



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 6BNL / pdb_00006bnl
Title : Crystal structure of TCR-MHC-like molecule
Authors : Le Nours, J.; Rossjohn, J.
Deposited on : 2017-11-16
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

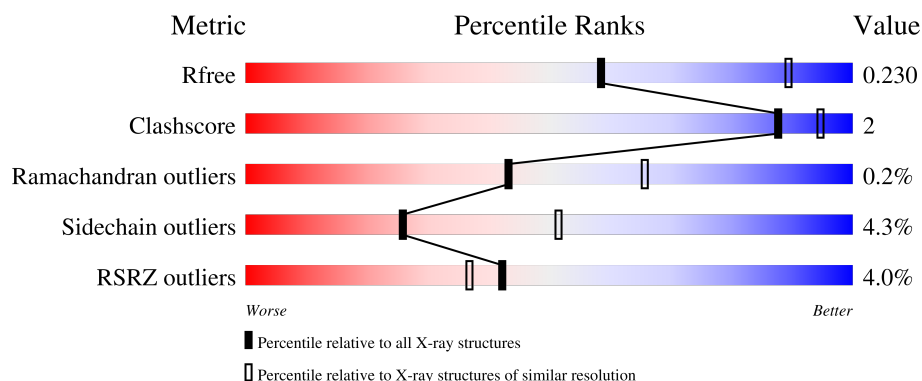
1 Overall quality at a glance

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	302	4% 75% 10% 16%
1	E	302	5% 75% 10% 14%
2	B	99	5% 79% 15% ...
2	F	99	19% 84% 10% 6%
3	C	207	2% 90% 7% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	207	% 88% 9% .
4	D	242	2% 90% 8% .
4	H	242	91% 8% .
5	I	2	50% 50%
5	J	2	50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12603 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1972	1263	330	366	13			
1	E	260	Total	C	N	O	S	0	1	0
			2011	1292	333	372	14			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	GLY	-	expression tag	UNP A0A0R4J090
A	281	SER	-	expression tag	UNP A0A0R4J090
A	282	LEU	-	expression tag	UNP A0A0R4J090
A	283	HIS	-	expression tag	UNP A0A0R4J090
A	284	HIS	-	expression tag	UNP A0A0R4J090
A	285	ILE	-	expression tag	UNP A0A0R4J090
A	286	LEU	-	expression tag	UNP A0A0R4J090
A	287	ASP	-	expression tag	UNP A0A0R4J090
A	288	ALA	-	expression tag	UNP A0A0R4J090
A	289	GLN	-	expression tag	UNP A0A0R4J090
A	290	LYS	-	expression tag	UNP A0A0R4J090
A	291	MET	-	expression tag	UNP A0A0R4J090
A	292	VAL	-	expression tag	UNP A0A0R4J090
A	293	TRP	-	expression tag	UNP A0A0R4J090
A	294	ASN	-	expression tag	UNP A0A0R4J090
A	295	HIS	-	expression tag	UNP A0A0R4J090
A	296	ARG	-	expression tag	UNP A0A0R4J090
A	297	HIS	-	expression tag	UNP A0A0R4J090
A	298	HIS	-	expression tag	UNP A0A0R4J090
A	299	HIS	-	expression tag	UNP A0A0R4J090
A	300	HIS	-	expression tag	UNP A0A0R4J090
A	301	HIS	-	expression tag	UNP A0A0R4J090
A	302	HIS	-	expression tag	UNP A0A0R4J090
E	280	GLY	-	expression tag	UNP A0A0R4J090
E	281	SER	-	expression tag	UNP A0A0R4J090

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	282	LEU	-	expression tag	UNP A0A0R4J090
E	283	HIS	-	expression tag	UNP A0A0R4J090
E	284	HIS	-	expression tag	UNP A0A0R4J090
E	285	ILE	-	expression tag	UNP A0A0R4J090
E	286	LEU	-	expression tag	UNP A0A0R4J090
E	287	ASP	-	expression tag	UNP A0A0R4J090
E	288	ALA	-	expression tag	UNP A0A0R4J090
E	289	GLN	-	expression tag	UNP A0A0R4J090
E	290	LYS	-	expression tag	UNP A0A0R4J090
E	291	MET	-	expression tag	UNP A0A0R4J090
E	292	VAL	-	expression tag	UNP A0A0R4J090
E	293	TRP	-	expression tag	UNP A0A0R4J090
E	294	ASN	-	expression tag	UNP A0A0R4J090
E	295	HIS	-	expression tag	UNP A0A0R4J090
E	296	ARG	-	expression tag	UNP A0A0R4J090
E	297	HIS	-	expression tag	UNP A0A0R4J090
E	298	HIS	-	expression tag	UNP A0A0R4J090
E	299	HIS	-	expression tag	UNP A0A0R4J090
E	300	HIS	-	expression tag	UNP A0A0R4J090
E	301	HIS	-	expression tag	UNP A0A0R4J090
E	302	HIS	-	expression tag	UNP A0A0R4J090

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			739	474	123	136	6			
2	F	93	Total	C	N	O	S	0	0	0
			669	427	116	120	6			

- Molecule 3 is a protein called NKT Valpha14 (MOUSE) - 2C12 TCR - Hybrid mouse variable and human constant domains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	202	Total	C	N	O	S	0	2	0
			1545	958	263	317	7			
3	G	203	Total	C	N	O	S	0	1	0
			1540	955	262	316	7			

- Molecule 4 is a protein called NKT Vbeta8.2 (MOUSE) - 2C12 TCR - hybrid mouse variable and human constant domains.

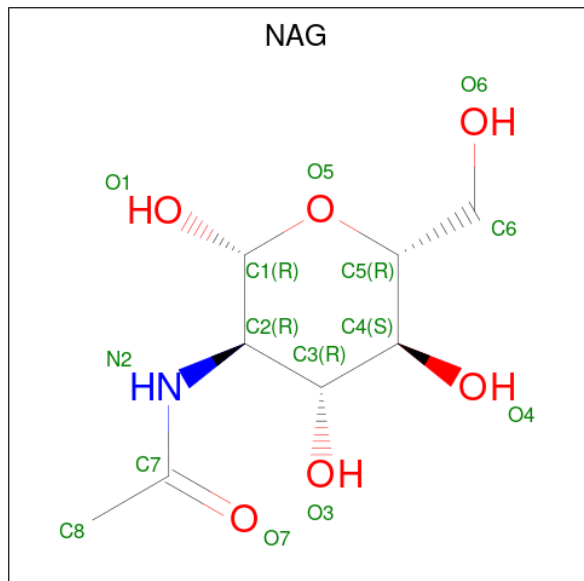
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	240	Total	C	N	O	S	0	0	0
			1853	1167	324	356	6			
4	H	240	Total	C	N	O	S	0	0	0
			1852	1167	325	354	6			

- Molecule 5 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
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



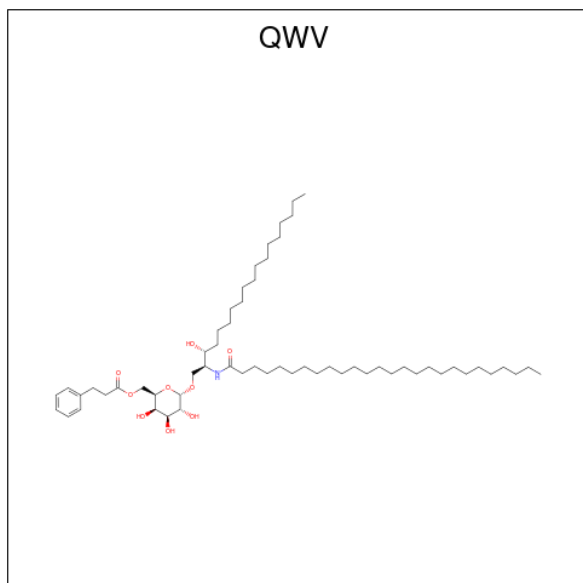
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is N-[(2S,3R)-3-hydroxy-1-{[6-O-(3-phenylpropanoyl)-alpha-D-galactopyranosyl]oxy}octadecan-2-yl]hexacosanamide (CCD ID: QWV) (formula: C₅₉H₁₀₇NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			69	59	1	9		
7	E	1	Total	C	N	O	0	0
			69	59	1	9		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	36	Total	O	0	0
			36	36		
8	B	7	Total	O	0	0
			7	7		
8	C	30	Total	O	0	0
			30	30		
8	D	26	Total	O	0	0
			26	26		
8	E	17	Total	O	0	0
			17	17		

Continued on next page...

