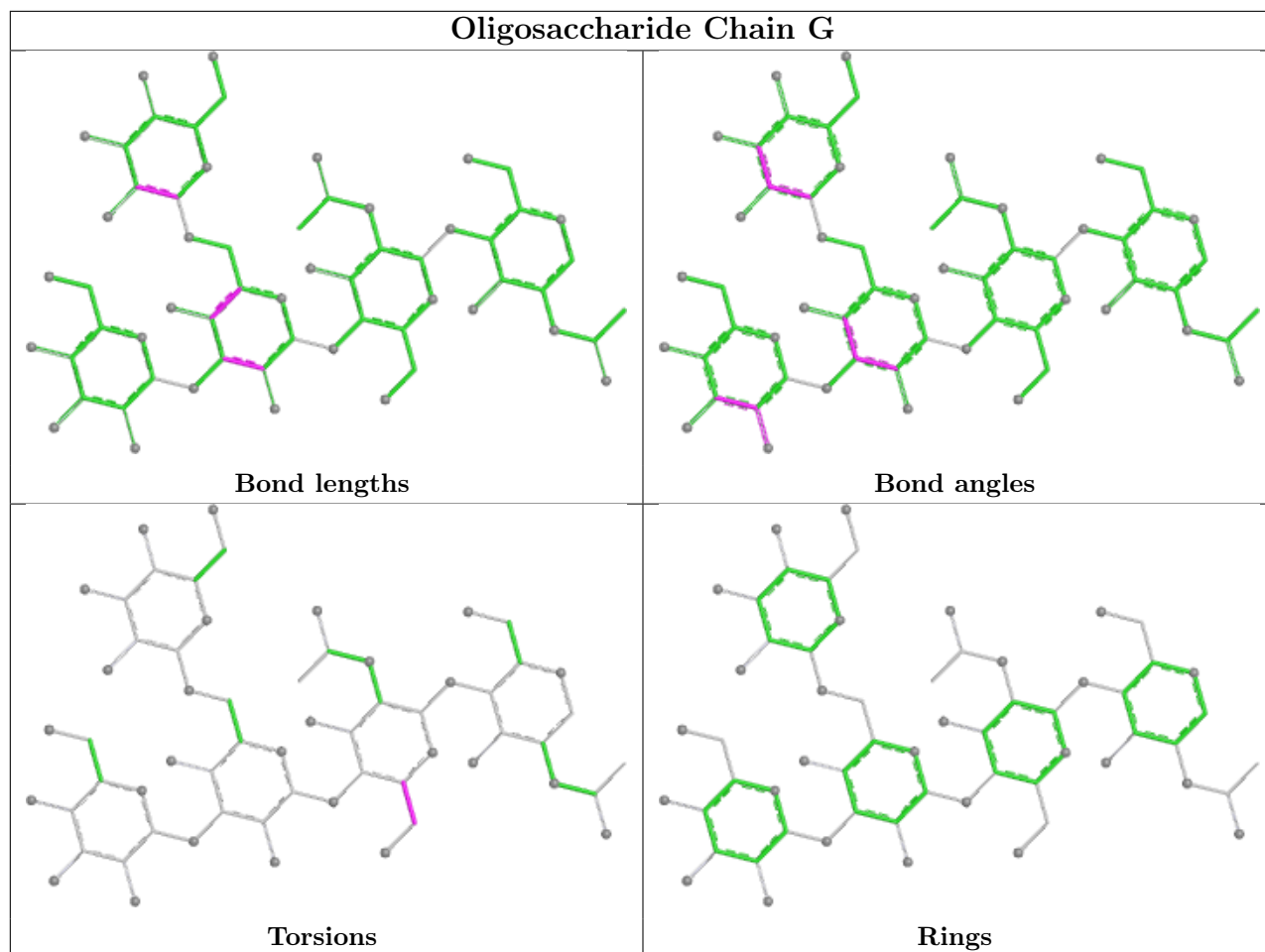
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6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

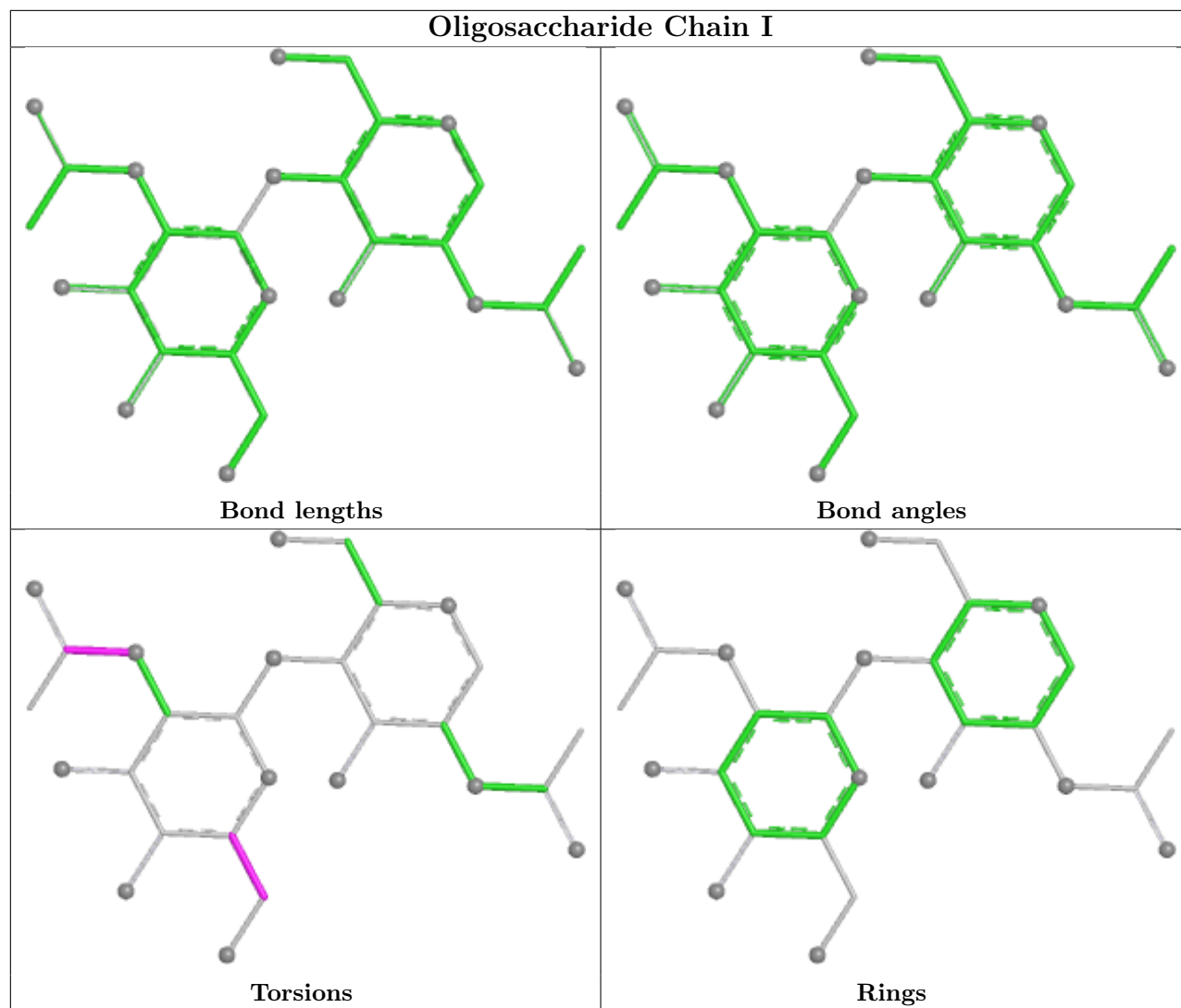
There are no ring outliers.

