



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:57 PM UTC

PDB ID : 3RTQ / pdb_00003rtq
Title : Structure of the mouse CD1d-HS44-iNKT TCR complex
Authors : Yu, E.D.; Zajonc, D.M.
Deposited on : 2011-05-03
Resolution : 2.80 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

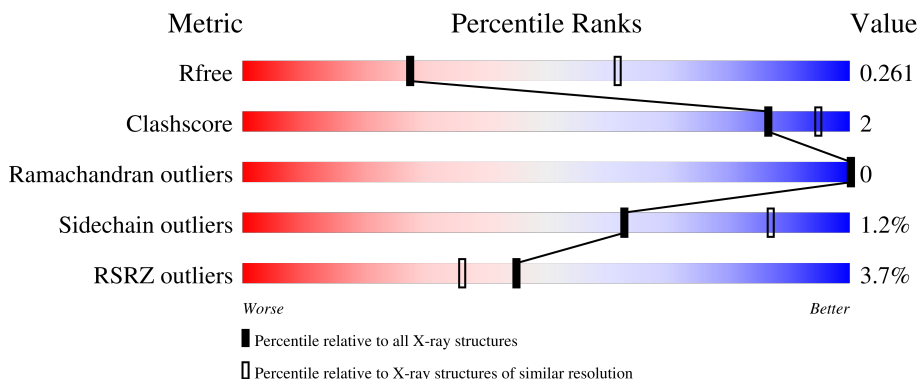
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	285	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 84% 10% 6%</p>
2	B	99	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 96% ..</p>
3	C	209	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10% 90% 7% .</p>
4	D	241	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">94% 5% .</p>
5	E	2	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">50% 50%</p>

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Mol	Chain	Length	Quality of chain
6	F	4	 25% 75%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6588 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
			Total	C	N	O	S			
1	A	268	2129	1359	363	394	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	96	775	495	130	144	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	variant	UNP P01887

- Molecule 3 is a protein called Valpha14 (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	203	1535	953	263	311	8	0	0	0

- Molecule 4 is a protein called V beta8.2 (mouse variable domain, human constant domain).

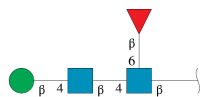
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	239	1873	1175	332	360	6	0	0	0

- 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
			Total	C	N	O	S			
5	E	2	28	16	2	10		0	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



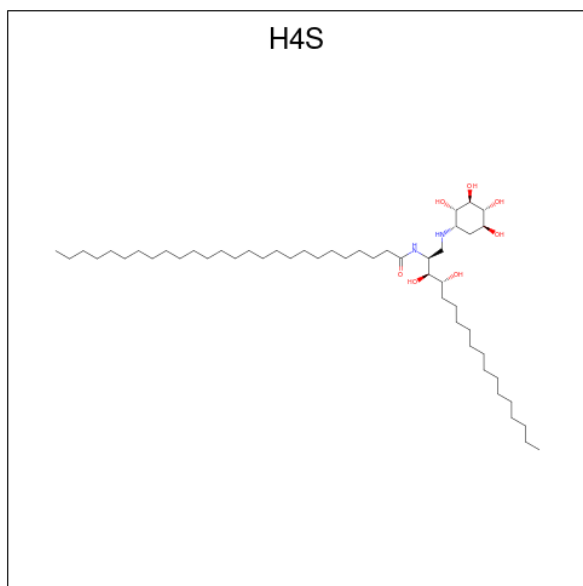
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	4	49	28	2	19		0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is N-[(2S,3S,4R)-3,4-dihydroxy-1-{[(1S,2S,3R,4R,5S)-2,3,4,5-tetrahydroxycyclohexyl]amino}octadecan-2-yl]hexacosanamide (CCD ID: H4S) (formula: $C_{50}H_{100}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			59	50	2	7		

