



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:40 AM EDT

PDB ID : 8XX0 / pdb_00008xx0
Title : Crystal structure of anti-IgE antibody HMK-12 Fab complexed with IgE F(ab')₂
Authors : Hirano, T.; Koyanagi, A.; Kasai, M.; Okumura, K.
Deposited on : 2024-01-17
Resolution : 2.90 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

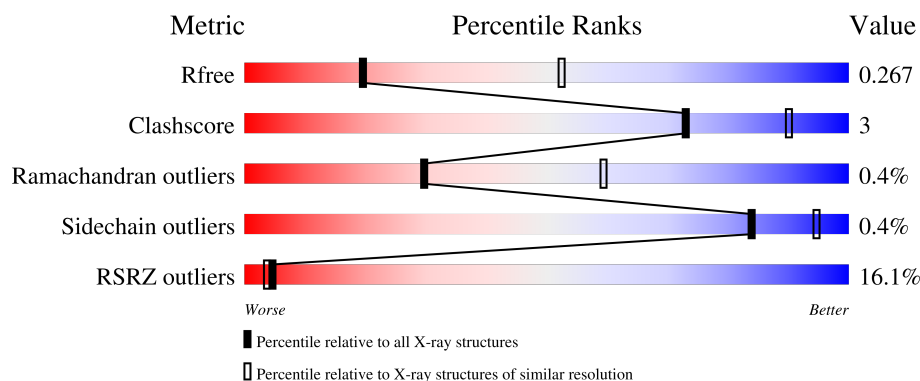
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	L	214	4% 93% 7%
2	H	225	3% 91% 8%
3	A	321	32% 84% 12%
4	B	215	16% 90% 8%
5	C	2	100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7558 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 anti-IgE antibody HMK-12 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	4	0
			1667	1036	284	341	6			

- Molecule 2 is a protein called anti-IgE antibody HMK-12 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1694	1076	279	332	7			

- Molecule 3 is a protein called SPE7 immunoglobulin E F(ab')₂ heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	311	Total	C	N	O	S	0	1	0
			2436	1547	402	470	17			

- Molecule 4 is a protein called SPE7 immunoglobulin E F(ab')₂ light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	211	Total	C	N	O	S	0	2	0
			1601	1002	270	323	6			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



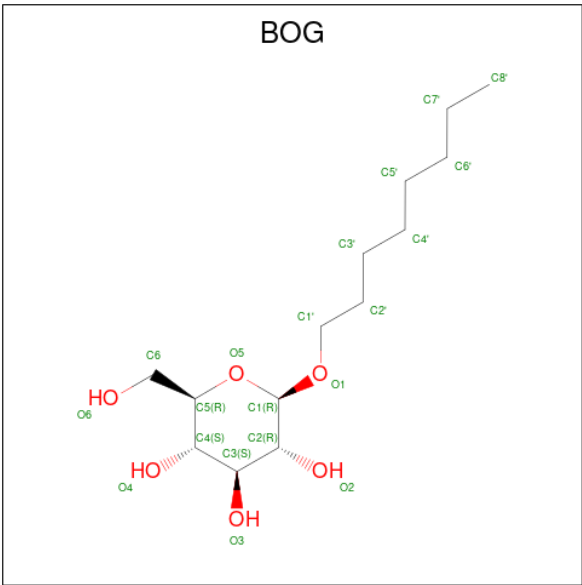
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	C O	0	0
			20	14 6		

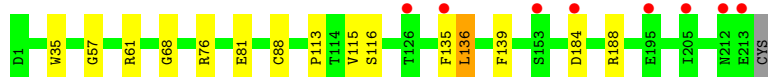
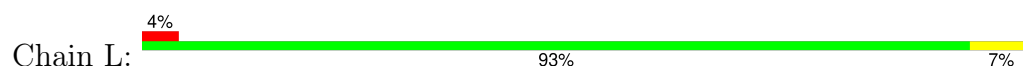
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	28	Total	O	0	0
			28	28		
8	H	22	Total	O	0	0
			22	22		
8	A	19	Total	O	0	0
			19	19		
8	B	7	Total	O	0	0
			7	7		

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.

