



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:29 AM UTC

PDB ID : 6BNK / pdb_00006bnk
Title : Crystal structure of TCR-MHC-like molecule
Authors : Le Nours, J.; Rossjohn, J.
Deposited on : 2017-11-16
Resolution : 3.20 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:

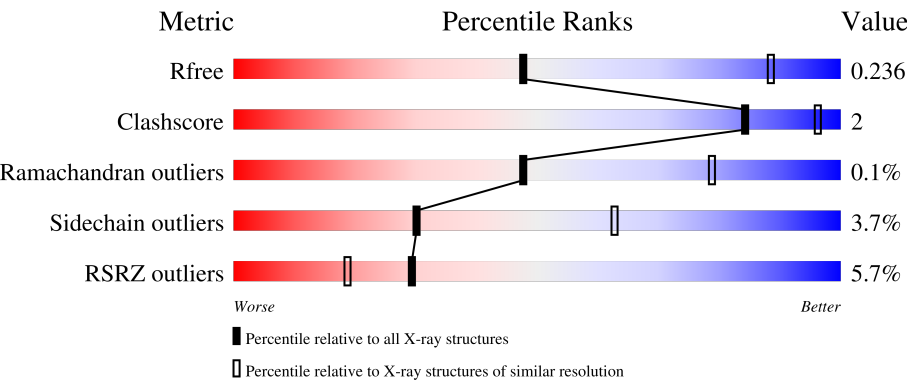
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	2% 81% 8% 10%
1	E	302	16% 82% 8% 10%
2	B	99	2% 94%
2	F	99	24% 89% 9%
3	C	207	2% 91% 7%

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Mol	Chain	Length	Quality of chain
3	G	207	3% 90% 6% ..
4	D	242	% 90% 8% ..
4	H	242	90% 7% ..
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 12526 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	272	Total	C	N	O	S	0	0	0
			2054	1312	345	384	13			
1	E	272	Total	C	N	O	S	0	1	0
			1969	1242	338	378	11			

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

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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	97	Total	C	N	O	S	0	0	0
			740	474	124	136	6			
2	F	97	Total	C	N	O	S	0	0	0
			694	446	119	123	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	203	Total	C	N	O	S	0	0	0
			1524	943	261	314	6			
3	G	203	Total	C	N	O	S	0	0	0
			1515	940	259	309	7			

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

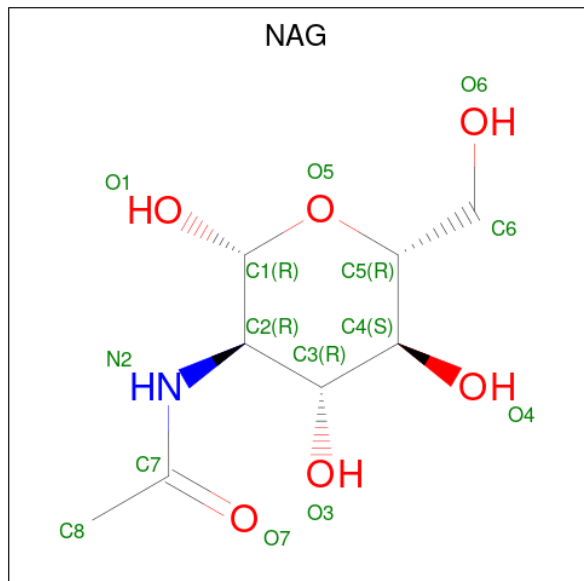
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1838	1160	321	351	6			
4	H	239	Total	C	N	O	S	0	0	0
			1858	1170	329	353	6			

- 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: $C_8H_{15}NO_6$).



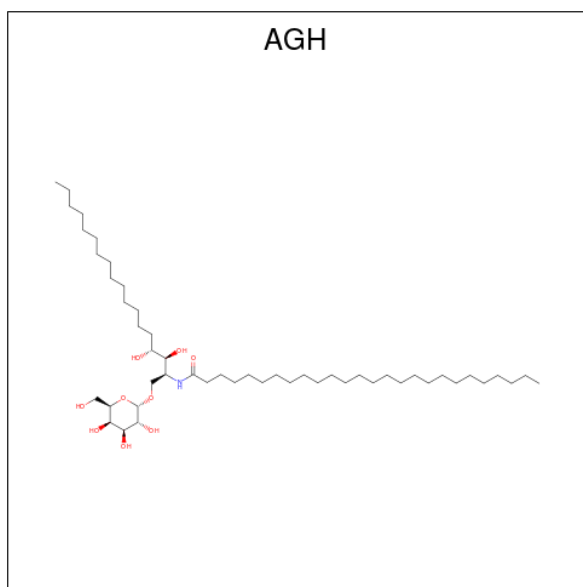
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (CCD ID: AGH) (formula: C₅₀H₉₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			60	50	1	9		
7	E	1	Total	C	N	O	0	0
			60	50	1	9		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O	0	0
			8	8		
8	B	4	Total	O	0	0
			4	4		
8	C	11	Total	O	0	0
			11	11		
8	D	32	Total	O	0	0
			32	32		

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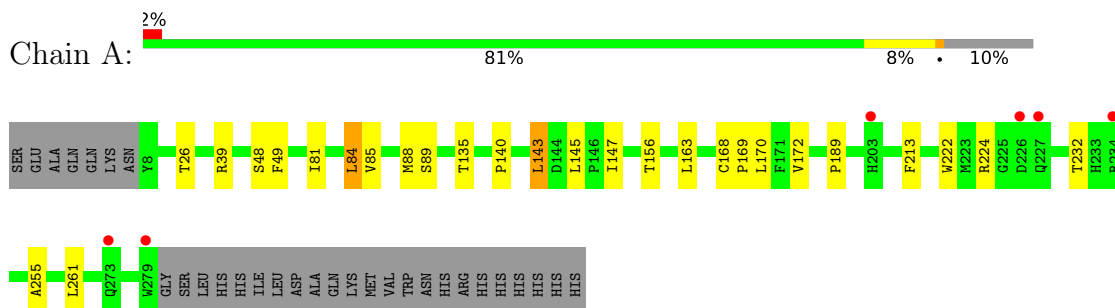
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	8	Total 8	O 8	0	0
8	F	2	Total 2	O 2	0	0
8	G	14	Total 14	O 14	0	0
8	H	23	Total 23	O 23	0	0

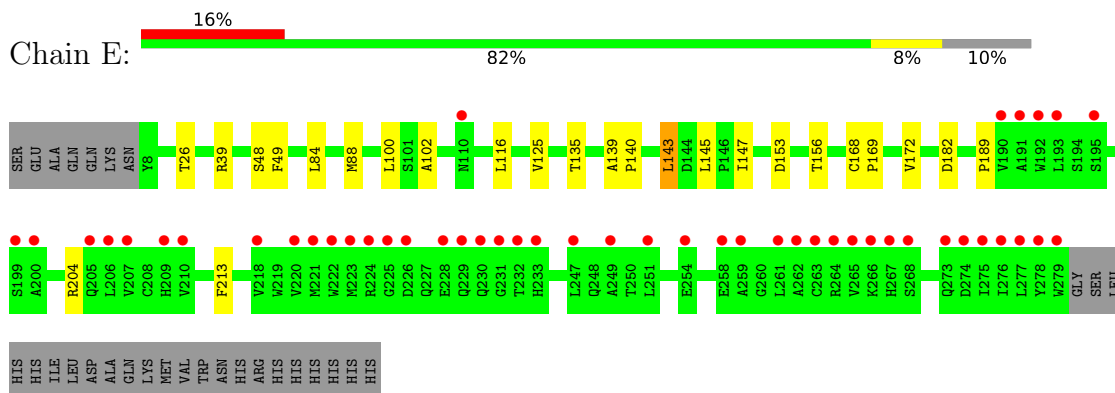
3 Residue-property plots [i](#)

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.