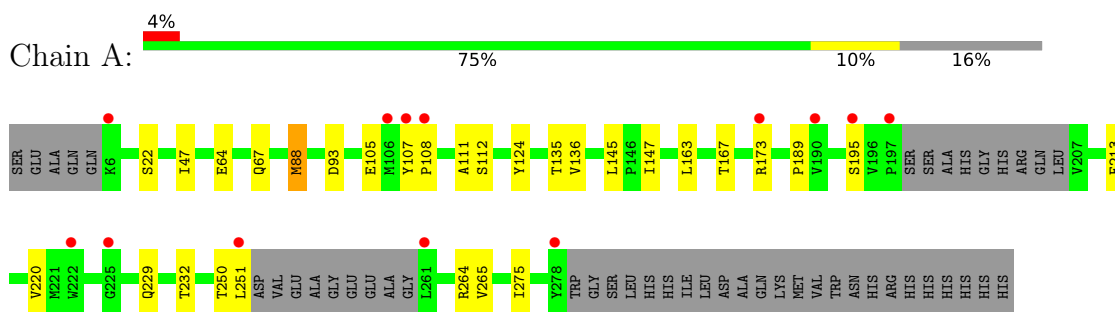
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	28	Total 28	O 28	0	0
8	H	28	Total 28	O 28	0	0

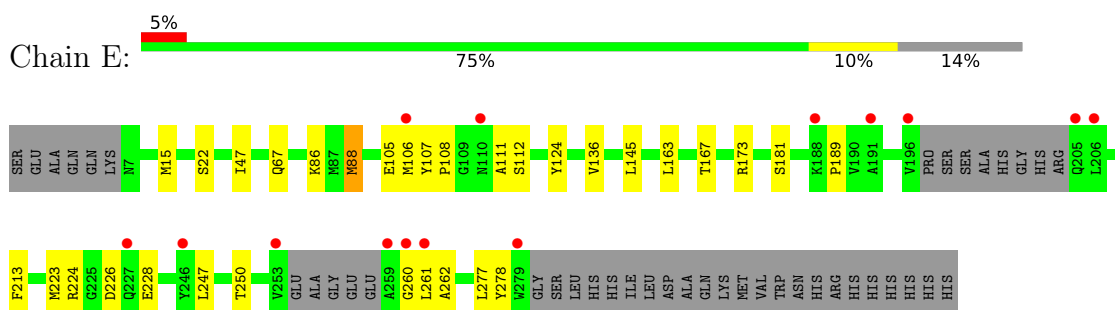
3 Residue-property plots [i](#)

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.

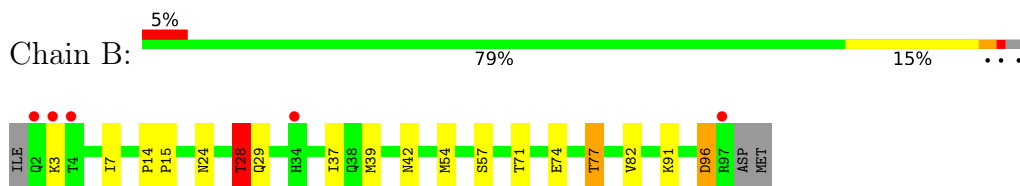
- Molecule 1: Antigen-presenting glycoprotein CD1d1



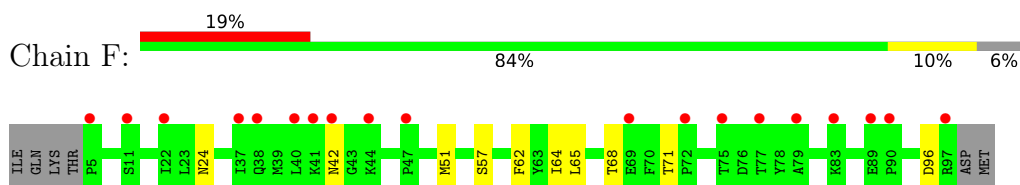
- Molecule 1: Antigen-presenting glycoprotein CD1d1



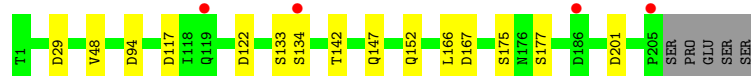
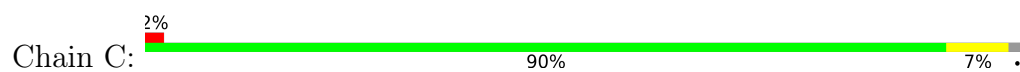
- Molecule 2: Beta-2-microglobulin



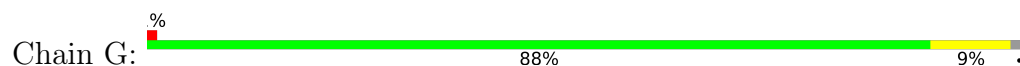
- Molecule 2: Beta-2-microglobulin



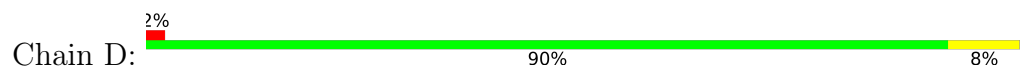
- Molecule 3: NKT Valpha14 (MOUSE) - 2C12 TCR - Hybrid mouse variable and human constant domains



- Molecule 3: NKT Valpha14 (MOUSE) - 2C12 TCR - Hybrid mouse variable and human constant domains



- Molecule 4: NKT Vbeta8.2 (MOUSE) - 2C12 TCR - hybrid mouse variable and human constant domains



- Molecule 4: NKT Vbeta8.2 (MOUSE) - 2C12 TCR - hybrid mouse variable and human constant domains



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.67Å 150.32Å 100.14Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	38.07 – 2.60 38.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.07-2.60) 99.8 (38.07-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.181 , 0.214 0.192 , 0.230	Depositor DCC
R_{free} test set	3637 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12603	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, QWV