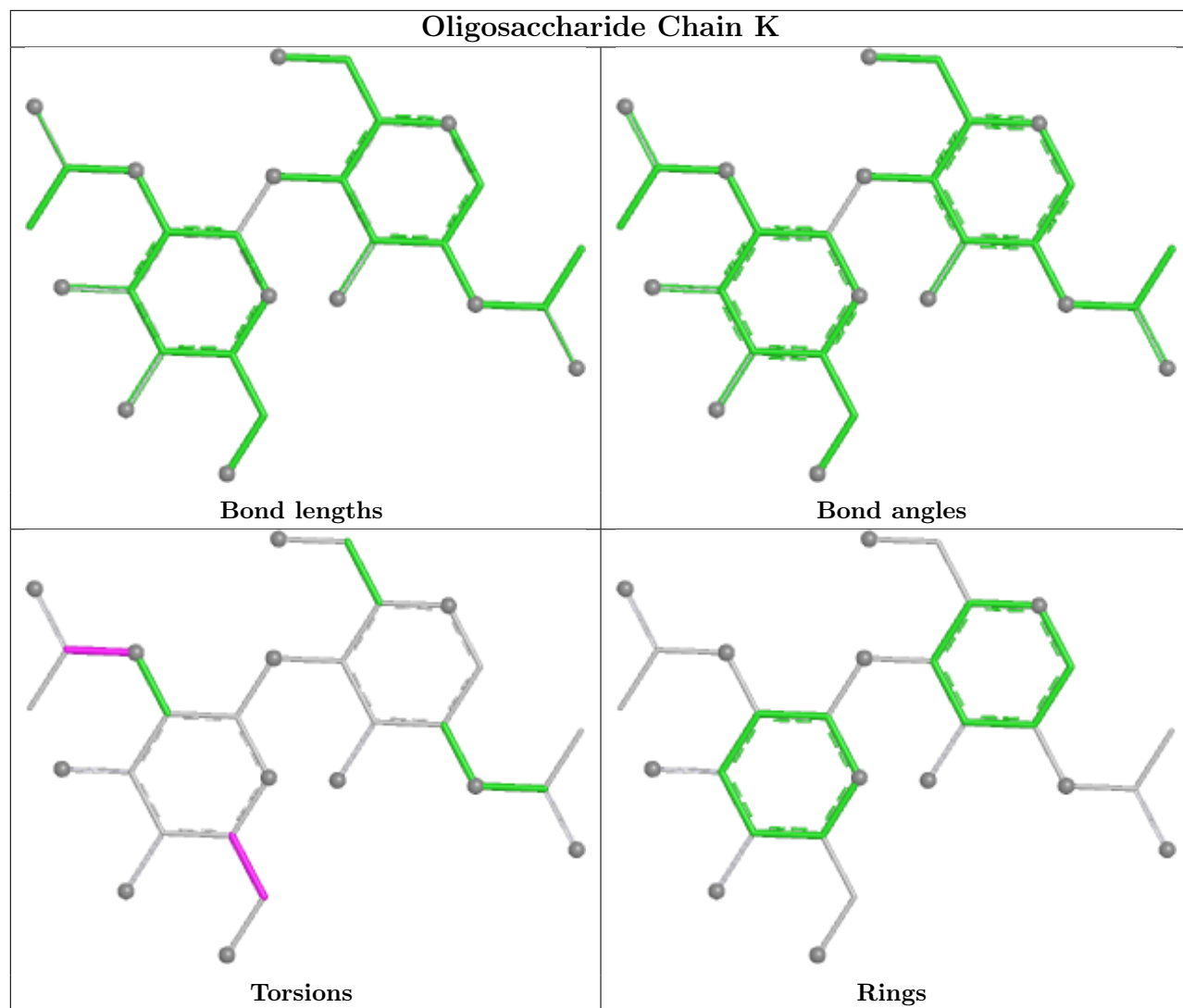
1 monomer is involved in 1 short contact:

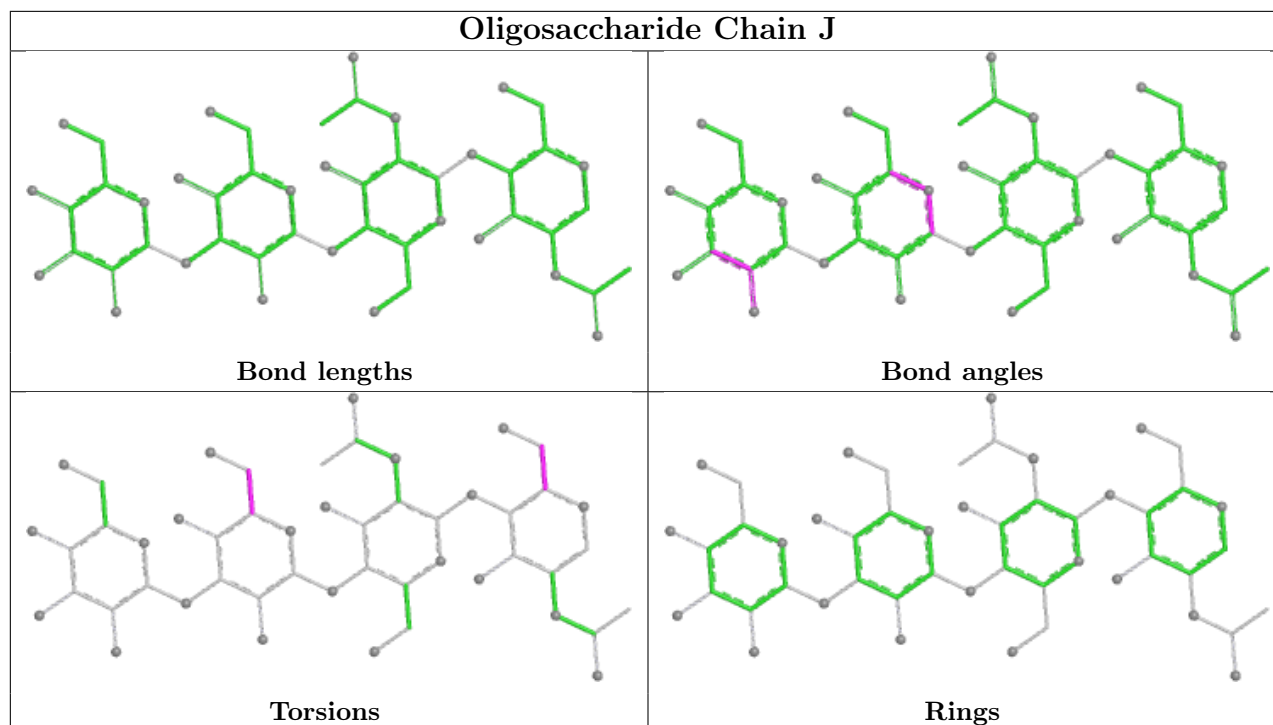
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 15 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	A	501	-	4,4,4	0.22	0	6,6,6	0.24	0
8	SO4	L	301	-	4,4,4	0.25	0	6,6,6	0.19	0
8	SO4	C	507	-	4,4,4	0.25	0	6,6,6	0.07	0
12	NAG	B	2004	2	14,14,15	0.33	0	17,19,21	0.54	0
8	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.16	0
12	NAG	D	2004	2	14,14,15	0.46	0	17,19,21	0.50	0
10	GOL	A	508	-	5,5,5	0.37	0	5,5,5	0.66	0
10	GOL	A	507	-	5,5,5	0.38	0	5,5,5	0.51	0
13	XQS	B	2005	11	28,28,28	3.10	10 (35%)	33,38,38	1.72	5 (15%)
8	SO4	A	506	-	4,4,4	0.26	0	6,6,6	0.48	0
13	XQS	D	2005	11	28,28,28	3.15	11 (39%)	33,38,38	1.61	4 (12%)

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	B	2004	2	-	2/6/23/26	0/1/1/1
12	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
10	GOL	A	508	-	-	4/4/4/4	-
10	GOL	A	507	-	-	0/4/4/4	-
13	XQS	B	2005	11	-	2/25/35/35	0/2/2/2
13	XQS	D	2005	11	-	3/25/35/35	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	2005	XQS	C22-C21	8.03	1.51	1.39
13	D	2005	XQS	C25-C23	7.97	1.51	1.38
13	D	2005	XQS	C24-C26	7.94	1.51	1.39
13	B	2005	XQS	C25-C23	7.81	1.51	1.38
13	B	2005	XQS	C22-C21	7.73	1.51	1.39
13	B	2005	XQS	C24-C26	7.61	1.50	1.39
13	D	2005	XQS	C15-N06	4.91	1.42	1.35
13	B	2005	XQS	C15-N06	4.56	1.41	1.35
13	D	2005	XQS	C19-N07	3.59	1.42	1.34
13	B	2005	XQS	C19-N07	3.49	1.42	1.34
13	B	2005	XQS	C23-C21	-2.97	1.34	1.39
13	B	2005	XQS	C25-C26	-2.95	1.34	1.39
13	D	2005	XQS	C23-C21	-2.87	1.35	1.39
13	D	2005	XQS	C25-C26	-2.82	1.35	1.39
13	B	2005	XQS	C24-C22	-2.77	1.34	1.38
13	B	2005	XQS	C14-N06	-2.41	1.42	1.47
13	D	2005	XQS	C14-N06	-2.40	1.42	1.47
13	D	2005	XQS	C24-C22	-2.39	1.34	1.38
13	B	2005	XQS	C13-N06	-2.21	1.43	1.47
13	D	2005	XQS	C26-C27	2.20	1.51	1.47
13	D	2005	XQS	C13-N06	-2.18	1.43	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	2005	XQS	C14-N06-C13	5.44	123.78	112.68
13	D	2005	XQS	C14-N06-C13	4.97	122.82	112.68
13	B	2005	XQS	C14-C12-C10	-4.11	105.88	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	2005	XQS	C11-C13-N06	4.09	118.68	110.66
13	B	2005	XQS	C11-C13-N06	3.64	117.79	110.66
13	D	2005	XQS	C14-C12-C10	-3.33	106.72	110.32
13	B	2005	XQS	C13-C11-C10	-2.94	107.14	110.32
13	B	2005	XQS	C12-C14-N06	2.92	116.39	110.66
13	D	2005	XQS	C12-C14-N06	2.90	116.35	110.66

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	508	GOL	C1-C2-C3-O3
10	A	508	GOL	O2-C2-C3-O3
13	B	2005	XQS	C24-C26-C27-N08
13	D	2005	XQS	C24-C26-C27-N08
10	A	508	GOL	O1-C1-C2-C3
13	D	2005	XQS	C11-C10-O01-C17
13	B	2005	XQS	C25-C26-C27-N08
13	D	2005	XQS	C25-C26-C27-N08
10	A	508	GOL	O1-C1-C2-O2
12	B	2004	NAG	C4-C5-C6-O6
12	B	2004	NAG	O5-C5-C6-O6