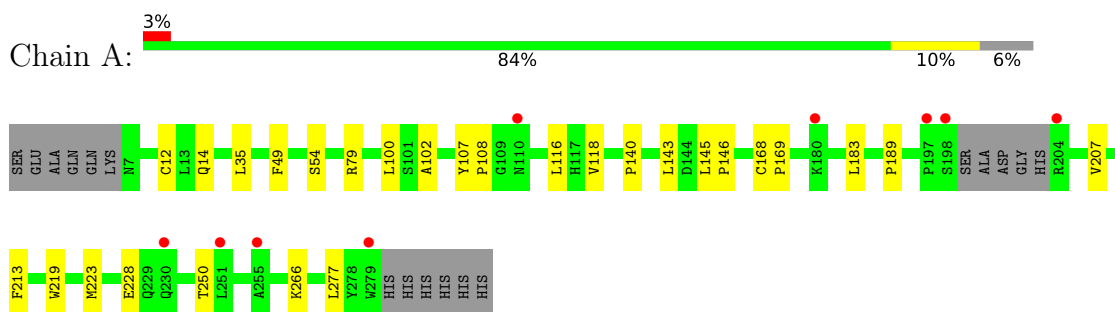
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	41	Total O 41 41	0	0
9	B	13	Total O 13 13	0	0
9	C	34	Total O 34 34	0	0
9	D	38	Total O 38 38	0	0

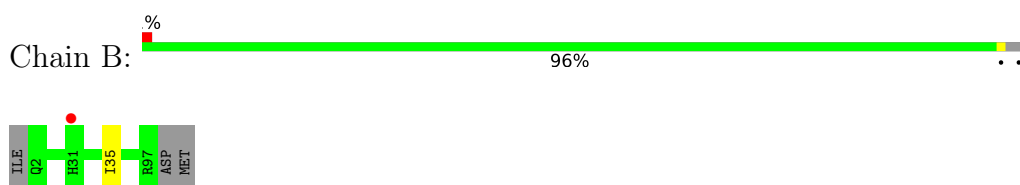
3 Residue-property plots [i](#)

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.

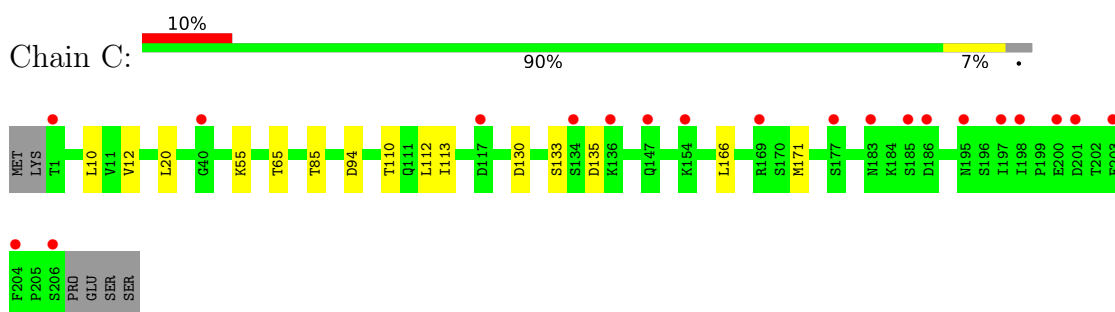
- Molecule 1: Antigen-presenting glycoprotein CD1d1



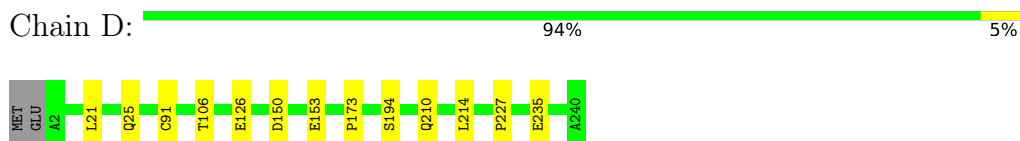
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Valpha14 (mouse variable domain, human constant domain)



- Molecule 4: V beta8.2 (mouse variable domain, human constant domain)




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

Chain E:  50% 50%

MAG1
MAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-a-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  25% 75%

MAG1
MAG2
BMA3
FUT4

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.78Å 191.66Å 150.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.41 – 2.80 35.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.41-2.80) 99.4 (35.41-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.227 , 0.268 0.222 , 0.261	Depositor DCC
R_{free} test set	1171 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6588	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: BMA, H4S, FUL, 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	0.38	0/2191	0.69	0/2983
2	B	0.41	0/801	0.66	0/1094
3	C	0.41	0/1563	0.69	0/2128
4	D	0.41	0/1924	0.68	2/2623 (0.1%)
All	All	0.40	0/6479	0.68	2/8828 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	126	GLU	CA-C-N	5.29	125.30	119.90
4	D	126	GLU	C-N-CA	5.29	125.30	119.90