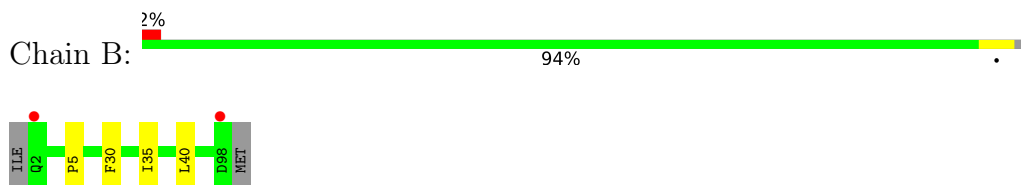
- Molecule 1: Antigen-presenting glycoprotein CD1d1



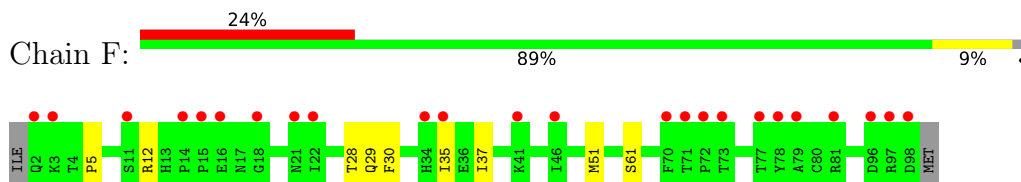
- Molecule 1: Antigen-presenting glycoprotein CD1d1



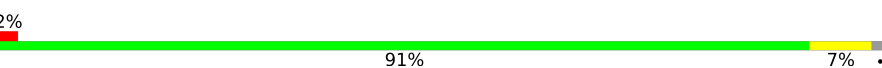
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

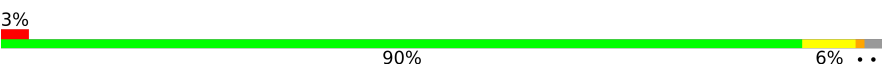


- Molecule 3: NKT Valpha14 (MOUSE) - 2C12 TCR - Hybrid mouse variable and human constant domains

Chain C:  91% 7% 2%

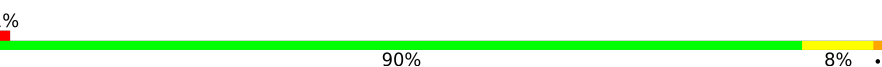


- Molecule 3: NKT Valpha14 (MOUSE) - 2C12 TCR - Hybrid mouse variable and human constant domains

Chain G:  90% 6% 3%



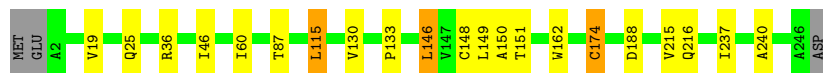
- Molecule 4: NKT Vbeta8.2 (MOUSE) - 2C12 TCR - hybrid mouse variable and human constant domains

Chain D:  90% 8% 1%



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

Chain H:  90% 7% 1%



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

Chain I:  50% 50%



- Molecule 5: 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.97Å 150.57Å 101.20Å 90.00° 95.23° 90.00°	Depositor
Resolution (Å)	44.45 – 3.20 44.45 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.45-3.20) 99.7 (44.45-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.201 , 0.220 0.215 , 0.236	Depositor DCC
R_{free} test set	2019 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.8	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	0.90	EDS
Total number of atoms	12526	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: AGH, 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	0.71	0/2113	1.15	1/2889 (0.0%)
1	E	0.72	0/2021	1.16	2/2770 (0.1%)
2	B	0.76	0/766	1.08	0/1055
2	F	0.79	0/718	1.05	0/992
3	C	0.73	0/1552	1.12	2/2118 (0.1%)
3	G	0.73	0/1543	1.12	3/2107 (0.1%)
4	D	0.66	0/1890	1.04	1/2583 (0.0%)
4	H	0.67	0/1910	1.04	1/2608 (0.0%)
All	All	0.71	0/12513	1.10	10/17122 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	119	ASP	CA-CB-CG	8.76	121.36	112.60
3	C	29	ASP	CA-CB-CG	6.73	119.33	112.60
3	G	29	ASP	CA-CB-CG	6.47	119.07	112.60
3	G	94	ASP	CA-CB-CG	5.25	117.85	112.60
3	C	94	ASP	CA-CB-CG	5.21	117.81	112.60
1	E	153	ASP	CA-CB-CG	5.19	117.79	112.60
4	H	188	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	49	PHE	CA-CB-CG	5.11	118.91	113.80
3	G	130	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	49	PHE	CA-CB-CG	5.00	118.80	113.80