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	0.84	1/2030 (0.0%)	1.18	4/2773 (0.1%)
1	E	0.84	1/2073 (0.0%)	1.21	2/2834 (0.1%)
2	B	0.94	1/765 (0.1%)	1.19	5/1052 (0.5%)
2	F	0.91	0/693	1.15	0/955
3	C	0.87	0/1579	1.24	8/2152 (0.4%)
3	G	0.93	0/1571	1.27	10/2141 (0.5%)
4	D	0.79	0/1905	1.12	5/2603 (0.2%)
4	H	0.78	0/1904	1.13	5/2601 (0.2%)
All	All	0.85	3/12520 (0.0%)	1.19	39/17111 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39	MET	SD-CE	-7.76	1.60	1.79
1	E	88	MET	SD-CE	-7.75	1.60	1.79
1	A	88	MET	SD-CE	-6.85	1.62	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	29	ASP	CA-CB-CG	7.18	119.78	112.60
4	D	96	ASP	CA-CB-CG	7.05	119.65	112.60
4	D	30	ASN	CA-CB-CG	6.71	119.31	112.60
3	G	186	ASP	CA-CB-CG	6.62	119.22	112.60
3	C	167	ASP	CA-CB-CG	6.58	119.18	112.60
4	H	30	ASN	CA-CB-CG	6.45	119.05	112.60
3	G	167	ASP	CA-CB-CG	6.40	119.00	112.60
3	G	134	SER	CA-C-N	6.38	128.82	120.28
3	G	134	SER	C-N-CA	6.38	128.82	120.28
3	C	133	SER	CA-C-N	6.29	133.56	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	133	SER	C-N-CA	6.29	133.56	121.54
2	B	24	ASN	CA-CB-CG	6.28	118.88	112.60
4	H	10	ASN	CA-CB-CG	6.17	118.77	112.60
4	H	96	ASP	CA-CB-CG	6.03	118.63	112.60
3	C	94	ASP	CA-CB-CG	5.91	118.51	112.60
3	C	29	ASP	CA-CB-CG	5.84	118.44	112.60
2	B	28	THR	N-CA-CB	-5.62	102.52	111.62
2	B	96	ASP	CA-CB-CG	5.53	118.13	112.60
1	E	86	LYS	CA-C-N	5.34	127.44	120.28
1	E	86	LYS	C-N-CA	5.34	127.44	120.28
4	H	156	ASP	CA-CB-CG	5.33	117.93	112.60
3	G	142	THR	CA-C-N	5.28	130.06	122.40
3	G	142	THR	C-N-CA	5.28	130.06	122.40
3	G	130	ASP	CA-CB-CG	5.24	117.84	112.60
2	B	3	LYS	CA-C-N	5.20	127.88	120.49
2	B	3	LYS	C-N-CA	5.20	127.88	120.49
1	A	93	ASP	CA-C-N	5.20	128.55	120.60
1	A	93	ASP	C-N-CA	5.20	128.55	120.60
3	C	142	THR	CA-C-N	5.19	129.92	122.40
3	C	142	THR	C-N-CA	5.19	129.92	122.40
4	H	119	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	173	ARG	CA-C-N	5.13	125.64	120.00
1	A	173	ARG	C-N-CA	5.13	125.64	120.00
3	G	168	MET	CA-C-N	5.08	127.35	120.38
3	G	168	MET	C-N-CA	5.08	127.35	120.38
4	D	124	PHE	CA-CB-CG	5.07	118.87	113.80
4	D	222	GLU	CA-C-N	5.06	127.56	120.28
4	D	222	GLU	C-N-CA	5.06	127.56	120.28
3	C	122	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1972	0	1810	12	0
1	E	2011	0	1846	14	0
2	B	739	0	658	7	0
2	F	669	0	553	3	0
3	C	1545	0	1464	2	0
3	G	1540	0	1452	2	0
4	D	1853	0	1719	7	0
4	H	1852	0	1724	5	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
6	A	28	0	26	0	0
6	E	28	0	26	0	0
7	A	69	0	0	0	0
7	E	69	0	0	0	0
8	A	36	0	0	0	0
8	B	7	0	0	1	0
8	C	30	0	0	0	0
8	D	26	0	0	0	0
8	E	17	0	0	0	0
8	G	28	0	0	0	0
8	H	28	0	0	0	0
All	All	12603	0	11328	48	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 (48) 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:E:189:PRO:HB3	1:E:213:PHE:HB3	1.70	0.74
1:E:88:MET:HE1	1:E:145:LEU:HD23	1.70	0.73
1:A:88:MET:HE1	1:A:145:LEU:HD23	1.73	0.70
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.73	0.70
1:E:223:MET:HG2	1:E:228:GLU:HA	1.78	0.66
1:A:265:VAL:HG22	1:A:275:ILE:HB	1.76	0.66
2:B:7:ILE:HD12	2:B:91:LYS:HD2	1.79	0.63
1:E:15[A]:MET:HG2	2:F:62:PHE:HE2	1.64	0.62
3:C:177:SER:OG	4:D:196:ARG:HD2	2.00	0.62
2:B:42:ASN:HA	2:B:77:THR:HG23	1.81	0.61
2:B:28:THR:HB	8:B:101:HOH:O	2.06	0.56
3:G:60:ARG:HH21	3:G:81:LEU:HG	1.73	0.53
3:G:133:SER:C	3:G:135:ASP:H	2.17	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.91	0.53
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.91	0.52
1:E:15[B]:MET:HG2	2:F:62:PHE:HE2	1.75	0.51
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.93	0.51
4:D:157:HIS:HB3	4:D:218:TYR:HB2	1.93	0.49
1:E:107:TYR:HB3	1:E:108:PRO:HD2	1.95	0.48
4:H:176:ASP:HB2	4:H:193:LEU:HD12	1.96	0.48
2:B:28:THR:HG23	2:B:29:GLN:HG2	1.97	0.47
1:E:124:TYR:CZ	1:E:136:VAL:HG11	2.50	0.47
1:A:229:GLN:O	1:A:232:THR:HG22	2.15	0.47
4:D:176:ASP:HB2	4:D:193:LEU:HD12	1.97	0.47
1:E:262:ALA:HB2	1:E:278:TYR:CE2	2.51	0.46
4:D:245:ARG:HD3	4:D:247:ASP:HB2	1.99	0.45
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.52	0.44
1:E:47:ILE:HD12	1:E:67:GLN:HG3	1.98	0.44
1:A:264:ARG:HA	1:A:275:ILE:O	2.17	0.44
2:B:37:ILE:HG12	2:B:82:VAL:HG22	1.99	0.44
1:A:47:ILE:HD12	1:A:67:GLN:HG3	2.01	0.43
4:D:21:LEU:HD22	4:D:112:THR:HG21	1.99	0.43
4:H:123:VAL:HG12	4:H:233:PRO:HB2	2.00	0.43
4:H:205:GLN:HA	4:H:245:ARG:O	2.18	0.43
1:E:277:LEU:HD23	1:E:277:LEU:HA	1.88	0.42
4:H:36:ARG:HB3	4:H:46:ILE:HD11	2.02	0.41
1:A:163:LEU:HA	1:A:167:THR:HB	2.03	0.41
1:E:15[B]:MET:HE2	1:E:15[B]:MET:HB2	1.85	0.41
4:D:36:ARG:HB3	4:D:46:ILE:HD11	2.01	0.41
1:A:220:VAL:HG13	1:A:265:VAL:HG12	2.01	0.41
1:E:107:TYR:HB2	1:E:111:ALA:HB3	2.03	0.41
4:H:133:PRO:HD3	4:H:146:LEU:HG	2.02	0.41
1:A:107:TYR:HB2	1:A:111:ALA:HB3	2.03	0.41
2:B:28:THR:CG2	2:B:29:GLN:HG2	2.51	0.41
1:A:135:THR:HG23	1:A:147:ILE:HG13	2.04	0.40
1:E:106:MET:HE2	1:E:173:ARG:HG3	2.03	0.40
2:B:14:PRO:HA	2:B:15:PRO:HD3	2.00	0.40
1:E:163:LEU:HA	1:E:167:THR:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/302 (82%)	246 (99%)	3 (1%)	0	100	100
1	E	255/302 (84%)	251 (98%)	3 (1%)	1 (0%)	30	51
2	B	94/99 (95%)	91 (97%)	3 (3%)	0	100	100
2	F	91/99 (92%)	88 (97%)	2 (2%)	1 (1%)	11	25
3	C	202/207 (98%)	189 (94%)	12 (6%)	1 (0%)	24	46
3	G	202/207 (98%)	190 (94%)	12 (6%)	0	100	100
4	D	238/242 (98%)	232 (98%)	6 (2%)	0	100	100
4	H	238/242 (98%)	233 (98%)	5 (2%)	0	100	100
All	All	1569/1700 (92%)	1520 (97%)	46 (3%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	42	ASN
3	C	134	SER
1	E	260	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	205/264 (78%)	198 (97%)	7 (3%)	32	60
1	E	208/264 (79%)	199 (96%)	9 (4%)	26	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	77/93 (83%)	70 (91%)	7 (9%)	9	19
2	F	61/93 (66%)	55 (90%)	6 (10%)	7	17
3	C	176/186 (95%)	170 (97%)	6 (3%)	32	60
3	G	174/186 (94%)	164 (94%)	10 (6%)	18	40
4	D	194/207 (94%)	188 (97%)	6 (3%)	35	63
4	H	194/207 (94%)	190 (98%)	4 (2%)	47	73
All	All	1289/1500 (86%)	1234 (96%)	55 (4%)	26	51