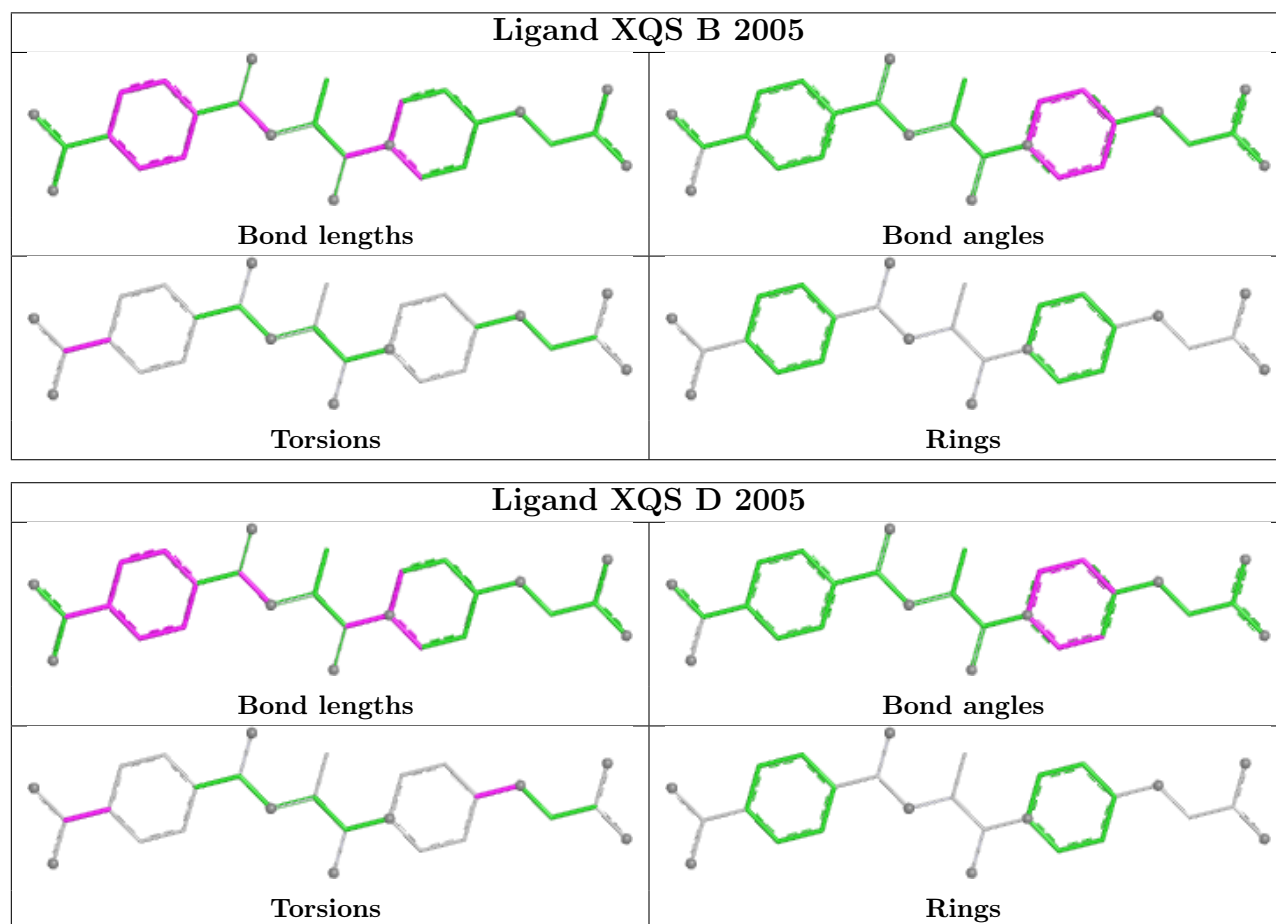
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	508	GOL	1	0
10	A	507	GOL	1	0
13	B	2005	XQS	1	0
13	D	2005	XQS	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 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%)	-0.26	7 (1%) 72 68	21, 35, 52, 72	5 (1%)
1	C	453/457 (99%)	0.05	5 (1%) 78 74	21, 49, 69, 91	3 (0%)
2	B	466/472 (98%)	0.37	21 (4%) 38 32	20, 57, 120, 136	4 (0%)
2	D	471/472 (99%)	0.54	26 (5%) 30 25	24, 67, 111, 128	2 (0%)
3	E	214/221 (96%)	1.45	51 (23%) 2 1	67, 112, 153, 163	0
3	H	216/221 (97%)	0.90	19 (8%) 15 12	47, 84, 118, 126	0
4	F	214/214 (100%)	1.30	48 (22%) 2 2	69, 111, 156, 175	0
4	L	214/214 (100%)	0.50	8 (3%) 45 39	51, 74, 89, 115	0
All	All	2702/2728 (99%)	0.45	185 (6%) 23 19	20, 63, 133, 175	14 (0%)