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	2054	0	1873	12	0
1	E	1969	0	1694	12	0
2	B	740	0	651	1	0
2	F	694	0	581	3	0
3	C	1524	0	1419	7	0
3	G	1515	0	1403	7	0
4	D	1838	0	1709	8	0
4	H	1858	0	1746	7	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	60	0	99	1	0
7	E	60	0	99	1	0
8	A	8	0	0	0	0
8	B	4	0	0	0	0
8	C	11	0	0	0	0
8	D	32	0	0	0	0
8	E	8	0	0	0	0
8	F	2	0	0	0	0
8	G	14	0	0	0	0
8	H	23	0	0	0	0
All	All	12526	0	11376	54	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 (54) 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:125:VAL:HG11	1:E:143:LEU:HD13	1.55	0.86
1:E:125:VAL:CG1	1:E:143:LEU:HD13	2.21	0.69
1:A:156:THR:HG23	7:A:405:AGH:HAB2	1.76	0.67
1:E:88:MET:HE1	1:E:145:LEU:HD23	1.77	0.67
3:C:28:PRO:HD2	3:C:94:ASP:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:VAL:HG11	1:E:143:LEU:CD1	2.27	0.64
3:G:28:PRO:HD2	3:G:94:ASP:HB2	1.80	0.63
4:H:130:VAL:HG23	4:H:240:ALA:HB3	1.82	0.60
4:D:130:VAL:HG23	4:D:240:ALA:HB3	1.84	0.59
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.86	0.56
1:E:189:PRO:HB3	1:E:213:PHE:HB3	1.86	0.56
1:E:125:VAL:HG13	1:E:139:ALA:HB1	1.89	0.55
1:A:88:MET:HE1	1:A:145:LEU:HD23	1.88	0.54
3:G:116:PRO:HG3	3:G:165:VAL:HG11	1.91	0.53
4:D:36:ARG:HB3	4:D:46:ILE:HD11	1.90	0.53
4:H:36:ARG:HB3	4:H:46:ILE:HD11	1.90	0.53
3:C:116:PRO:HG3	3:C:165:VAL:HG11	1.92	0.51
3:G:166:LEU:HB3	4:H:174:CYS:HB3	1.92	0.51
1:E:156:THR:HG23	7:E:405:AGH:HAB2	1.93	0.51
1:A:81:ILE:O	1:A:85:VAL:HG23	2.11	0.50
4:D:133:PRO:HD3	4:D:146:LEU:HG	1.93	0.50
4:H:133:PRO:HD3	4:H:146:LEU:HG	1.94	0.48
3:G:94:ASP:O	3:G:95:ARG:HD3	2.13	0.48
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.96	0.48
1:A:224:ARG:HA	1:A:261:LEU:HD12	1.96	0.47
2:F:37:ILE:HB	2:F:51:MET:HE1	1.96	0.47
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.97	0.46
3:C:85:THR:HG23	3:C:113:ILE:HA	1.97	0.46
3:G:85:THR:HG23	3:G:113:ILE:HA	1.97	0.45
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.97	0.45
1:E:168:CYS:HB3	1:E:169:PRO:HD3	1.98	0.44
1:E:102:ALA:HB2	1:E:116:LEU:HD13	1.99	0.44
3:C:55:LYS:HG2	3:C:65:THR:HG22	1.99	0.44
1:A:168:CYS:O	1:A:172:VAL:HG23	2.19	0.43
1:A:84:LEU:HD13	3:C:99:LEU:HD21	2.00	0.43
2:F:29:GLN:HA	2:F:61:SER:HB2	2.00	0.43
1:A:39:ARG:HG3	1:A:48:SER:HB2	2.01	0.43
1:E:168:CYS:O	1:E:172:VAL:HG23	2.19	0.43
2:F:5:PRO:HB3	2:F:30:PHE:HB3	2.01	0.42
4:D:148:CYS:HB2	4:D:162:TRP:CZ2	2.55	0.42
4:H:150:ALA:HB2	4:H:215:VAL:HG21	2.01	0.42
4:D:123:VAL:HG12	4:D:233:PRO:HB2	2.02	0.42
4:D:150:ALA:HB2	4:D:215:VAL:HG21	2.02	0.42
4:H:87:THR:HG23	4:H:115:LEU:HA	2.02	0.42
4:H:148:CYS:HB2	4:H:162:TRP:CZ2	2.55	0.42
1:E:39:ARG:HG3	1:E:48:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:PRO:HG2	1:E:143:LEU:HD12	2.02	0.41
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.96	0.41
3:C:31:HIS:CE1	3:C:93:GLY:HA3	2.56	0.41
3:G:31:HIS:CE1	3:G:93:GLY:HA3	2.56	0.41
1:A:140:PRO:HG2	1:A:143:LEU:HD12	2.03	0.41
1:A:222:TRP:HD1	1:A:232:THR:HG23	1.86	0.41
3:G:33:ARG:HG3	3:G:48:VAL:HG23	2.03	0.41
4:D:87:THR:HG23	4:D:115:LEU:HA	2.02	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	270/302 (89%)	262 (97%)	7 (3%)	1 (0%)	30	62
1	E	271/302 (90%)	263 (97%)	8 (3%)	0	100	100
2	B	95/99 (96%)	91 (96%)	4 (4%)	0	100	100
2	F	95/99 (96%)	92 (97%)	3 (3%)	0	100	100
3	C	201/207 (97%)	192 (96%)	9 (4%)	0	100	100
3	G	201/207 (97%)	191 (95%)	10 (5%)	0	100	100
4	D	237/242 (98%)	230 (97%)	7 (3%)	0	100	100
4	H	237/242 (98%)	233 (98%)	4 (2%)	0	100	100
All	All	1607/1700 (94%)	1554 (97%)	52 (3%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ALA

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	207/264 (78%)	199 (96%)	8 (4%)	28	62
1	E	183/264 (69%)	175 (96%)	8 (4%)	25	59
2	B	76/93 (82%)	74 (97%)	2 (3%)	40	69
2	F	63/93 (68%)	60 (95%)	3 (5%)	23	56
3	C	170/186 (91%)	168 (99%)	2 (1%)	63	79
3	G	166/186 (89%)	162 (98%)	4 (2%)	43	70
4	D	192/207 (93%)	183 (95%)	9 (5%)	23	57
4	H	197/207 (95%)	187 (95%)	10 (5%)	21	54
All	All	1254/1500 (84%)	1208 (96%)	46 (4%)	30	63

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	84	LEU
1	A	89	SER
1	A	135	THR
1	A	143	LEU
1	A	147	ILE
1	A	163	LEU
1	A	170	LEU
2	B	35	ILE
2	B	40	LEU
3	C	74	THR
3	C	198	ILE
4	D	19	VAL
4	D	25	GLN
4	D	60	ILE
4	D	115	LEU
4	D	119	ASP
4	D	146	LEU
4	D	149	LEU

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Mol	Chain	Res	Type
4	D	151	THR
4	D	237	ILE
1	E	26	THR
1	E	84	LEU
1	E	100	LEU
1	E	135	THR
1	E	143	LEU
1	E	147	ILE
1	E	182	ASP
1	E	204	ARG
2	F	12	ARG
2	F	28	THR
2	F	35	ILE
3	G	48	VAL
3	G	74	THR
3	G	95	ARG
3	G	198	ILE
4	H	19	VAL
4	H	25	GLN
4	H	60	ILE
4	H	115	LEU
4	H	146	LEU
4	H	149	LEU
4	H	151	THR
4	H	174	CYS
4	H	216	GLN
4	H	237	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	134	GLN
1	A	186	GLN
3	C	37	GLN
3	C	58	ASN
3	C	127	GLN
4	D	27	ASN
4	D	28	ASN
4	D	37	GLN
4	D	206	ASN
4	D	236	GLN

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Mol	Chain	Res	Type
1	E	186	GLN
2	F	13	HIS
2	F	67	HIS
3	G	30	ASN
3	G	37	GLN
3	G	127	GLN
4	H	28	ASN
4	H	37	GLN
4	H	74	ASN
4	H	228	GLN
4	H	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	5,1	14,14,15	0.31	0	17,19,21	0.58	0
5	NAG	I	2	5	14,14,15	0.31	0	17,19,21	0.79	1 (5%)
5	NAG	J	1	5,1	14,14,15	0.30	0	17,19,21	0.58	0
5	NAG	J	2	5	14,14,15	0.31	0	17,19,21	0.73	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
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	C1-O5-C5	2.44	115.45	112.19
5	J	2	NAG	C1-O5-C5	2.18	115.11	112.19