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	64	GLU
1	A	105	GLU
1	A	112	SER
1	A	195	SER
1	A	250	THR
1	A	251	LEU
2	B	28	THR
2	B	54	MET
2	B	57	SER
2	B	71	THR
2	B	74	GLU
2	B	77	THR
2	B	96	ASP
3	C	48	VAL
3	C	117	ASP
3	C	147	GLN
3	C	152	GLN
3	C	175	SER
3	C	201	ASP
4	D	54	SER
4	D	80	GLU
4	D	122	ASN
4	D	196	ARG
4	D	205	GLN
4	D	228	GLN
1	E	22	SER
1	E	105	GLU
1	E	112	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	181	SER
1	E	224	ARG
1	E	226	ASP
1	E	247	LEU
1	E	250	THR
1	E	261	LEU
2	F	51	MET
2	F	57	SER
2	F	64	ILE
2	F	68	THR
2	F	71	THR
2	F	96	ASP
3	G	48	VAL
3	G	95	ARG
3	G	117	ASP
3	G	134	SER
3	G	136	LYS
3	G	147	GLN
3	G	151	SER
3	G	175	SER
3	G	195	ASN
3	G	201	ASP
4	H	54	SER
4	H	80	GLU
4	H	174	CYS
4	H	228	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	14	GLN
1	A	55	GLN
1	A	60	ASN
1	A	186	GLN
2	B	8	GLN
2	B	17	ASN
2	B	38	GLN
3	C	37	GLN
3	C	195	ASN
4	D	24	ASN
4	D	37	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	178	GLN
4	D	205	GLN
1	E	14	GLN
1	E	55	GLN
1	E	60	ASN
1	E	186	GLN
1	E	240	ASN
2	F	8	GLN
2	F	17	ASN
2	F	24	ASN
2	F	29	GLN
3	G	37	GLN
3	G	149	ASN
4	H	24	ASN
4	H	37	GLN
4	H	74	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 ⓘ

4 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	I	1	1,5	14,14,15	0.34	0	17,19,21	0.69	0
5	NAG	I	2	5	14,14,15	0.35	0	17,19,21	1.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	1	1,5	14,14,15	0.30	0	17,19,21	0.64	0
5	NAG	J	2	5	14,14,15	0.35	0	17,19,21	1.03	2 (11%)

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	I	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	O5-C1-C2	-2.84	106.90	111.29
5	J	2	NAG	C1-O5-C5	2.68	115.78	112.19
5	J	2	NAG	O5-C1-C2	-2.58	107.30	111.29
5	I	2	NAG	C1-O5-C5	2.32	115.29	112.19

There are no chirality outliers.

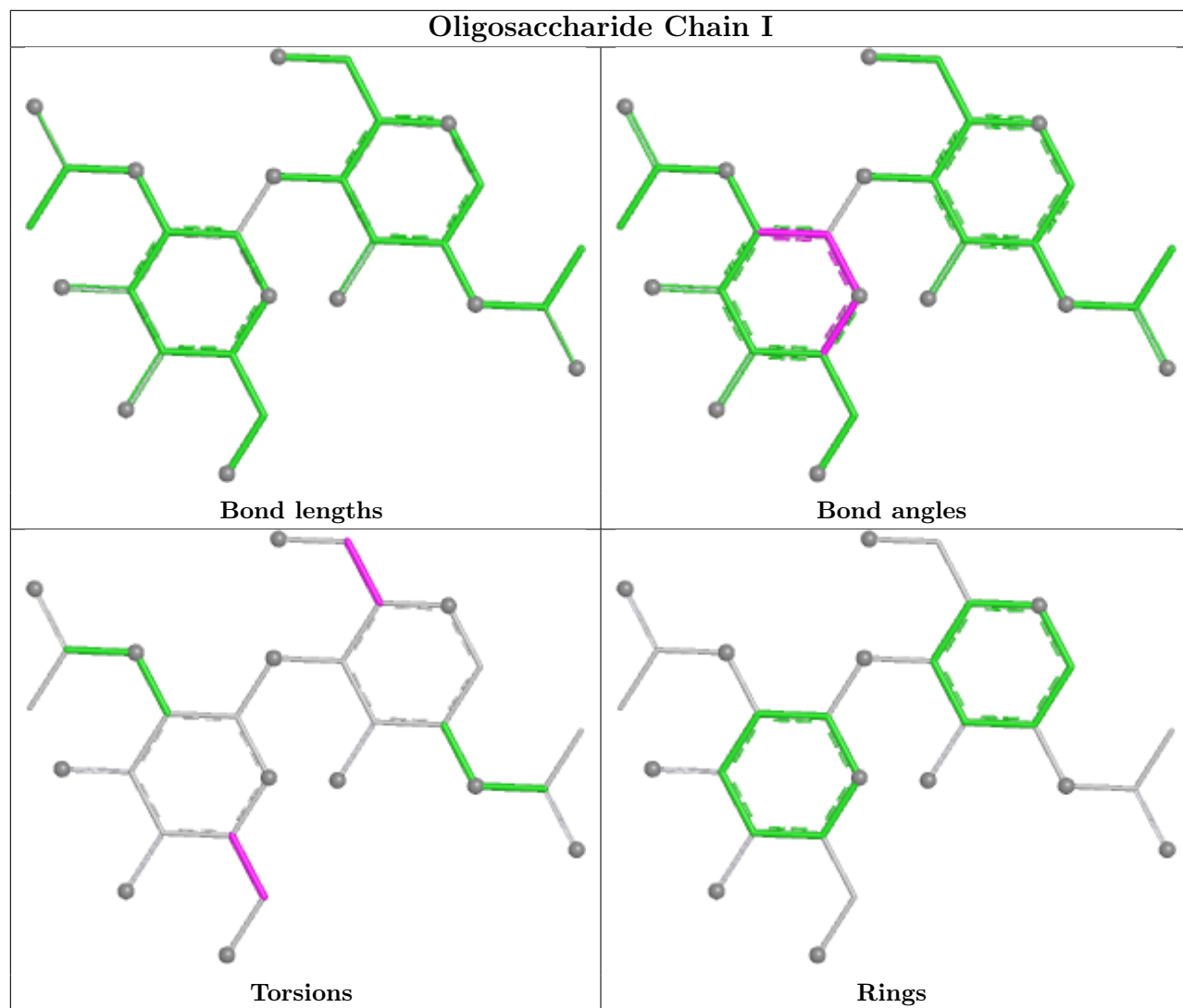
All (3) torsion outliers are listed below:

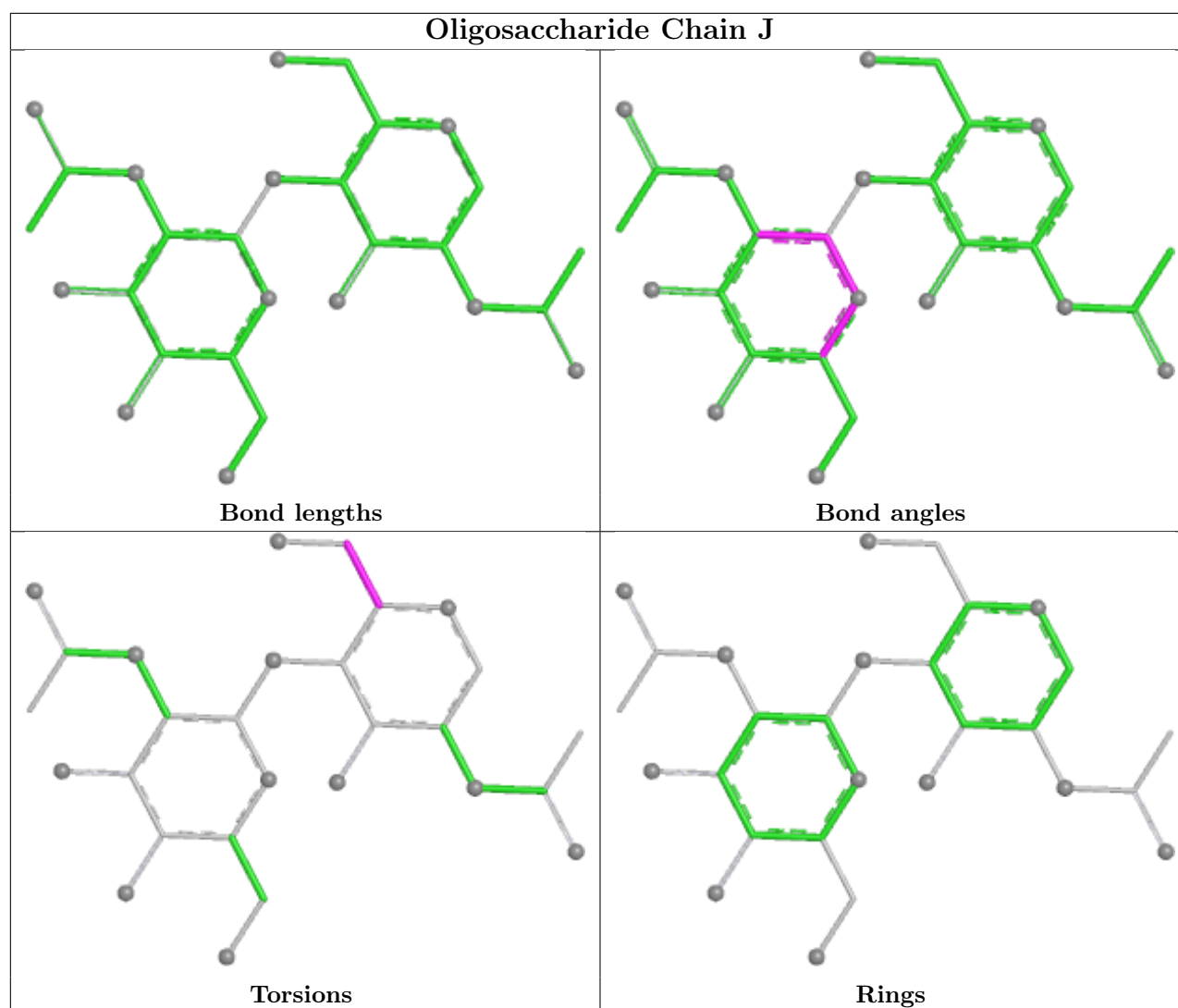
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6

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](#)

6 ligands 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	$\# Z > 2$
6	NAG	A	401	1	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
6	NAG	E	401	1	14,14,15	0.33	0	17,19,21	0.70	1 (5%)
6	NAG	A	402	1	14,14,15	0.38	0	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	QWV	A	405	-	70,70,70	0.84	4 (5%)	78,81,81	0.99	1 (1%)
7	QWV	E	405	-	70,70,70	0.69	2 (2%)	78,81,81	0.88	2 (2%)
6	NAG	E	402	1	14,14,15	0.38	0	17,19,21	1.08	1 (5%)

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
6	NAG	A	401	1	-	1/6/23/26	0/1/1/1
6	NAG	E	401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	402	1	-	2/6/23/26	0/1/1/1
7	QWV	A	405	-	-	22/63/83/83	0/2/2/2
7	QWV	E	405	-	-	28/63/83/83	0/2/2/2
6	NAG	E	402	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	405	QWV	C1-C2	2.41	1.56	1.51
7	E	405	QWV	CCJ-CCI	2.18	1.57	1.50
7	A	405	QWV	C1-C2	2.15	1.55	1.51
7	A	405	QWV	O6A-C1A	2.13	1.47	1.41
7	A	405	QWV	C4-C3	2.11	1.56	1.52
7	A	405	QWV	C3A-C2A	2.01	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	402	NAG	C1-O5-C5	4.01	117.56	112.19
6	E	402	NAG	C1-O5-C5	3.74	117.20	112.19
7	A	405	QWV	C5-C4-C3	-2.63	109.81	114.11
7	E	405	QWV	O3-C3-C2	-2.62	104.73	109.88
6	E	401	NAG	C1-O5-C5	2.53	115.58	112.19
6	A	401	NAG	C1-O5-C5	2.41	115.41	112.19
7	E	405	QWV	C1A-O6A-C5M	2.12	117.86	113.72

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	405	QWV	O6A-C5M-C6C-O6C
6	E	402	NAG	O5-C5-C6-O6
6	A	402	NAG	C4-C5-C6-O6
6	A	402	NAG	O5-C5-C6-O6
6	E	402	NAG	C4-C5-C6-O6
7	E	405	QWV	O6A-C5M-C6C-O6C
7	A	405	QWV	CAQ-CAR-CAS-CAT
7	A	405	QWV	CAV-CAW-CAX-CAY
7	A	405	QWV	CAK-CAL-CAM-CAN
7	E	405	QWV	CAN-CAO-CAP-CAQ
7	E	405	QWV	C12-C13-C14-C15
7	E	405	QWV	CAG-CAH-CAI-CAJ
7	E	405	QWV	CAK-CAL-CAM-CAN
7	E	405	QWV	CCJ-CCI-O6C-C6C
7	E	405	QWV	C11-C12-C13-C14
7	A	405	QWV	CAL-CAM-CAN-CAO
7	E	405	QWV	C13-C14-C15-C16
7	E	405	QWV	C11-C10-C9-C8
7	A	405	QWV	C7-C8-C9-C10
7	E	405	QWV	C5-C6-C7-C8
7	E	405	QWV	C4-C5-C6-C7
7	E	405	QWV	OCI-CCI-O6C-C6C
7	A	405	QWV	CAO-CAP-CAQ-CAR
7	A	405	QWV	CAU-CAV-CAW-CAX
7	E	405	QWV	CAE-CAF-CAG-CAH
7	A	405	QWV	C11-C10-C9-C8
7	A	405	QWV	C4A-C5M-C6C-O6C
7	E	405	QWV	CAJ-CAK-CAL-CAM
7	A	405	QWV	C11-C12-C13-C14
7	E	405	QWV	CAU-CAV-CAW-CAX
7	E	405	QWV	CAV-CAW-CAX-CAY
7	E	405	QWV	C4A-C5M-C6C-O6C
7	E	405	QWV	CAC-CAD-CAE-CAF
7	A	405	QWV	CAN-CAO-CAP-CAQ
7	E	405	QWV	CAL-CAM-CAN-CAO
7	A	405	QWV	CAH-CAI-CAJ-CAK
7	E	405	QWV	CAQ-CAR-CAS-CAT
7	A	405	QWV	CAR-CAS-CAT-CAU
7	A	405	QWV	CAG-CAH-CAI-CAJ
7	E	405	QWV	C6-C7-C8-C9
7	E	405	QWV	C14-C15-C16-C17
7	A	405	QWV	C15-C16-C17-C18
7	E	405	QWV	CAT-CAU-CAV-CAW

Continued on next page...