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	165	LEU	5.2
2	D	471	CYS	5.1
2	D	375	LEU	5.0
3	E	147	LEU	4.9
4	F	130	ALA	4.7
1	A	454	VAL	4.4
2	B	33	LEU	4.4
3	E	212	VAL	4.4
3	E	176	LEU	4.2
4	F	125	LEU	4.1
2	D	2	PRO	4.0
4	F	180	THR	4.0
4	F	126	THR	3.7
2	B	129	TRP	3.7
1	A	217	SER	3.7
4	F	193	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	466	TRP	3.5
1	A	46	SER	3.5
2	D	469	SER	3.5
4	F	181	LEU	3.5
3	H	198	SER	3.5
2	B	77	SER	3.4
3	E	201	CYS	3.4
1	C	453	VAL	3.4
3	E	203	VAL	3.4
4	F	136	LEU	3.4
3	E	216	ILE	3.3
2	B	466	TRP	3.3
4	F	152	GLY	3.3
2	B	74	SER	3.2
4	F	131	SER	3.2
3	E	149	LYS	3.2
3	E	214	LYS	3.2
2	D	468	GLY	3.2
4	F	135	PHE	3.2
4	F	134	CYS	3.2
3	E	194	TRP	3.2
4	F	150	ILE	3.2
4	L	145	ASN	3.1
1	C	217	SER	3.1
4	F	160	LEU	3.1
3	H	189	VAL	3.1
4	F	209	PHE	3.1
2	B	4	ILE	3.0
1	C	1	LEU	3.0
2	D	376	ASN	3.0
4	L	157	ASN	3.0
3	E	144	LEU	3.0
3	E	142	VAL	3.0
3	E	189	VAL	3.0
2	D	33	LEU	3.0
4	F	179	LEU	3.0
4	F	204	PRO	3.0
1	C	47	GLN	2.9
4	F	115	VAL	2.9
4	F	132	VAL	2.9
3	E	134	CYS	2.9
4	F	133	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	H	177	GLN	2.9
3	E	199	ILE	2.9
4	F	182	THR	2.9
2	B	375	LEU	2.9
4	F	205	ILE	2.8
3	H	134	CYS	2.8
4	F	194	CYS	2.8
2	D	467	LEU	2.8
3	H	192	SER	2.8
3	H	196	SER	2.8
4	F	186	TYR	2.8
4	F	202	THR	2.8
4	F	163	TRP	2.8
2	D	446	HIS	2.7
3	E	128	TYR	2.7
2	B	181	LYS	2.7
4	F	178	THR	2.7
4	F	159	VAL	2.7
4	F	199	LYS	2.7
2	D	178	TYR	2.7
4	F	203	SER	2.7
2	B	458	GLY	2.6
4	F	195	GLU	2.6
4	F	157	ASN	2.6
3	E	182	THR	2.6
1	A	319	ASP	2.6
3	E	11	LEU	2.6
2	D	374	CYS	2.6
3	E	127	VAL	2.6
3	E	129	PRO	2.6
3	E	161	ASN	2.6
4	L	7	SER	2.6
2	B	76	ASP	2.5
2	D	378	GLU	2.5
3	H	166	SER	2.5
3	H	206	PRO	2.5
3	H	203	VAL	2.5
2	B	452	ASN	2.5
3	E	164	SER	2.5
2	D	380	ILE	2.5
4	F	192	TYR	2.5
2	B	46	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	451	GLY	2.5
3	E	153	PRO	2.5
3	E	195	PRO	2.5
2	D	143	ARG	2.4
3	E	175	VAL	2.4
2	B	378	GLU	2.4
3	E	215	LYS	2.4
4	F	169	LYS	2.4
3	E	148	VAL	2.4
3	H	133	VAL	2.4
2	D	1	GLY	2.4
3	E	204	ALA	2.4
4	F	197	THR	2.4
3	E	140	SER	2.4
3	H	178	SER	2.4
2	B	2	PRO	2.4
2	B	446	HIS	2.3
3	E	206	PRO	2.3
1	A	339	ALA	2.3
4	F	117	ILE	2.3
4	L	191	SER	2.3
4	F	148	TRP	2.3
2	D	452	ASN	2.3
3	E	163	GLY	2.3
3	E	167	SER	2.3
3	E	210	THR	2.2
4	F	212	ASN	2.2
4	L	212	ASN	2.2
2	D	8	ARG	2.2
3	E	168	GLY	2.2
3	E	158	LEU	2.2
2	D	312	GLU	2.2
3	E	184	SER	2.2
1	C	216	VAL	2.2
3	E	156	VAL	2.2
3	E	174	ALA	2.2
4	F	114	THR	2.2
3	E	166	SER	2.2
2	D	129	TRP	2.2
4	F	188	ARG	2.2
2	D	79	GLN	2.2
3	E	121	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	198	SER	2.2
3	H	142	VAL	2.2
4	F	213	GLU	2.1
2	D	145	LEU	2.1
3	E	115	VAL	2.1
3	E	133	VAL	2.1
4	L	81	GLU	2.1
3	E	74	THR	2.1
2	B	32	PRO	2.1
4	F	147	LYS	2.1
3	H	5	GLN	2.1
4	L	214	CYS	2.1
3	E	180	LEU	2.1
3	H	176	LEU	2.1
2	B	75	GLY	2.1
4	F	158	GLY	2.1
3	H	141	SER	2.1
4	F	153	SER	2.1
3	E	219	ARG	2.1
3	H	138	THR	2.1
1	A	47	GLN	2.1
4	L	45	MET	2.1
2	B	5	CYS	2.1
3	H	212	VAL	2.1
4	F	116	SER	2.1
3	E	4	LEU	2.1
4	F	210	ASN	2.1
3	E	51	ILE	2.1
4	F	146	VAL	2.1
4	F	206	VAL	2.1
2	B	67	ARG	2.0
2	B	432	ASP	2.0
2	D	77	SER	2.0
4	F	149	LYS	2.0
3	E	193	THR	2.0
3	H	195	PRO	2.0
3	E	145	GLY	2.0
3	H	168	GLY	2.0
2	D	72	LYS	2.0
3	E	120	ALA	2.0
1	A	45	PRO	2.0
2	D	4	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	75	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

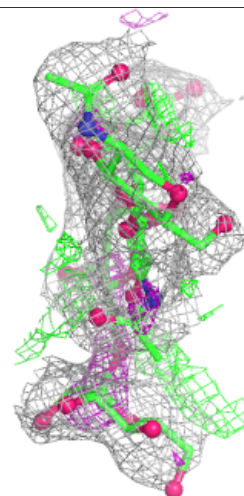
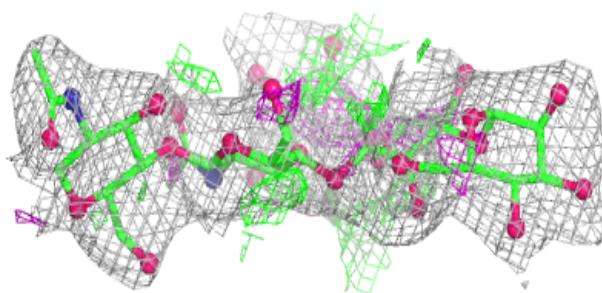
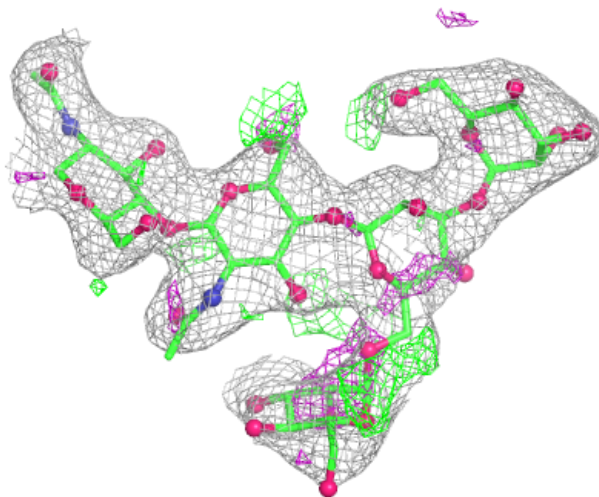
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