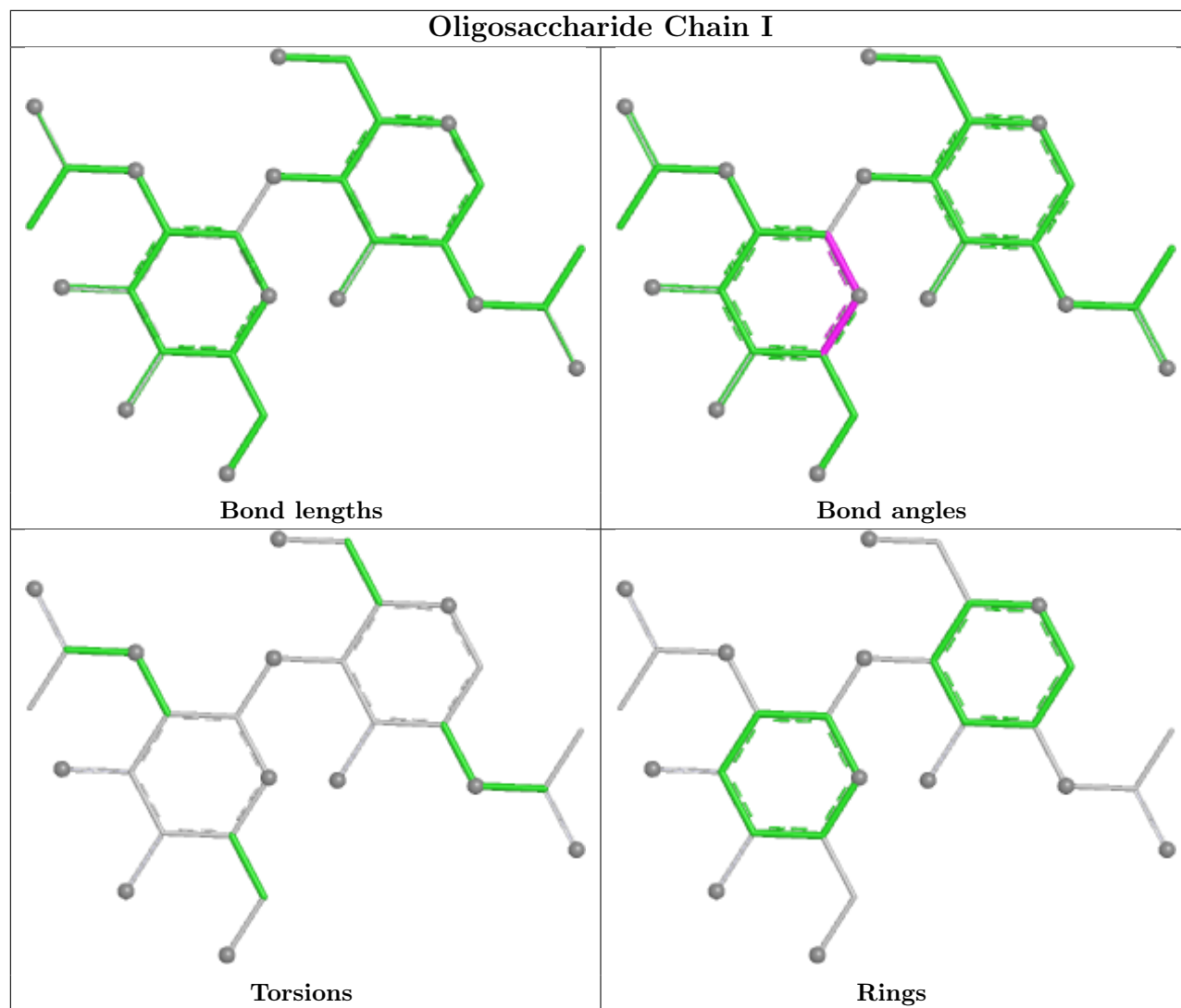
There are no chirality outliers.

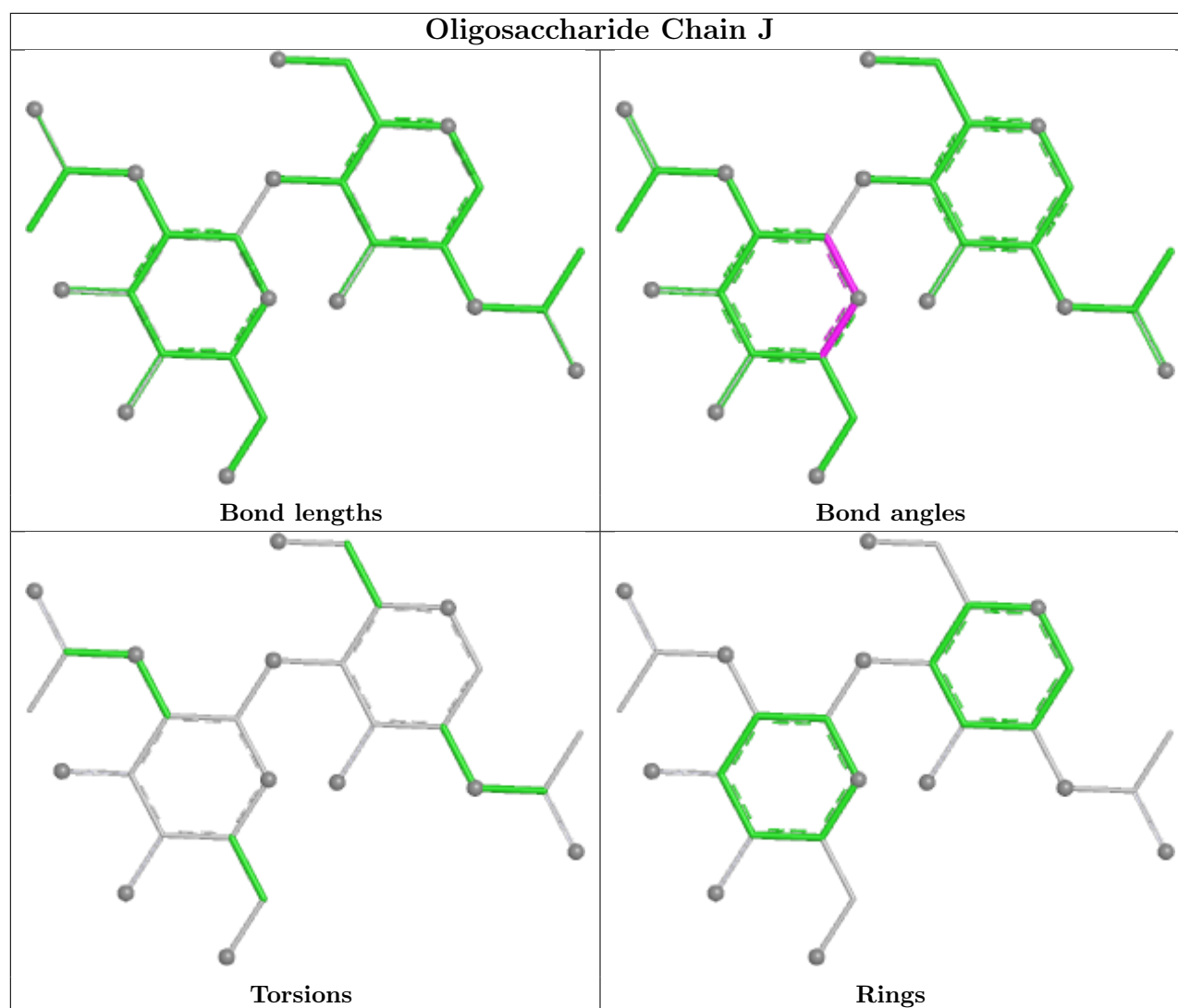
There are no torsion outliers.