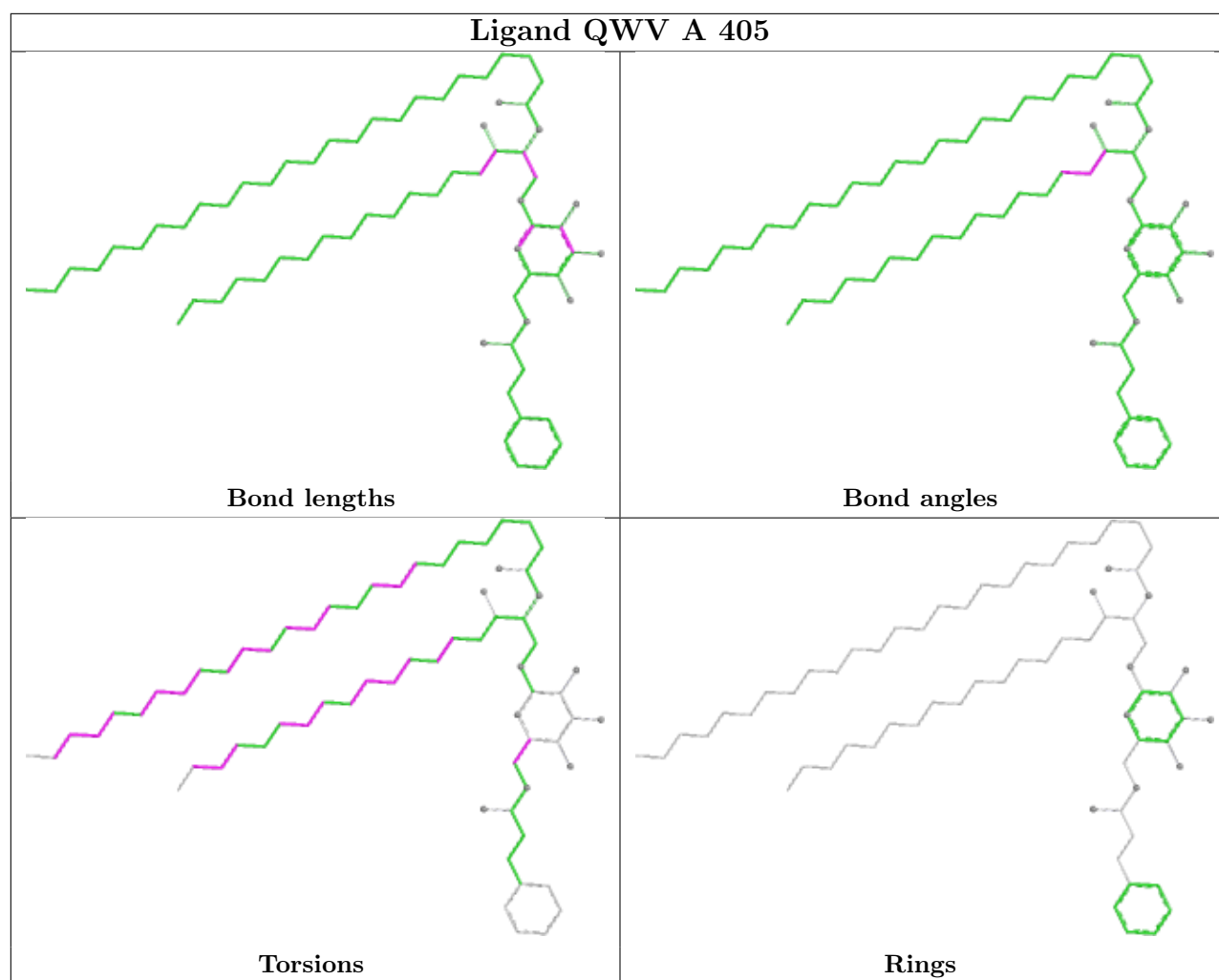
Continued from previous page...

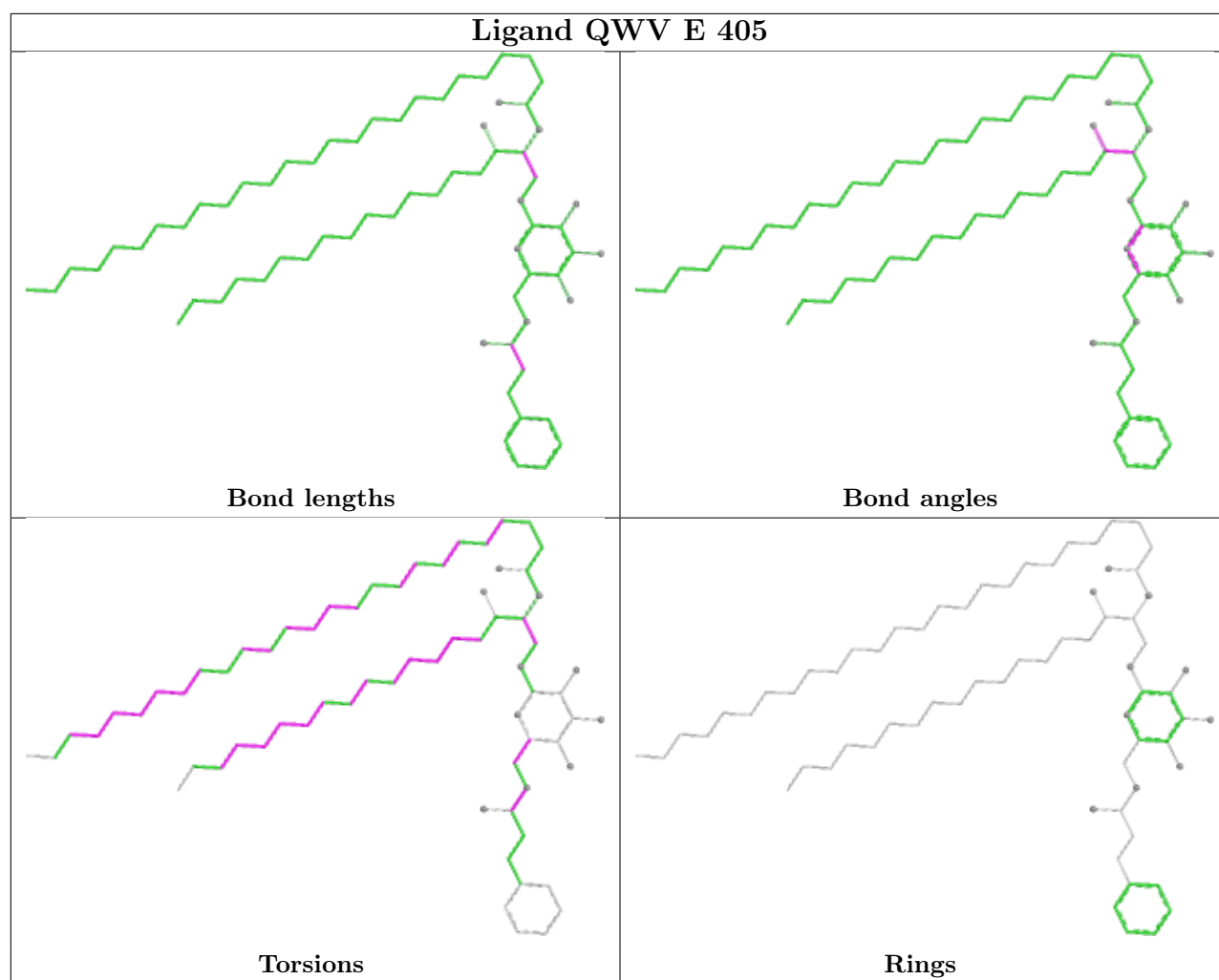
Mol	Chain	Res	Type	Atoms
7	A	405	QWV	C6-C7-C8-C9
7	A	405	QWV	C14-C15-C16-C17
7	A	405	QWV	C10-C11-C12-C13
7	A	405	QWV	CAS-CAT-CAU-CAV
6	E	401	NAG	C4-C5-C6-O6
7	A	405	QWV	CAW-CAX-CAY-CAZ
7	E	405	QWV	CAS-CAT-CAU-CAV
6	A	401	NAG	C4-C5-C6-O6
7	E	405	QWV	CAR-CAS-CAT-CAU
7	A	405	QWV	C4-C5-C6-C7
7	E	405	QWV	O1A-C1-C2-C3
7	E	405	QWV	C10-C11-C12-C13
6	E	401	NAG	O5-C5-C6-O6
7	E	405	QWV	C3-C4-C5-C6