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	2129	0	2009	16	0
2	B	775	0	719	0	0
3	C	1535	0	1447	7	0
4	D	1873	0	1770	5	0
5	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	49	0	43	0	0
7	A	14	0	13	0	0
8	A	59	0	100	2	0
9	A	41	0	0	0	0
9	B	13	0	0	0	0
9	C	34	0	0	0	0
9	D	38	0	0	0	0
All	All	6588	0	6126	26	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 (26) 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:A:219:TRP:HB3	1:A:266:LYS:HB2	1.83	0.61
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.87	0.55
1:A:140:PRO:HD2	1:A:143:LEU:HD12	1.89	0.54
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.92	0.52
3:C:85:THR:HG23	3:C:113:ILE:HA	1.92	0.51
4:D:150:ASP:HB2	4:D:173:PRO:HG2	1.92	0.51
4:D:214:LEU:HD13	4:D:227:PRO:HG2	1.92	0.50
3:C:20:LEU:HD22	3:C:110:THR:HG21	1.93	0.50
1:A:102:ALA:HB2	1:A:116:LEU:HD13	1.93	0.49
1:A:12:CYS:HB3	8:A:293:H4S:HBSA	1.94	0.49
3:C:130:ASP:HB3	3:C:133:SER:O	2.12	0.49
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.94	0.48
3:C:10:LEU:HD23	3:C:112:LEU:HD13	1.95	0.48
1:A:223:MET:HG2	1:A:228:GLU:HA	1.94	0.48
3:C:171:MET:HE1	4:D:194:SER:HB3	1.96	0.47
1:A:207:VAL:HG22	1:A:250:THR:HG22	1.99	0.45
3:C:55:LYS:HG2	3:C:65:THR:HG22	1.99	0.45
1:A:79:ARG:HH22	3:C:94:ASP:CG	2.26	0.44
4:D:21:LEU:HD22	4:D:106:THR:HG21	1.98	0.44
4:D:153:GLU:HB2	4:D:210:GLN:HB3	2.00	0.43
1:A:14:GLN:HB3	1:A:100:LEU:HB2	2.00	0.43
1:A:14:GLN:HB2	8:A:293:H4S:HBR	2.01	0.42
1:A:35:LEU:HD12	1:A:183:LEU:HD23	2.02	0.41
1:A:49:PHE:CD1	1:A:54:SER:HB2	2.56	0.41
1:A:145:LEU:HB3	1:A:146:PRO:HD3	2.01	0.41
1:A:100:LEU:HG	1:A:118:VAL:HG22	2.01	0.41

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	264/285 (93%)	261 (99%)	3 (1%)	0	100	100
2	B	94/99 (95%)	94 (100%)	0	0	100	100
3	C	201/209 (96%)	191 (95%)	10 (5%)	0	100	100
4	D	237/241 (98%)	235 (99%)	2 (1%)	0	100	100
All	All	796/834 (95%)	781 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/249 (91%)	226 (100%)	1 (0%)	84	94
2	B	85/93 (91%)	84 (99%)	1 (1%)	63	87
3	C	171/188 (91%)	168 (98%)	3 (2%)	51	82
4	D	202/208 (97%)	199 (98%)	3 (2%)	57	84
All	All	685/738 (93%)	677 (99%)	8 (1%)	63	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	LEU
2	B	35	ILE
3	C	12	VAL
3	C	135	ASP
3	C	166	LEU
4	D	25	GLN
4	D	91	CYS
4	D	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	55	GLN
1	A	186	GLN
1	A	240	ASN
1	A	248	GLN
1	A	273	GLN
2	B	24	ASN
2	B	34	HIS
2	B	67	HIS
3	C	2	GLN
3	C	23	ASN
3	C	30	ASN
4	D	172	GLN
4	D	208	GLN
4	D	210	GLN

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](#)