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	0.32	0	17,19,21	0.68	0
6	NAG	E	401	1	14,14,15	0.32	0	17,19,21	0.67	0
6	NAG	A	402	1	14,14,15	0.29	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	AGH	A	405	-	60,60,60	0.90	3 (5%)	66,69,69	0.82	0
6	NAG	E	402	1	14,14,15	0.31	0	17,19,21	0.98	1 (5%)
7	AGH	E	405	-	60,60,60	0.87	2 (3%)	66,69,69	0.86	3 (4%)

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	-	1/6/23/26	0/1/1/1
6	NAG	A	402	1	-	2/6/23/26	0/1/1/1
7	AGH	A	405	-	-	18/58/78/78	0/1/1/1
6	NAG	E	402	1	-	2/6/23/26	0/1/1/1
7	AGH	E	405	-	-	24/58/78/78	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	405	AGH	O1A-C1A	3.51	1.46	1.40
7	E	405	AGH	O1A-C1A	3.11	1.45	1.40
7	E	405	AGH	O6A-C1A	2.62	1.48	1.41
7	A	405	AGH	O6A-C1A	2.30	1.47	1.41
7	A	405	AGH	C2A-C3A	2.16	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	402	NAG	C1-O5-C5	3.53	116.92	112.19
6	E	402	NAG	C1-O5-C5	3.37	116.70	112.19
7	E	405	AGH	O6A-C5M-C6A	2.56	112.79	106.44
7	E	405	AGH	C1-C2-N2	2.10	112.65	109.66
7	E	405	AGH	O6A-C1A-O1A	2.08	114.95	110.04

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	405	AGH	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
7	E	405	AGH	O6A-C5M-C6A-O5A
7	E	405	AGH	C4A-C5M-C6A-O5A
7	E	405	AGH	CAA-CAB-CAC-CAD
7	E	405	AGH	C11-C12-C13-C14
7	E	405	AGH	C9-C10-C11-C12
7	A	405	AGH	CAH-CAI-CAJ-CAK
7	A	405	AGH	CAV-CAW-CAX-CAY
7	E	405	AGH	CAC-CAD-CAE-CAF
7	E	405	AGH	CAO-CAP-CAQ-CAR
7	A	405	AGH	CAI-CAJ-CAK-CAL
7	A	405	AGH	CAN-CAO-CAP-CAQ
7	A	405	AGH	CAQ-CAR-CAS-CAT
7	E	405	AGH	CAH-CAI-CAJ-CAK
7	E	405	AGH	CAQ-CAR-CAS-CAT
7	A	405	AGH	CAE-CAF-CAG-CAH
7	E	405	AGH	CAB-CAC-CAD-CAE
7	A	405	AGH	CAD-CAE-CAF-CAG
7	A	405	AGH	C9-C10-C11-C12
7	E	405	AGH	CAN-CAO-CAP-CAQ
7	E	405	AGH	C14-C15-C16-C17
7	E	405	AGH	CAL-CAM-CAN-CAO
7	A	405	AGH	CAU-CAV-CAW-CAX
7	E	405	AGH	CAI-CAJ-CAK-CAL
7	E	405	AGH	CAR-CAS-CAT-CAU
6	E	402	NAG	C4-C5-C6-O6
6	A	402	NAG	C4-C5-C6-O6
7	A	405	AGH	C12-C13-C14-C15
7	A	405	AGH	CAR-CAS-CAT-CAU
7	A	405	AGH	CAL-CAM-CAN-CAO
6	E	402	NAG	O5-C5-C6-O6
7	E	405	AGH	CAU-CAV-CAW-CAX
6	A	402	NAG	O5-C5-C6-O6
7	A	405	AGH	CAC-CAD-CAE-CAF
7	E	405	AGH	C6-C7-C8-C9
7	E	405	AGH	CAT-CAU-CAV-CAW
7	E	405	AGH	CAV-CAW-CAX-CAY
7	E	405	AGH	CAJ-CAK-CAL-CAM
7	A	405	AGH	CAS-CAT-CAU-CAV
7	A	405	AGH	C6-C7-C8-C9
7	E	405	AGH	O4-C4-C5-C6
7	A	405	AGH	C13-C14-C15-C16
7	E	405	AGH	CAS-CAT-CAU-CAV