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 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	255/302 (84%)	-0.03	13 (5%) 33 28	29, 54, 126, 150	1 (0%)
1	E	260/302 (86%)	0.08	14 (5%) 31 26	30, 60, 115, 139	1 (0%)
2	B	96/99 (96%)	0.21	5 (5%) 33 27	43, 71, 107, 126	0
2	F	93/99 (93%)	1.09	19 (20%) 3 2	52, 103, 130, 135	0
3	C	202/207 (97%)	-0.13	4 (1%) 65 60	27, 53, 100, 110	2 (0%)
3	G	203/207 (98%)	-0.20	3 (1%) 72 68	33, 53, 93, 110	1 (0%)
4	D	240/242 (99%)	-0.32	6 (2%) 58 52	32, 53, 83, 125	0
4	H	240/242 (99%)	-0.38	0 100 100	35, 51, 81, 93	0
All	All	1589/1700 (93%)	-0.06	64 (4%) 42 37	27, 57, 112, 150	5 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	97	ARG	6.6
1	E	196	VAL	4.7
1	E	279	TRP	4.6
2	B	2	GLN	4.5
1	E	253	VAL	4.2
1	E	259	ALA	3.8
2	B	97	ARG	3.8
1	A	197	PRO	3.8
3	G	133	SER	3.6
2	F	22	ILE	3.6
1	E	260	GLY	3.6
1	A	107	TYR	3.6
2	F	79	ALA	3.5
1	E	205	GLN	3.5
1	A	173	ARG	3.4
3	C	186	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	261	LEU	3.3
1	A	6	LYS	3.1
2	F	75	THR	3.0
2	F	38	GLN	3.0
2	F	11	SER	2.9
4	D	188	ASP	2.8
1	A	225	GLY	2.8
2	B	4	THR	2.8
2	F	72	PRO	2.7
2	F	37	ILE	2.7
1	A	251	LEU	2.7
2	F	44	LYS	2.7
1	A	108	PRO	2.6
2	F	90	PRO	2.6
4	D	229	ASP	2.6
2	B	34	HIS	2.6
1	E	191	ALA	2.6
4	D	185	ALA	2.6
2	B	3	LYS	2.6
2	F	89	GLU	2.5
3	C	119	GLN	2.5
1	E	206	LEU	2.5
2	F	77	THR	2.4
3	G	195	ASN	2.4
1	E	227	GLN	2.4
3	C	134	SER	2.3
4	D	187	ASN	2.3
2	F	40	LEU	2.3
1	A	106	MET	2.2
2	F	83	LYS	2.2
1	E	110	ASN	2.2
1	E	261	LEU	2.2
3	G	154	LYS	2.2
1	A	222	TRP	2.2
4	D	247	ASP	2.2
4	D	2	ALA	2.2
1	A	278	TYR	2.2
2	F	5	PRO	2.2
1	E	106	MET	2.2
2	F	69	GLU	2.1
1	E	188	LYS	2.1
2	F	41	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	47	PRO	2.1
1	E	246	TYR	2.1
1	A	190	VAL	2.1
1	A	195	SER	2.1
2	F	42	ASN	2.1
3	C	205	PRO	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](#)

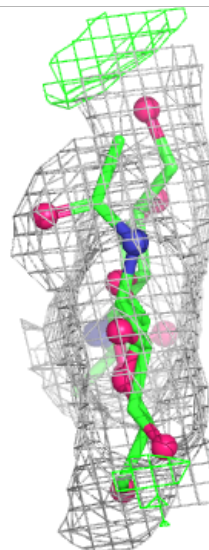
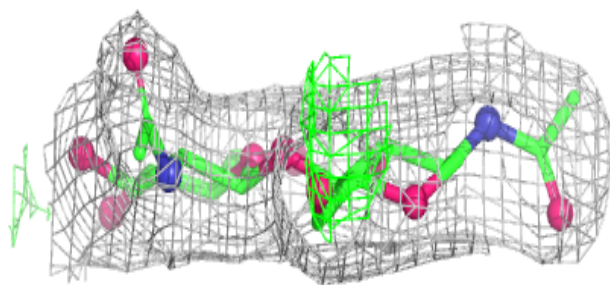
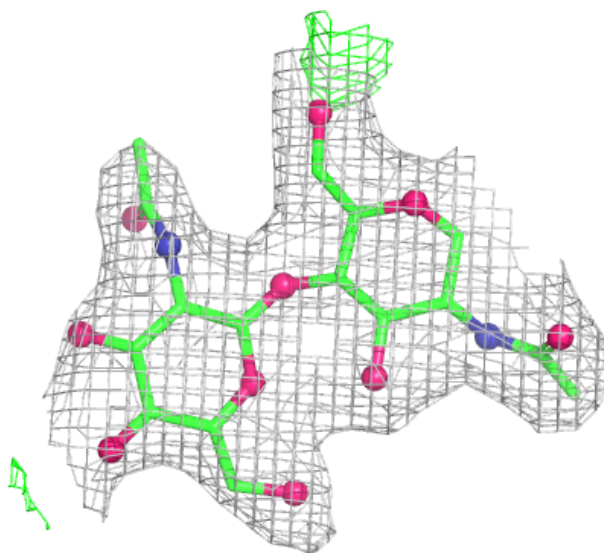
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

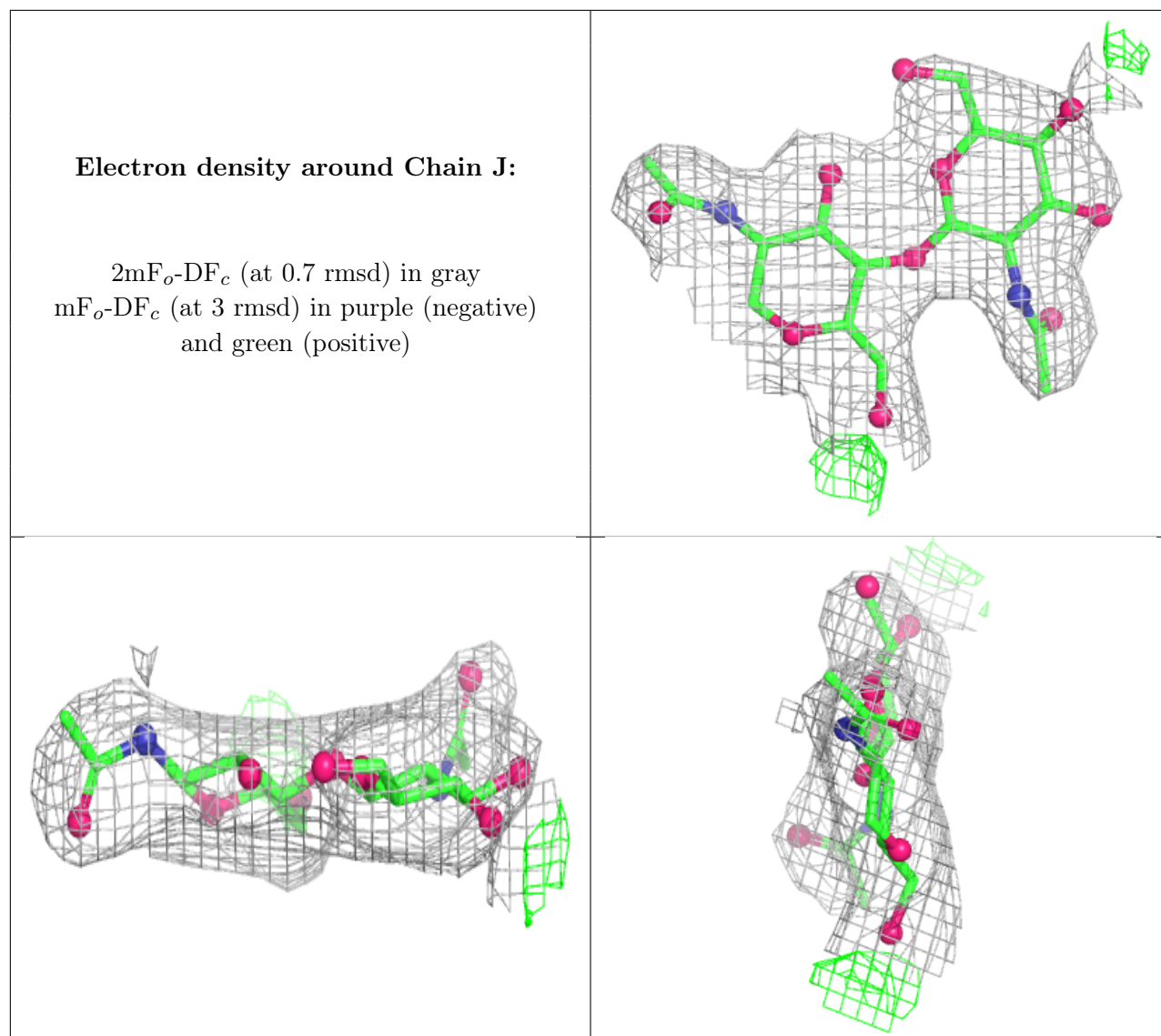
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	J	2	14/15	0.80	0.12	73,86,93,98	0
5	NAG	J	1	14/15	0.87	0.10	68,72,77,77	0
5	NAG	I	2	14/15	0.87	0.11	63,77,83,88	0
5	NAG	I	1	14/15	0.92	0.08	56,60,63,65	0