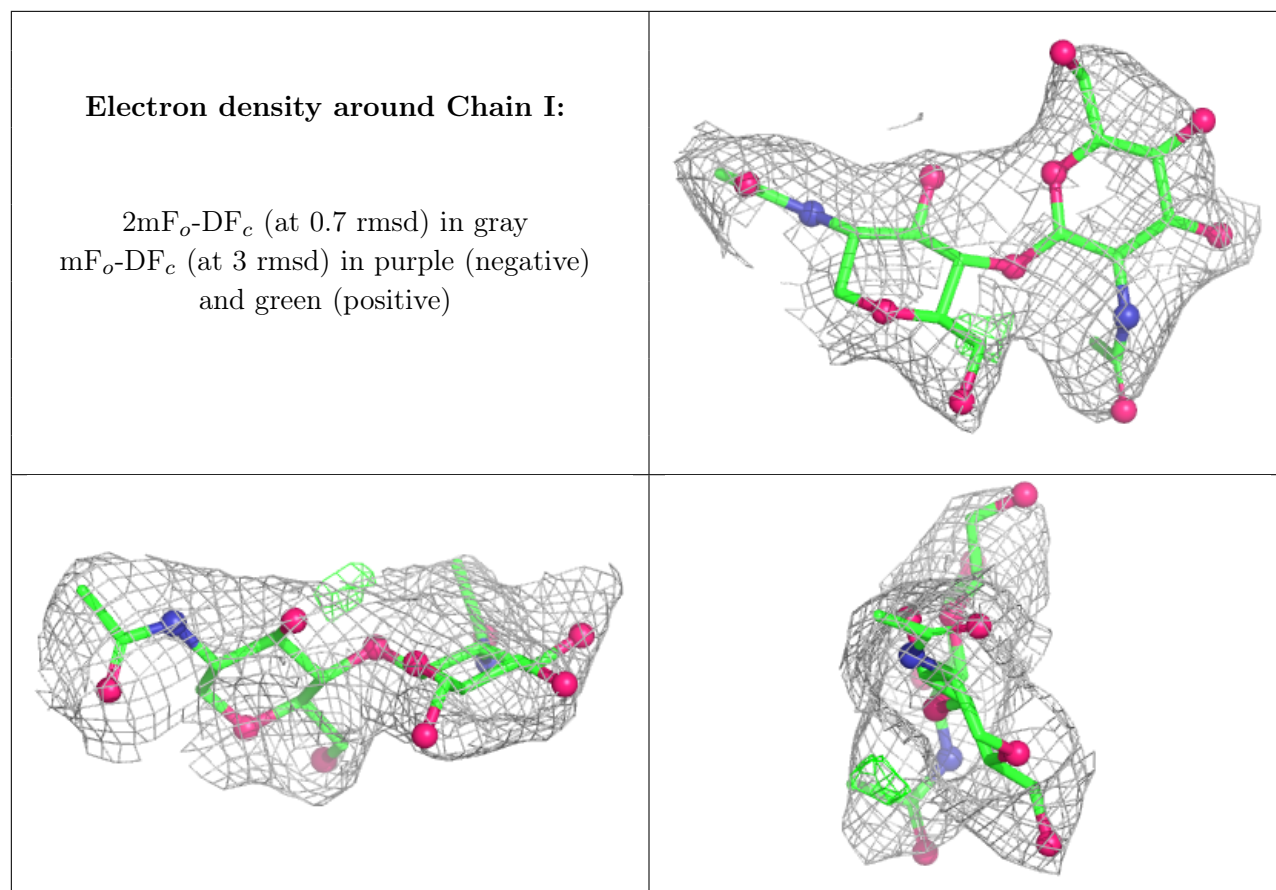
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	46,46,46,46	0
5	NAG	G	2	14/15	-	-	59,59,59,59	0
5	BMA	G	3	11/12	-	-	68,68,68,68	0
5	MAN	G	4	11/12	-	-	65,65,65,65	0
5	MAN	G	5	11/12	-	-	72,72,72,72	0
7	NAG	J	2	14/15	0.64	0.15	66,66,66,66	0
6	NAG	K	2	14/15	0.78	0.13	89,89,89,89	0
6	NAG	I	2	14/15	0.79	0.14	87,87,87,87	0
7	NAG	J	1	14/15	0.81	0.11	57,57,57,57	0
6	NAG	K	1	14/15	0.90	0.09	85,85,85,85	0
6	NAG	I	1	14/15	0.91	0.10	84,84,84,84	0
7	BMA	J	3	11/12	-	-	73,73,73,73	0
7	MAN	J	4	11/12	-	-	74,74,74,74	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:

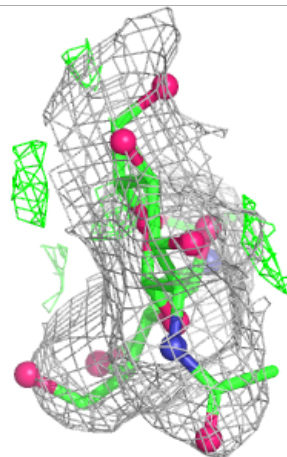
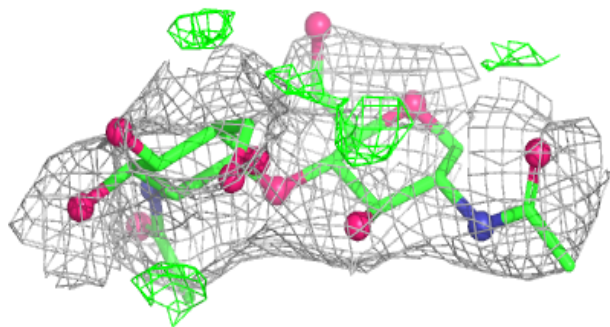
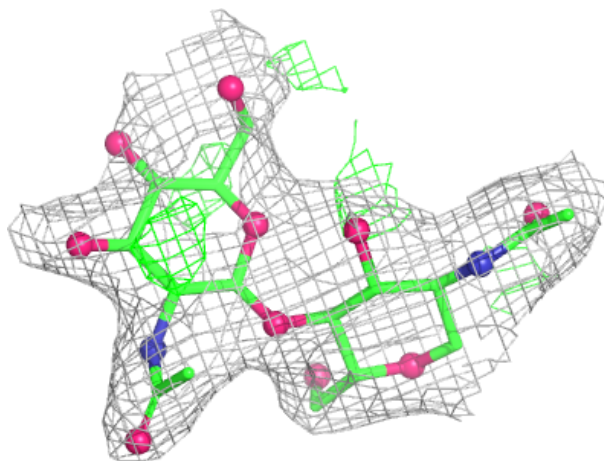
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