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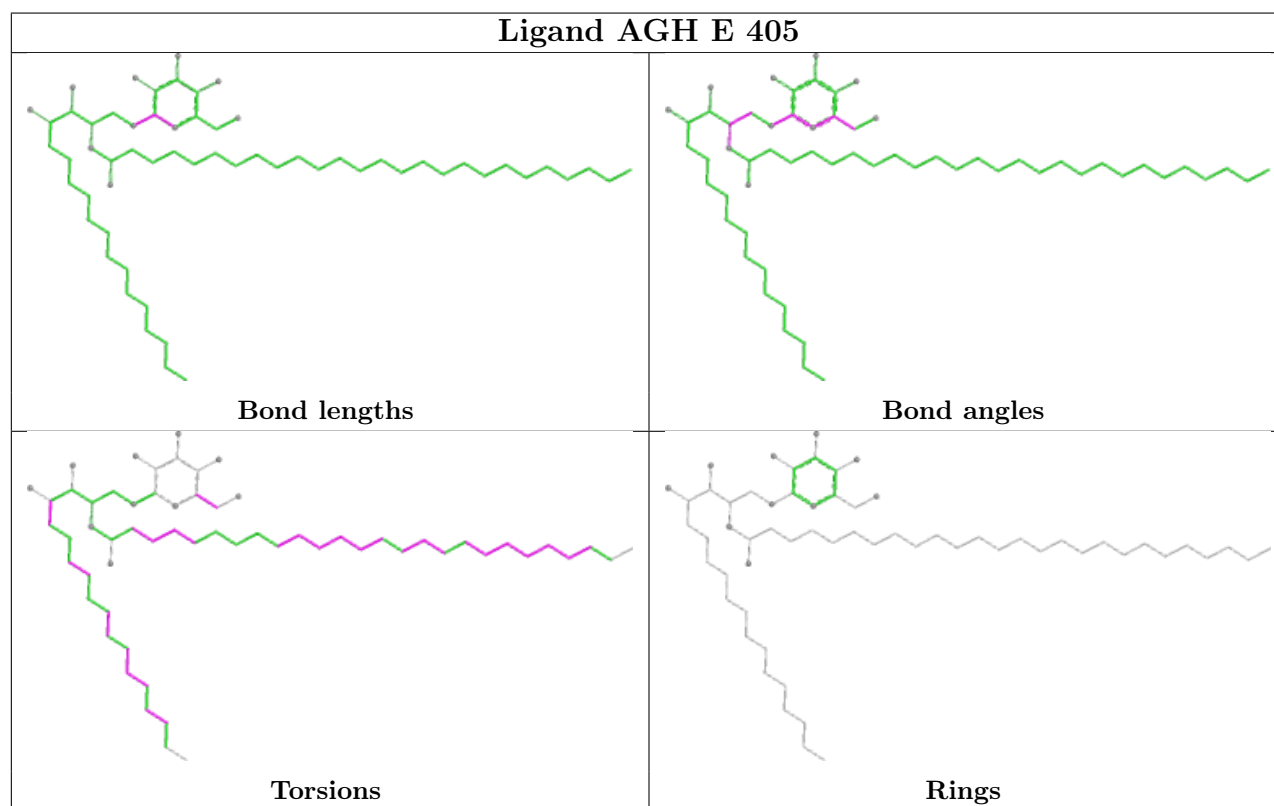
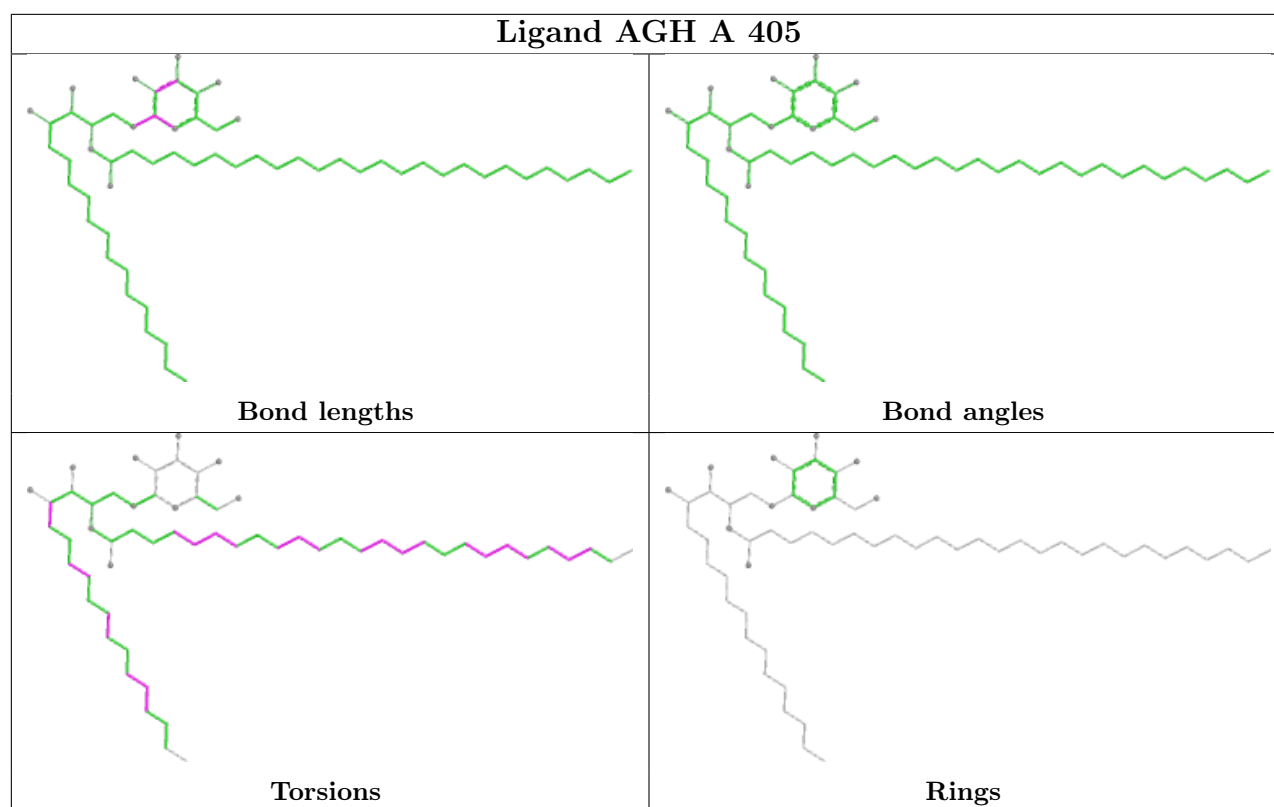
Mol	Chain	Res	Type	Atoms
7	A	405	AGH	CAM-CAN-CAO-CAP
7	E	405	AGH	C12-C13-C14-C15
6	E	401	NAG	C4-C5-C6-O6
7	E	405	AGH	CAK-CAL-CAM-CAN
6	A	401	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	405	AGH	1	0
7	E	405	AGH	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 ⓘ