6 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	E	1	5,1	14,14,15	0.51	0	17,19,21	0.86	1 (5%)
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.75	0
6	NAG	F	1	6,1	14,14,15	0.53	0	17,19,21	0.93	1 (5%)
6	NAG	F	2	6	14,14,15	0.60	0	17,19,21	1.06	1 (5%)
6	BMA	F	3	6	11,11,12	0.58	0	15,15,17	1.00	1 (6%)
6	FUL	F	4	6	10,10,11	0.68	0	14,14,16	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	FUL	F	4	6	-	-	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(°)
6	F	2	NAG	C4-C3-C2	3.30	115.85	111.02
6	F	3	BMA	C1-O5-C5	3.01	116.23	112.19
5	E	1	NAG	C1-O5-C5	2.62	115.69	112.19
6	F	1	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

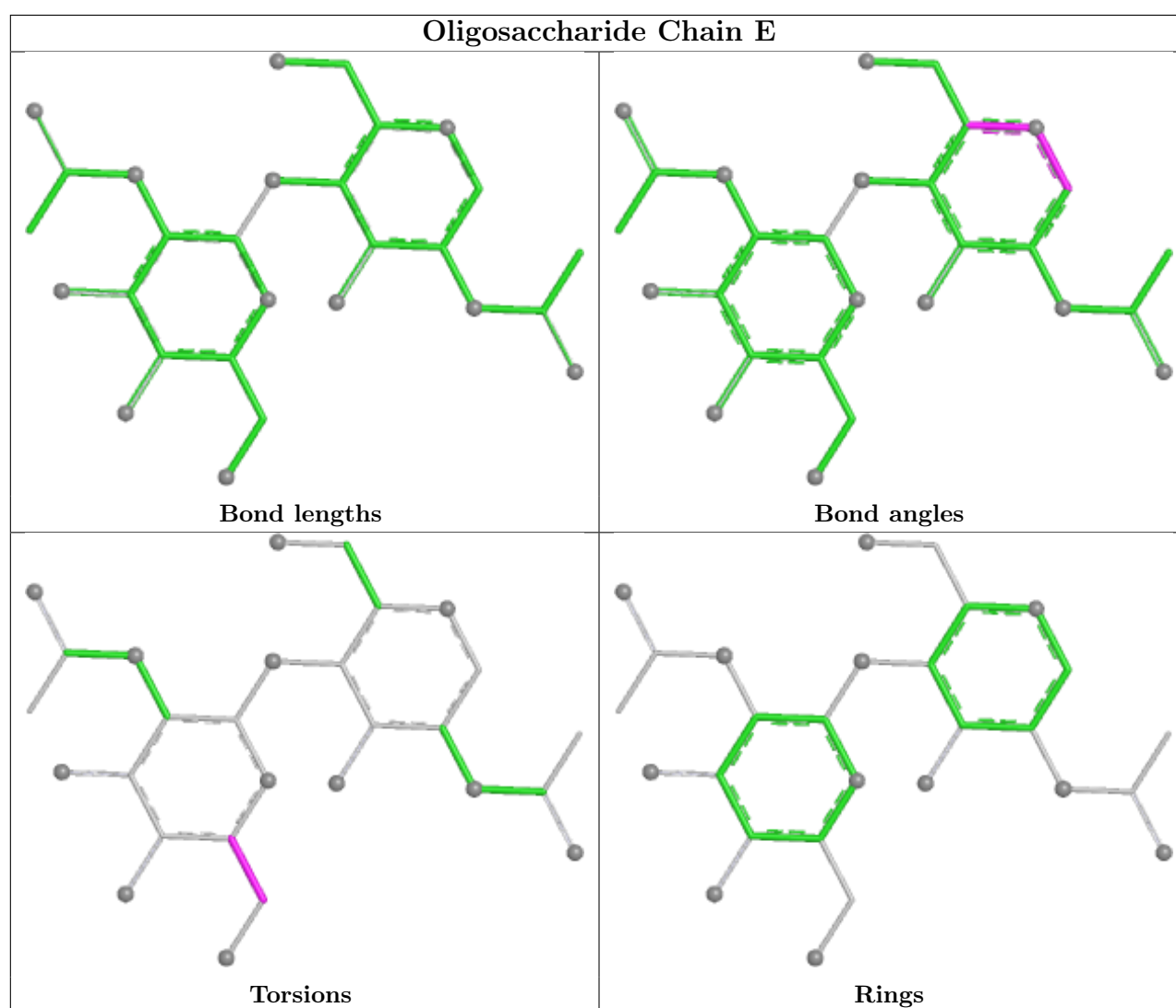
All (6) torsion outliers are listed below:

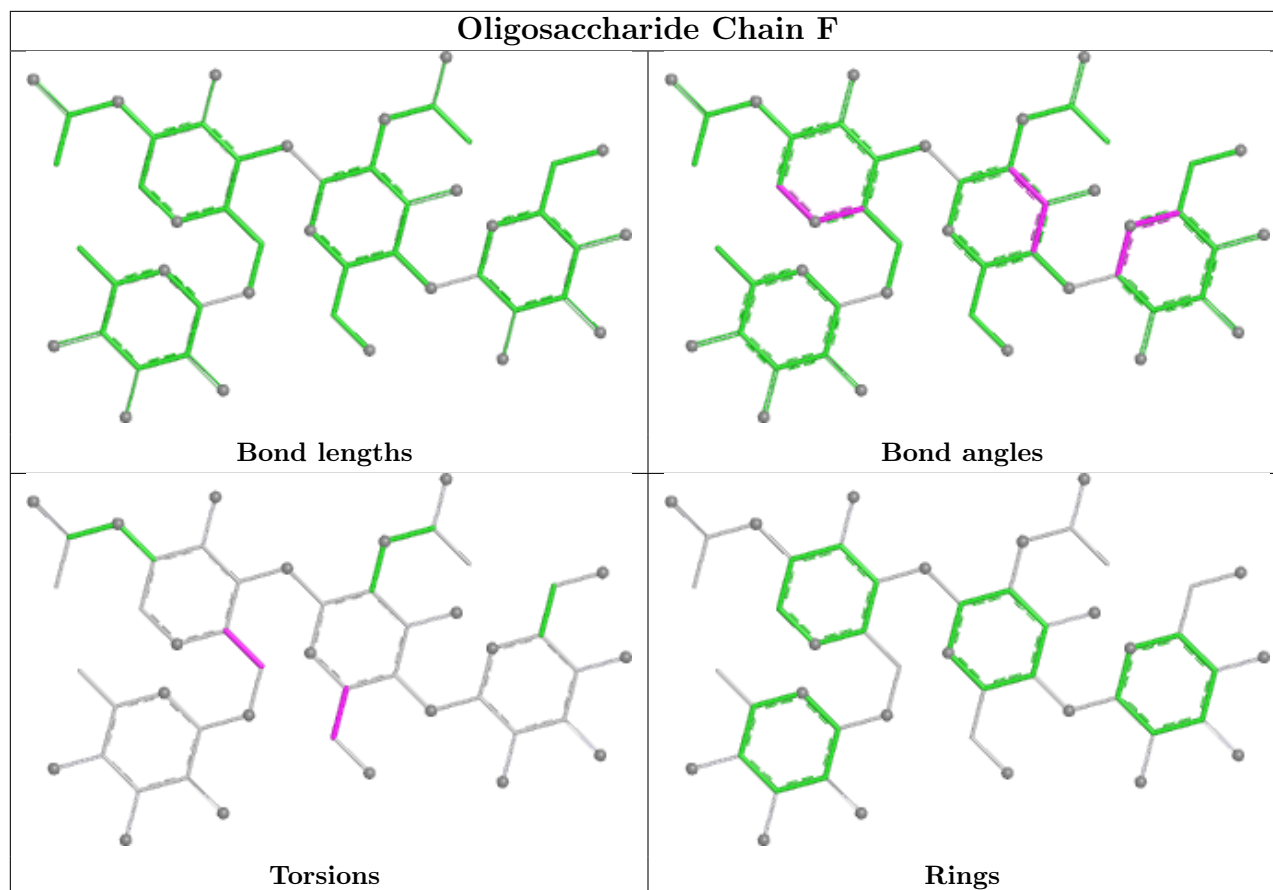
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
7	NAG	A	286	1	14,14,15	0.50	0	17,19,21	0.82	0
8	H4S	A	293	-	59,59,59	0.44	0	65,68,68	0.68	1 (1%)

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
7	NAG	A	286	1	-	2/6/23/26	0/1/1/1
8	H4S	A	293	-	-	23/56/76/76	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	293	H4S	CAC-CAB-NAA	-2.44	107.63	112.68

There are no chirality outliers.