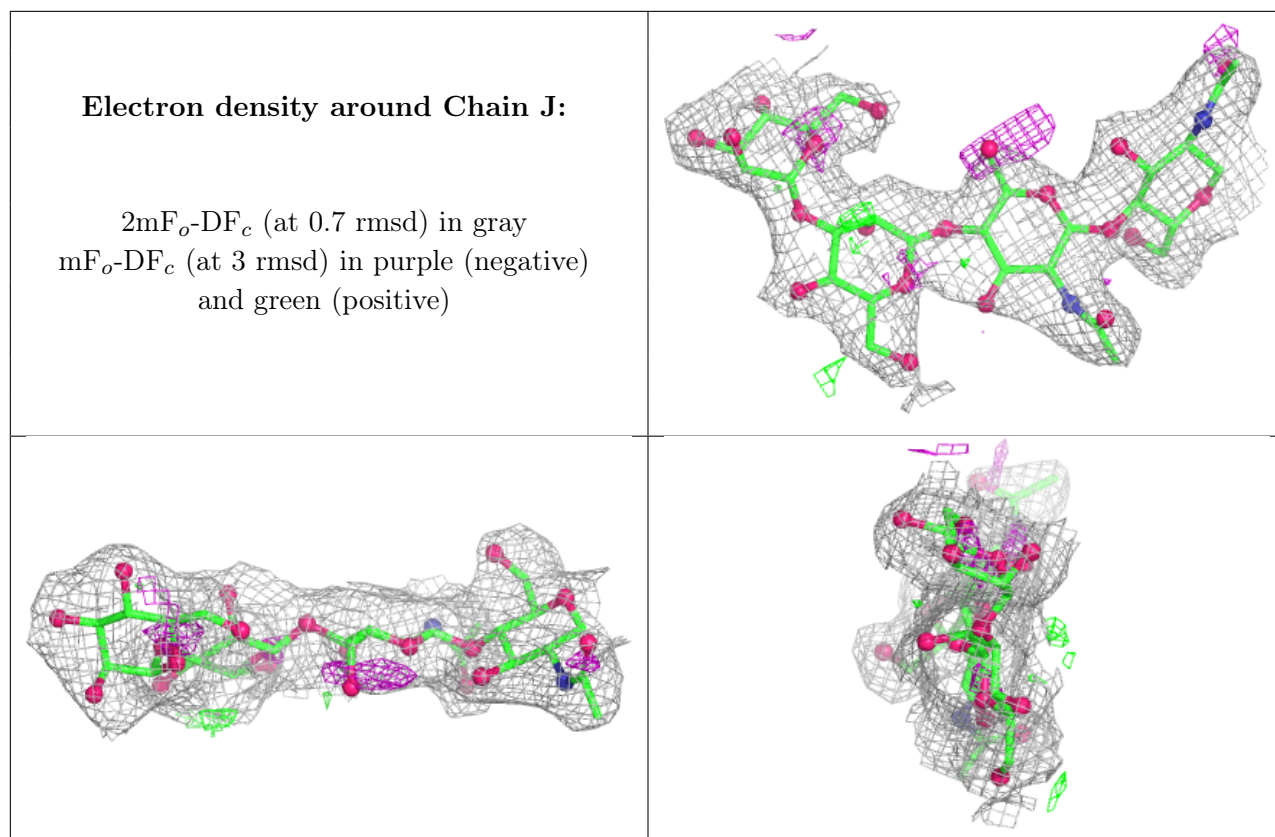




Electron density around Chain K:

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





6.4 Ligands [i](#)

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

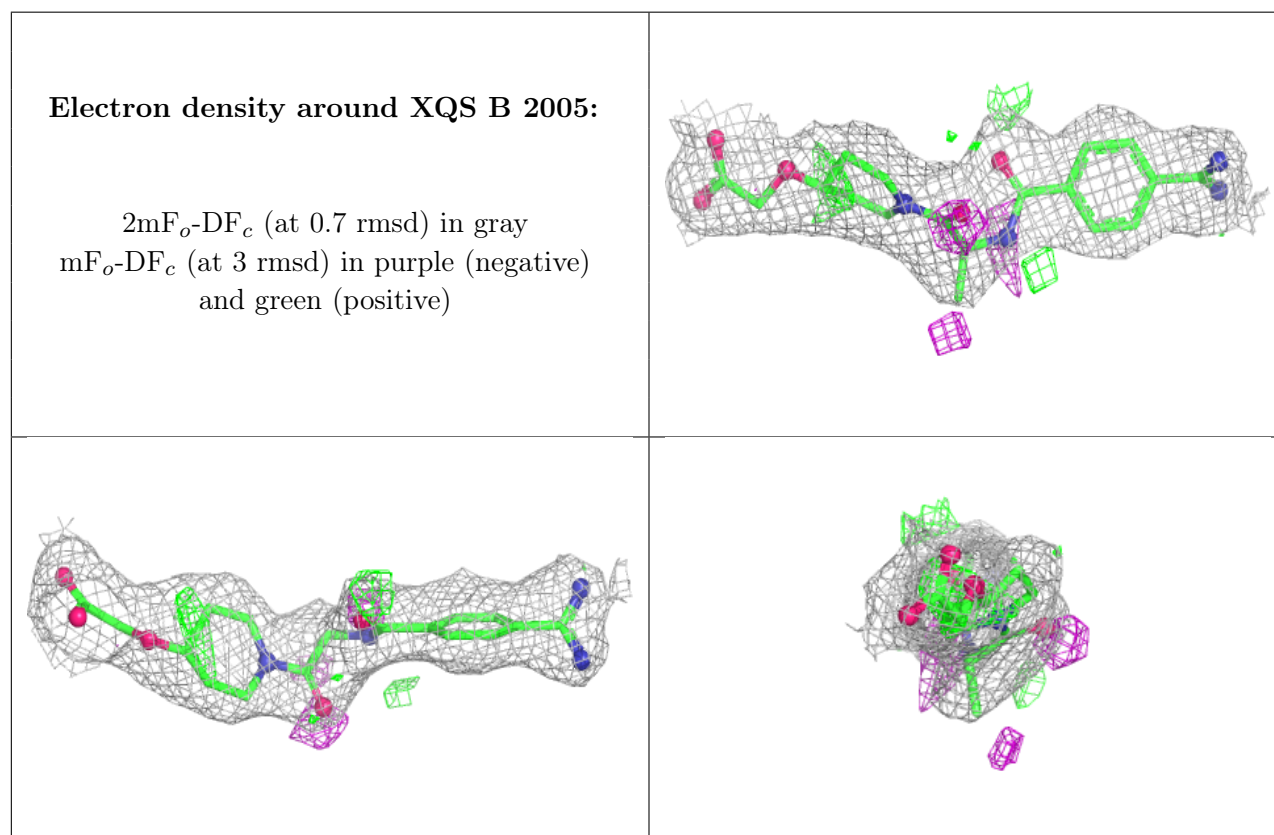
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	NAG	B	2004	14/15	0.69	0.15	86,86,86,86	0
12	NAG	D	2004	14/15	0.72	0.15	81,81,81,81	0
11	MN	B	2002	1/1	0.79	0.35	66,66,66,66	0
10	GOL	A	508	6/6	0.81	0.14	39,39,39,39	0
8	SO4	C	507	5/5	0.83	0.21	73,73,73,73	0
10	GOL	A	507	6/6	0.87	0.14	35,35,35,35	0
8	SO4	L	301	5/5	0.89	0.22	70,70,70,70	0
8	SO4	A	506	5/5	0.89	0.20	58,58,58,58	0
13	XQS	B	2005	27/27	0.90	0.11	33,33,33,33	0
8	SO4	A	501	5/5	0.91	0.13	49,49,49,49	0
8	SO4	C	501	5/5	0.91	0.16	69,69,69,69	0
13	XQS	D	2005	27/27	0.91	0.11	48,48,48,48	0
11	MN	D	2002	1/1	0.95	0.16	65,65,65,65	0
14	CL	C	502	1/1	0.97	0.05	53,53,53,53	0