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	272/302 (90%)	0.19	6 (2%) 62 42	21, 46, 100, 118	0
1	E	272/302 (90%)	0.78	48 (17%) 4 3	21, 54, 148, 161	2 (0%)
2	B	97/99 (97%)	0.19	2 (2%) 63 43	36, 56, 77, 82	1 (1%)
2	F	97/99 (97%)	1.42	24 (24%) 2 2	48, 93, 122, 129	0
3	C	203/207 (98%)	0.13	4 (1%) 65 45	22, 42, 77, 105	0
3	G	203/207 (98%)	0.19	6 (2%) 52 33	24, 42, 72, 84	0
4	D	239/242 (98%)	0.01	2 (0%) 82 67	23, 39, 62, 78	0
4	H	239/242 (98%)	-0.07	0 100 100	21, 39, 65, 78	0
All	All	1622/1700 (95%)	0.29	92 (5%) 29 19	21, 45, 109, 161	3 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	191	ALA	11.6
2	F	98	ASP	5.8
1	E	262	ALA	5.4
1	E	226	ASP	5.2
1	E	259	ALA	5.0
1	E	229	GLN	5.0
1	E	279	TRP	4.9
1	E	221	MET	4.7
1	E	222	TRP	4.7
3	G	206	SER	4.6
1	E	278	TYR	4.5
1	E	267	HIS	4.5
1	E	220	VAL	4.4
1	E	249	ALA	4.0
2	F	79	ALA	3.9
1	E	258	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	274	ASP	3.6
2	F	2	GLN	3.6
1	E	264	ARG	3.5
1	E	223	MET	3.5
1	E	261	LEU	3.4
3	C	206	SER	3.3
1	E	224	ARG	3.3
3	G	135	ASP	3.3
1	A	227	GLN	3.2
1	E	199	SER	3.2
2	F	15	PRO	3.2
2	F	78	TYR	3.1
4	D	246	ALA	3.0
2	F	72	PRO	3.0
1	E	225	GLY	3.0
1	E	265	VAL	3.0
2	F	73	THR	2.9
1	E	209	HIS	2.8
3	C	119	GLN	2.8
1	E	254	GLU	2.8
1	E	232	THR	2.8
2	F	21	ASN	2.8
1	E	277	LEU	2.8
1	E	231	GLY	2.7
2	F	3	LYS	2.7
1	E	206	LEU	2.7
1	E	192	TRP	2.7
2	F	96	ASP	2.7
2	F	97	ARG	2.7
1	E	276	ILE	2.7
1	A	279	TRP	2.7
4	D	188	ASP	2.7
3	G	133	SER	2.6
1	E	275	ILE	2.6
2	F	16	GLU	2.6
1	E	247	LEU	2.6
2	F	22	ILE	2.6
2	F	70	PHE	2.6
1	E	263	CYS	2.6
1	E	193	LEU	2.6
1	E	200	ALA	2.6
2	F	81	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	11	SER	2.5
1	E	230	GLN	2.5
1	E	210	VAL	2.5
3	G	134	SER	2.4
1	E	110	ASN	2.4
2	F	71	THR	2.4
1	E	273	GLN	2.4
1	E	205	GLN	2.4
3	C	183	ASN	2.4
1	E	268	SER	2.4
1	E	233	HIS	2.3
1	E	195	SER	2.3
1	E	266	LYS	2.3
2	B	2	GLN	2.3
2	F	46	ILE	2.3
3	G	183	ASN	2.3
2	F	14	PRO	2.2
1	E	228	GLU	2.2
2	F	34	HIS	2.2
2	F	77	THR	2.2
2	F	41	LYS	2.2
3	C	135	ASP	2.2
1	E	207	VAL	2.2
1	A	226	ASP	2.2
1	E	218	VAL	2.1
2	B	98	ASP	2.1
2	F	35	ILE	2.1
1	A	273	GLN	2.1
1	E	251	LEU	2.0
3	G	197	ILE	2.0
1	A	203	HIS	2.0
2	F	18	GLY	2.0
1	A	234	ARG	2.0
1	E	190	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

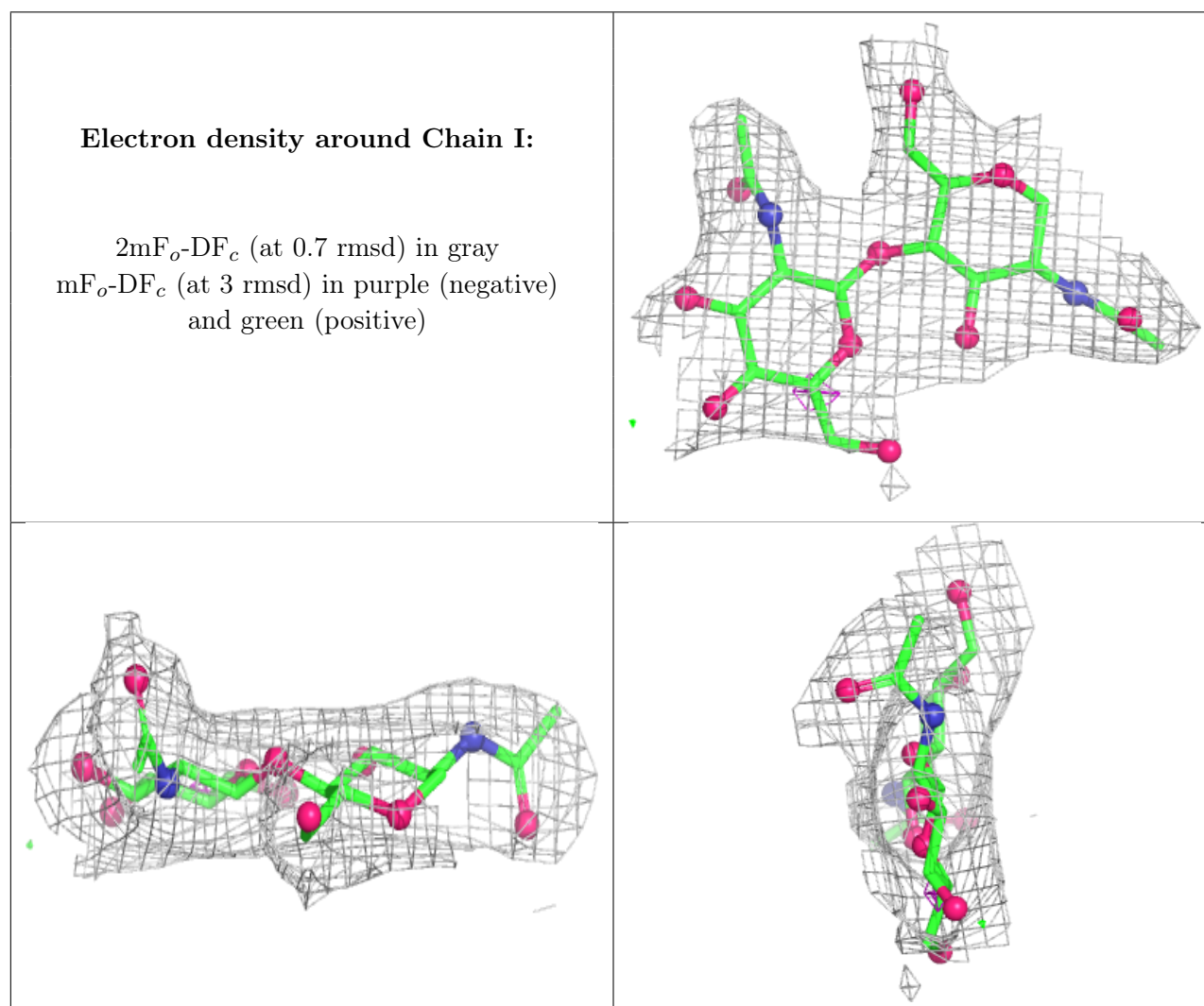
There are no non-standard protein/DNA/RNA residues in this entry.