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

Electron density around Chain I:

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



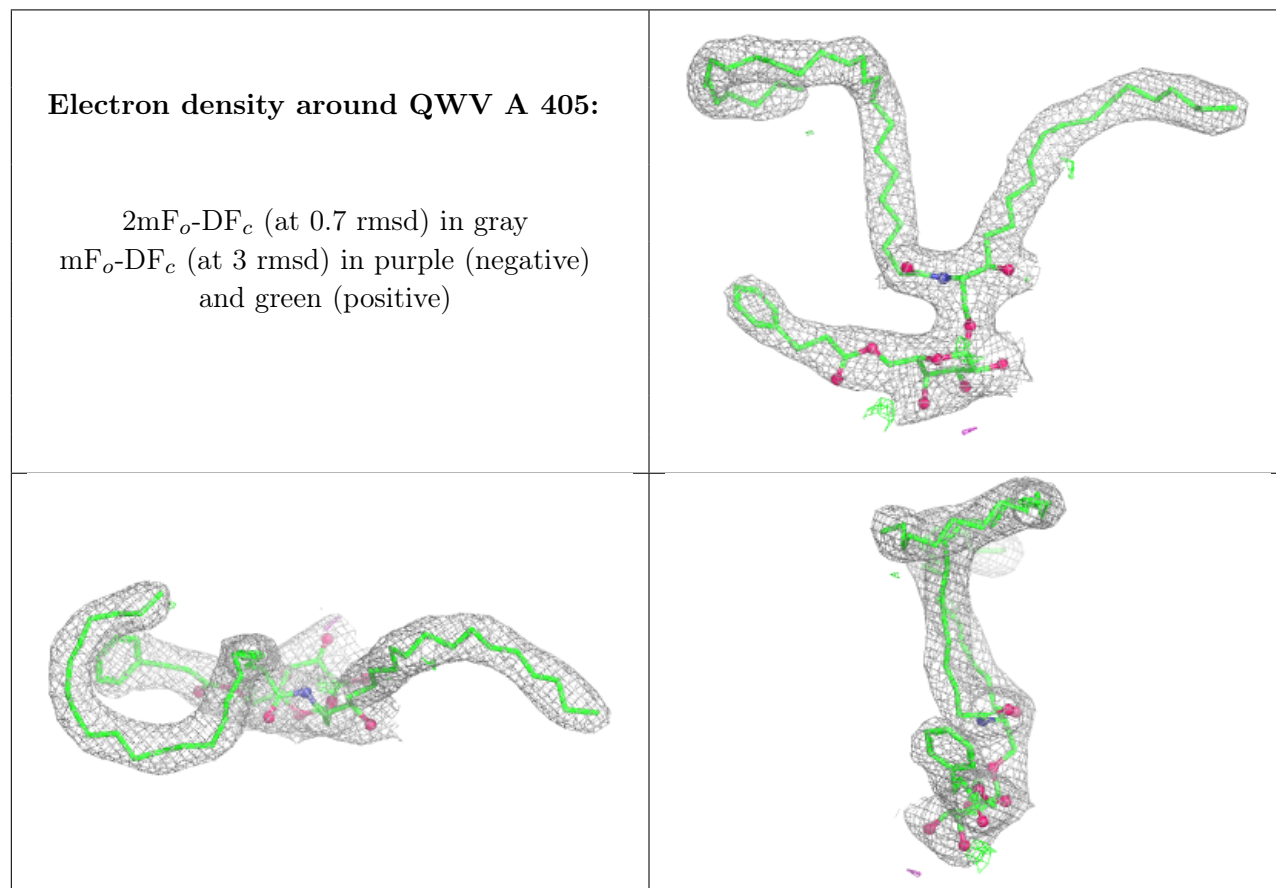


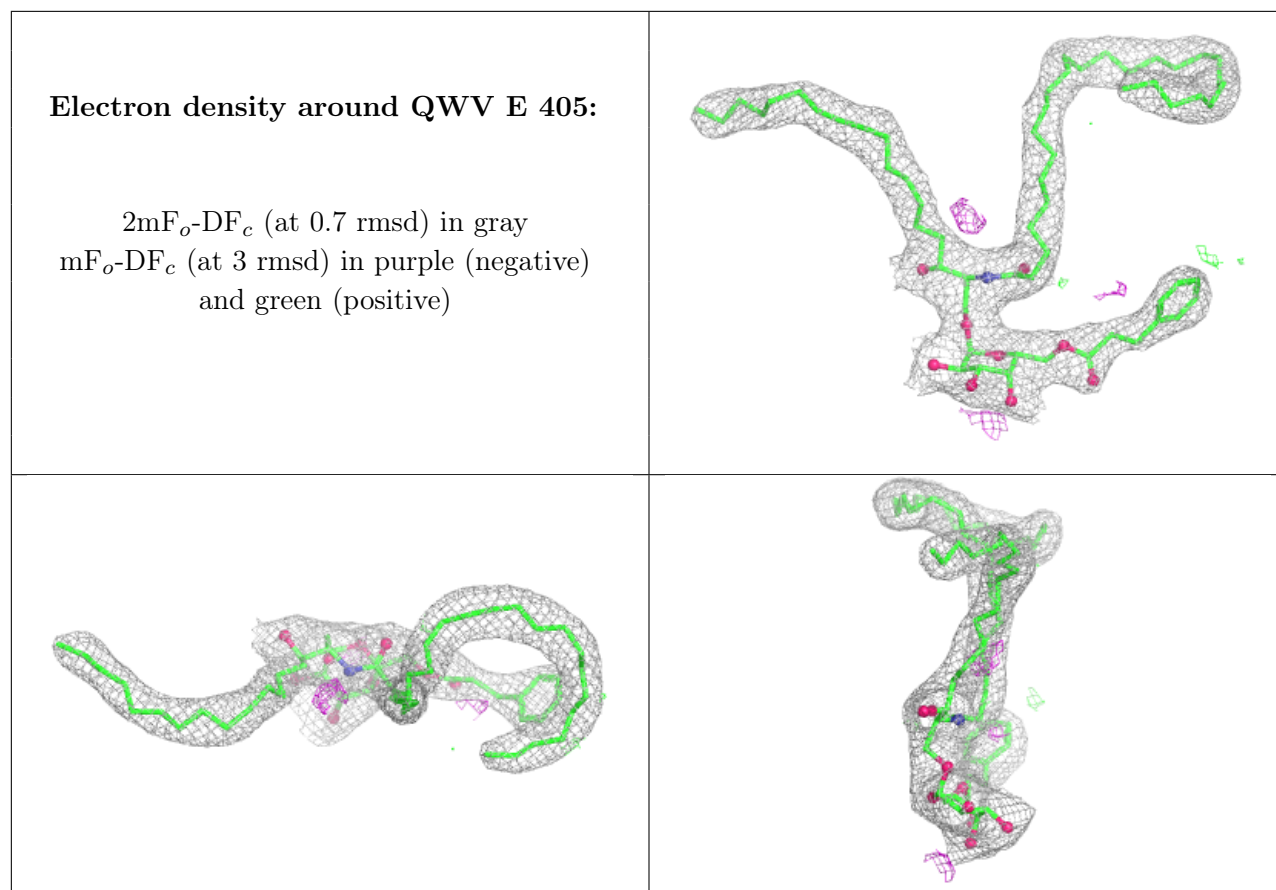
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
6	NAG	E	401	14/15	0.77	0.12	107,116,118,120	0
6	NAG	A	401	14/15	0.78	0.13	83,87,95,99	0
6	NAG	E	402	14/15	0.89	0.08	64,69,72,76	0
6	NAG	A	402	14/15	0.95	0.07	50,57,63,69	0
7	QWV	A	405	69/69	0.96	0.09	27,41,75,77	0
7	QWV	E	405	69/69	0.96	0.10	36,46,75,77	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.