All (25) torsion outliers are listed below:

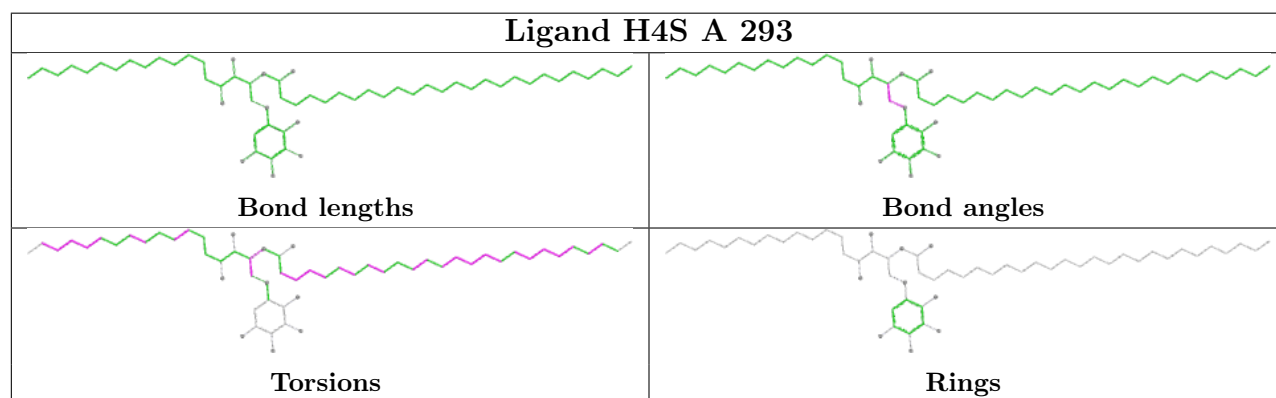
Mol	Chain	Res	Type	Atoms
8	A	293	H4S	CAO-CBH-CBI-CBJ
8	A	293	H4S	NAA-CAB-CAC-CAD
8	A	293	H4S	CBK-CBL-CBM-CBN
8	A	293	H4S	CBT-CBU-CBV-CBW
8	A	293	H4S	CAX-CAY-CAZ-CBA
8	A	293	H4S	CCB-CCC-CCD-CCE
8	A	293	H4S	CBY-CBZ-CCA-CCB
8	A	293	H4S	CBP-CBQ-CBR-CBS
8	A	293	H4S	CBB-CBC-CBD-CBE
8	A	293	H4S	CBS-CBT-CBU-CBV
7	A	286	NAG	C4-C5-C6-O6
8	A	293	H4S	CBH-CBI-CBJ-CBK
8	A	293	H4S	CBW-CBX-CBY-CBZ
8	A	293	H4S	CBC-CBD-CBE-CBF
8	A	293	H4S	CBM-CBN-CBO-CBP
8	A	293	H4S	CBU-CBV-CBW-CBX
8	A	293	H4S	CBR-CBS-CBT-CBU
7	A	286	NAG	O5-C5-C6-O6
8	A	293	H4S	CAB-CAC-NAN-CAO
8	A	293	H4S	CBI-CBJ-CBK-CBL
8	A	293	H4S	CBZ-CCA-CCB-CCC
8	A	293	H4S	CAU-CAV-CAW-CAX
8	A	293	H4S	CBD-CBE-CBF-CBG
8	A	293	H4S	CBA-CBB-CBC-CBD
8	A	293	H4S	CBX-CBY-CBZ-CCA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	293	H4S	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

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	268/285 (94%)	0.16	9 (3%) 48 39	23, 38, 86, 105	0
2	B	96/99 (96%)	0.34	1 (1%) 79 72	21, 48, 66, 74	1 (1%)
3	C	203/209 (97%)	0.41	20 (9%) 13 9	24, 39, 90, 114	0
4	D	239/241 (99%)	-0.04	0 100 100	24, 35, 57, 79	0
All	All	806/834 (96%)	0.18	30 (3%) 45 36	21, 38, 80, 114	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	31	HIS	8.4
3	C	197	ILE	4.9
3	C	186	ASP	4.0
1	A	255	ALA	3.6
1	A	197	PRO	3.3
3	C	206	SER	3.3
3	C	185	SER	3.3
3	C	183	ASN	3.2
1	A	279	TRP	3.2
1	A	230	GLN	3.0
3	C	203	PHE	2.9
1	A	198	SER	2.9
3	C	198	ILE	2.9
3	C	200	GLU	2.7
3	C	195	ASN	2.6
1	A	204	ARG	2.6
1	A	110	ASN	2.5
3	C	154	LYS	2.4
3	C	40	GLY	2.3
3	C	177	SER	2.3
3	C	201	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	204	PHE	2.2
3	C	136	LYS	2.2
3	C	134	SER	2.2
1	A	251	LEU	2.2
3	C	169	ARG	2.1
3	C	117	ASP	2.1
3	C	147	GLN	2.0
3	C	1	THR	2.0
1	A	180	LYS	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 [\(i\)](#)