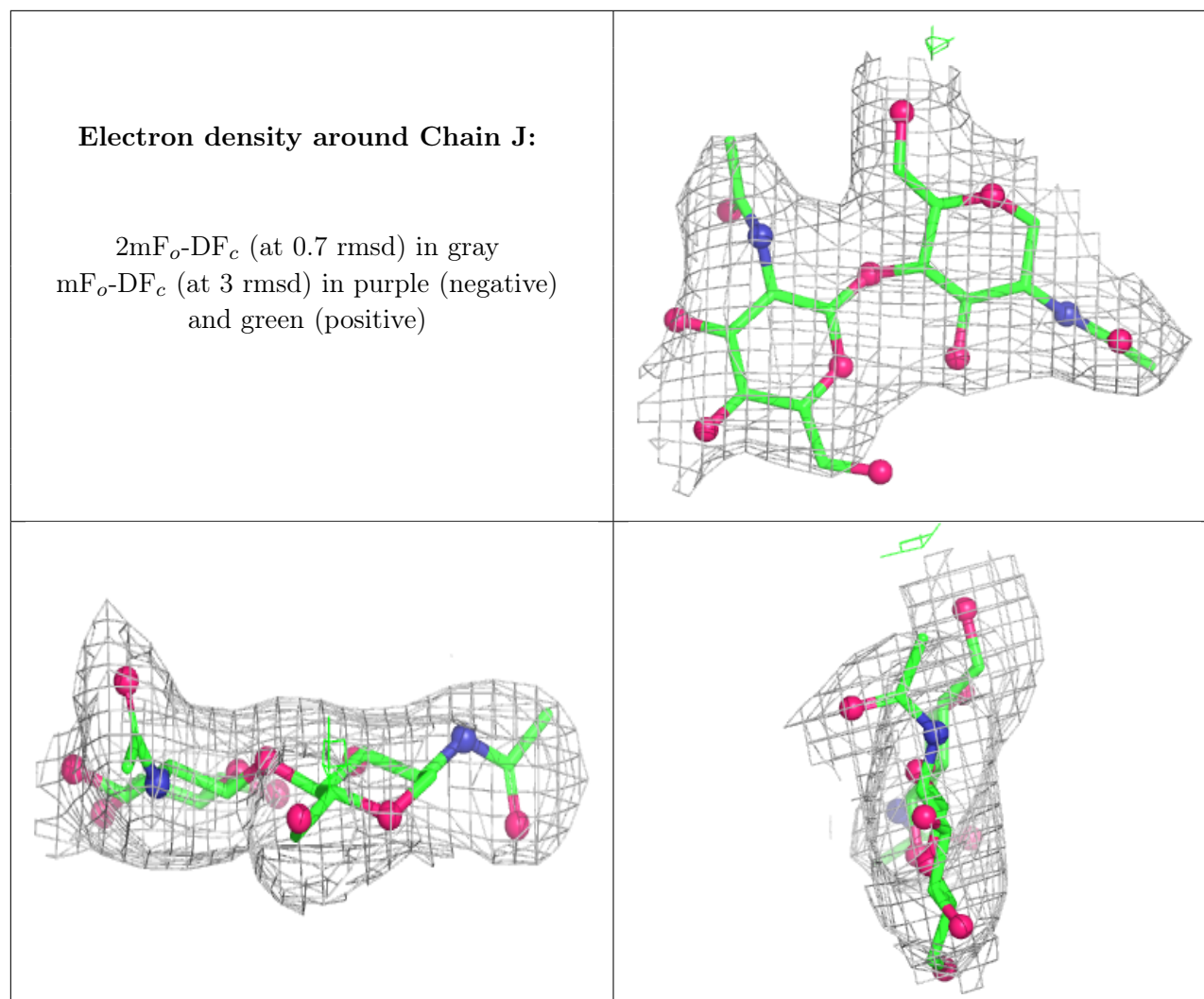
6.3 Carbohydrates [i](#)

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	I	2	14/15	0.84	0.12	50,55,59,60	0
5	NAG	J	2	14/15	0.84	0.11	62,69,76,78	0
5	NAG	J	1	14/15	0.92	0.08	52,57,60,62	0
5	NAG	I	1	14/15	0.94	0.08	46,48,49,51	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.





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.

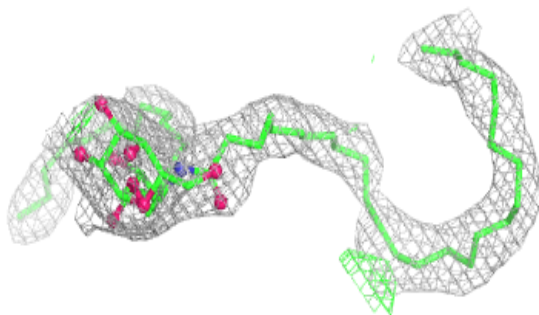
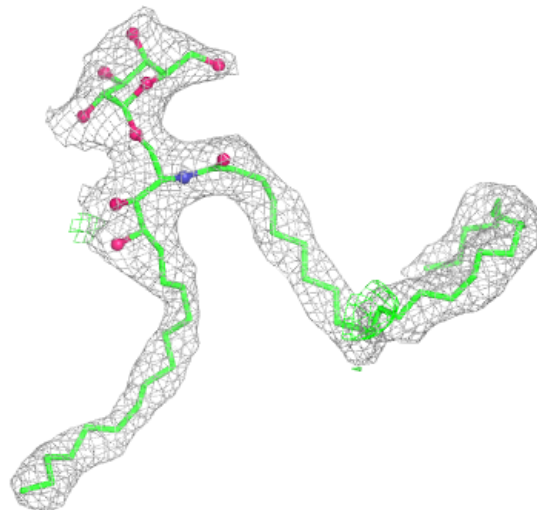
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	E	401	14/15	0.74	0.13	74,78,81,82	0
6	NAG	A	401	14/15	0.77	0.12	70,73,76,76	0
6	NAG	E	402	14/15	0.87	0.11	49,51,53,54	0
6	NAG	A	402	14/15	0.89	0.11	45,48,51,51	0
7	AGH	E	405	60/60	0.94	0.12	23,28,40,41	0
7	AGH	A	405	60/60	0.95	0.10	14,22,36,37	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.

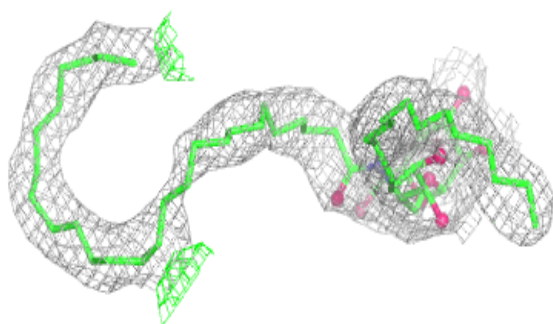
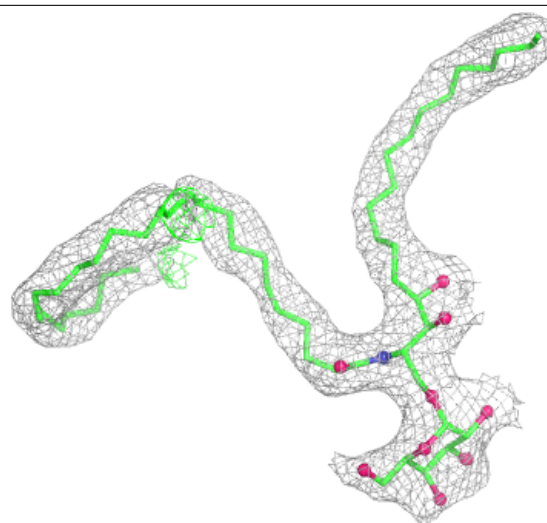
Electron density around AGH E 405:

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



Electron density around AGH A 405:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.