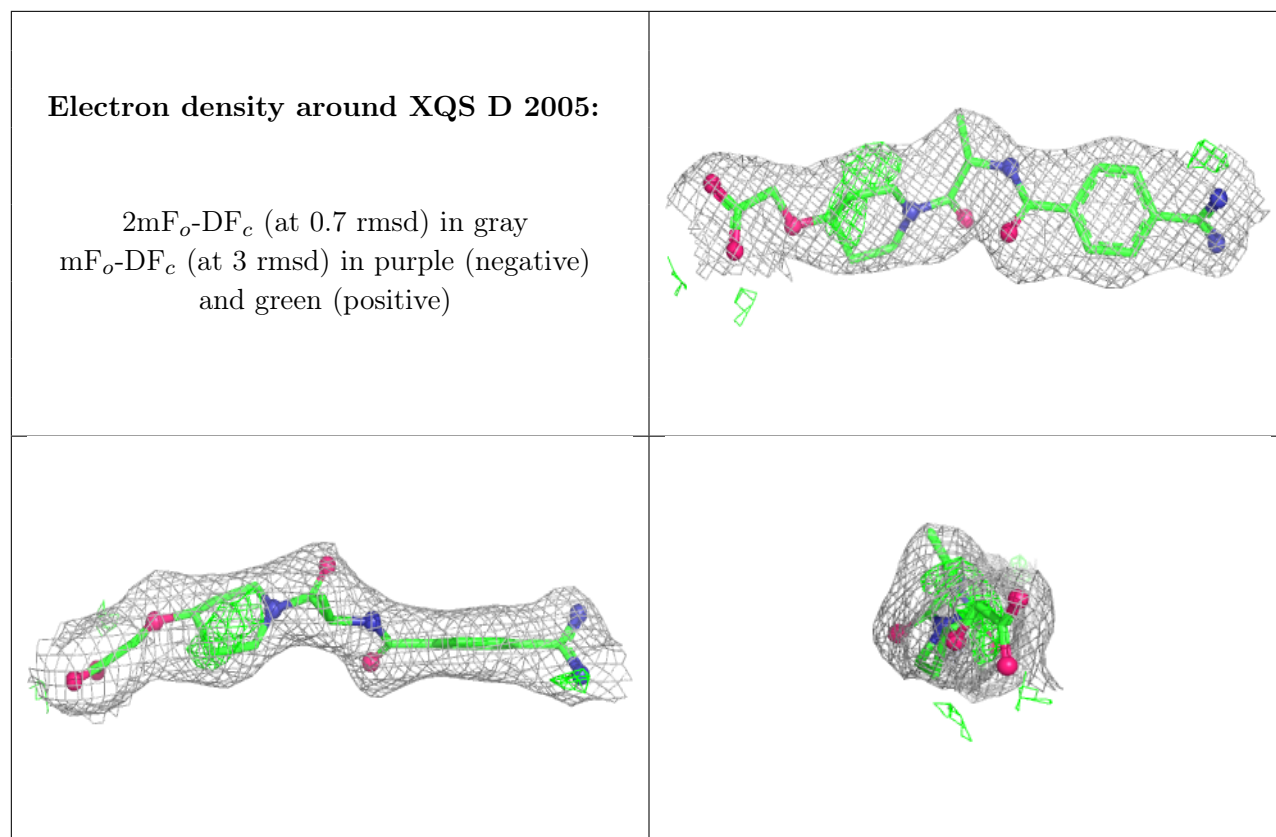
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CA	C	505	1/1	0.98	0.04	50,50,50,50	0
9	CA	A	502	1/1	0.98	0.03	44,44,44,44	0
9	CA	A	504	1/1	0.98	0.05	31,31,31,31	0
9	CA	C	503	1/1	0.98	0.04	67,67,67,67	0
9	CA	C	504	1/1	0.98	0.05	55,55,55,55	0
11	MN	D	2003	1/1	0.99	0.07	45,45,45,45	0
9	CA	A	503	1/1	0.99	0.06	33,33,33,33	0
9	CA	C	506	1/1	0.99	0.02	49,49,49,49	0
11	MN	B	2003	1/1	0.99	0.07	32,32,32,32	0
11	MN	D	2001	1/1	0.99	0.04	44,44,44,44	0
9	CA	A	505	1/1	0.99	0.02	31,31,31,31	0
11	MN	B	2001	1/1	1.00	0.04	29,29,29,29	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.