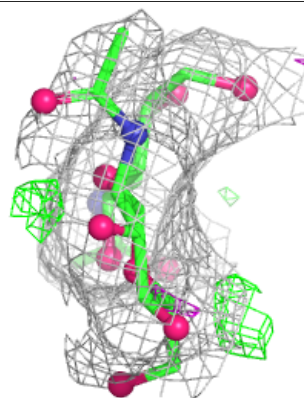
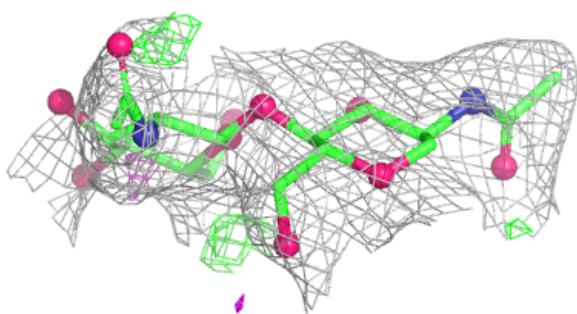
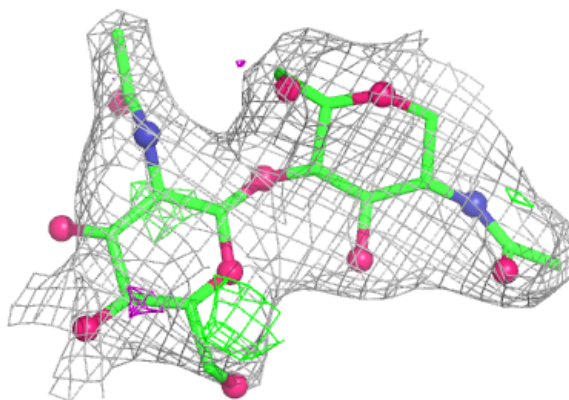
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	F	3	11/12	0.49	0.17	73,77,82,85	0
5	NAG	E	2	14/15	0.68	0.17	51,58,64,64	0
6	FUL	F	4	10/11	0.76	0.14	49,53,56,59	0
6	NAG	F	2	14/15	0.83	0.11	58,62,67,71	0
6	NAG	F	1	14/15	0.92	0.09	50,54,57,57	0
5	NAG	E	1	14/15	0.92	0.10	43,47,51,51	0

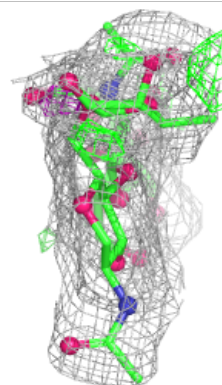
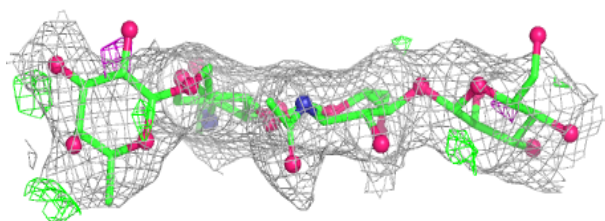
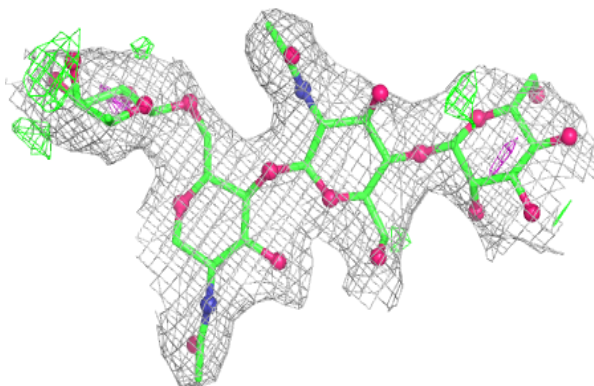
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

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

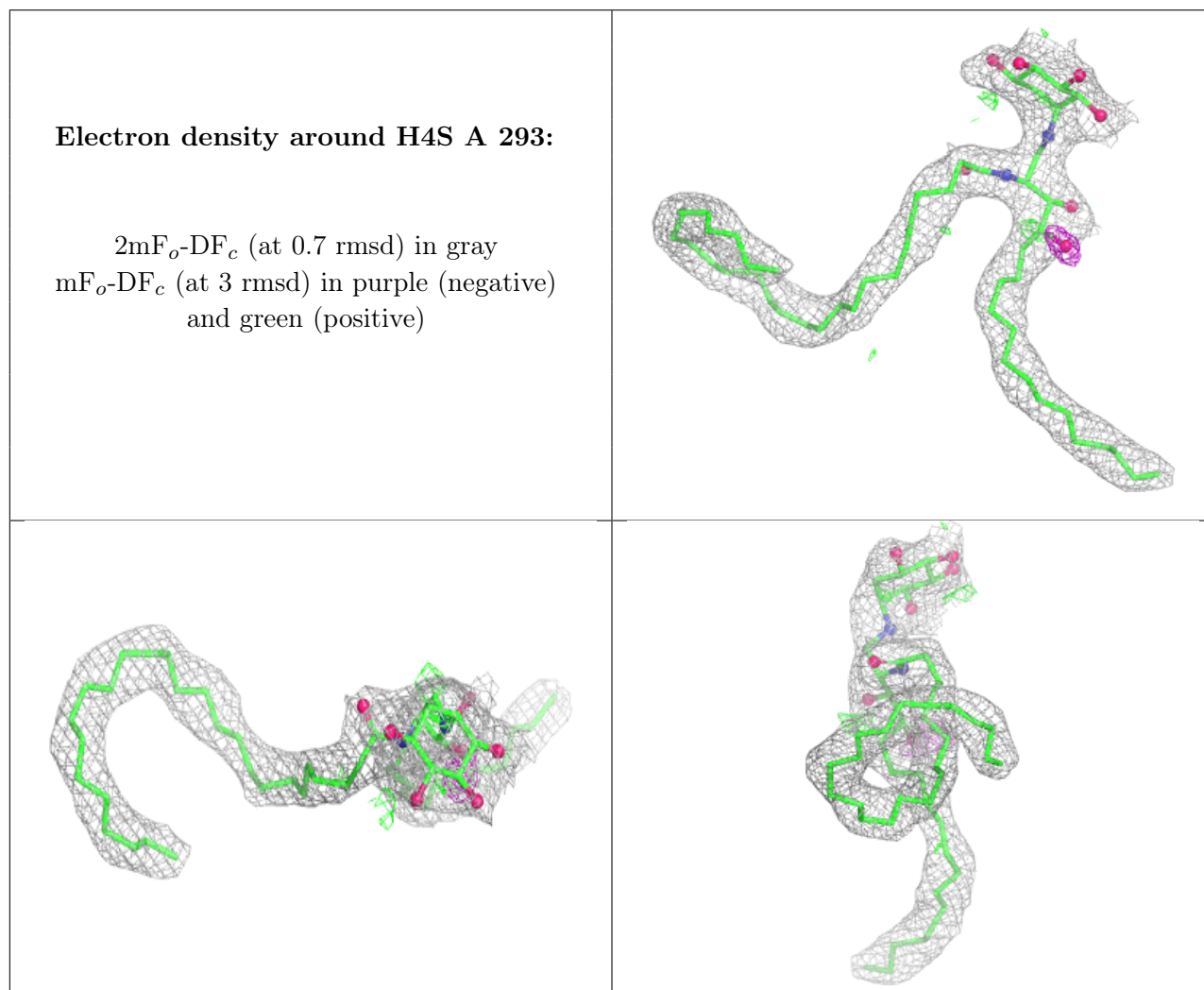


6.4 Ligands [i](#)

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
7	NAG	A	286	14/15	0.84	0.10	56,61,65,67	0
8	H4S	A	293	59/59	0.92	0.11	29,31,35,36	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.