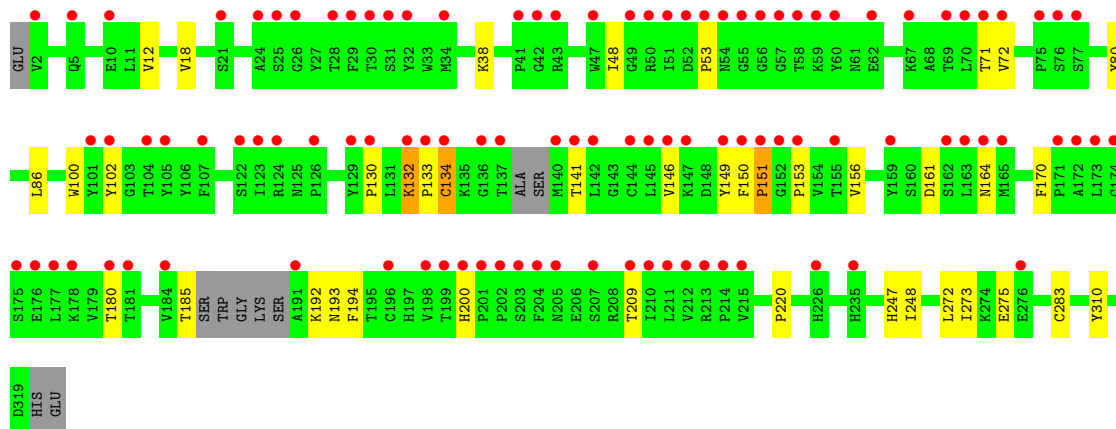
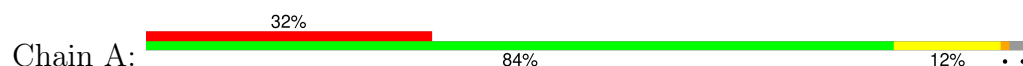
- Molecule 1: anti-IgE antibody HMK-12 Fab light chain



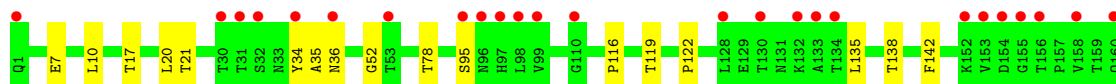
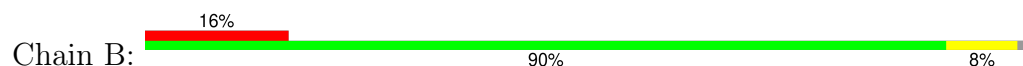
- Molecule 2: anti-IgE antibody HMK-12 Fab heavy chain

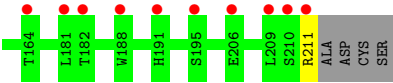


- Molecule 3: SPE7 immunoglobulin E F(ab')₂ heavy chain



- Molecule 4: SPE7 immunoglobulin E F(ab')₂ light chain





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

Chain C:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	282.05Å 86.09Å 56.06Å 90.00° 97.19° 90.00°	Depositor
Resolution (Å)	49.60 – 2.90 49.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.60-2.90) 99.9 (49.60-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.267 0.225 , 0.267	Depositor DCC
R_{free} test set	1920 reflections (6.46%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	1.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7558	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: EDO, BOG, 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	L	0.11	0/1714	0.31	0/2320
2	H	0.11	0/1742	0.37	0/2383
3	A	0.12	0/2503	0.36	0/3409
4	B	0.11	0/1642	0.33	0/2242
All	All	0.11	0/7601	0.34	0/10354

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	150	PHE	Peptide

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	L	1667	0	1608	8	0
2	H	1694	0	1646	9	0
3	A	2436	0	2336	23	0
4	B	1601	0	1561	11	0
5	C	28	0	25	0	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
6	H	16	0	24	0	0
6	L	12	0	18	1	0
7	H	20	0	28	0	0
8	A	19	0	0	0	0
8	B	7	0	0	0	0
8	H	22	0	0	0	0
8	L	28	0	0	0	0
All	All	7558	0	7258	47	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 3.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:151:PRO:HG2	3:A:153:PRO:HD2	1.72	0.72
3:A:161:ASP:HB2	3:A:192:LYS:HB3	1.69	0.71
3:A:273:ILE:HD11	3:A:283:CYS:HB2	1.74	0.68
1:L:57:GLY:H	6:L:303:EDO:H12	1.59	0.68
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.82	0.61
3:A:38:LYS:HB2	3:A:48:ILE:HD11	1.84	0.58
2:H:61:TYR:HB3	2:H:69:ILE:HD11	1.87	0.57
3:A:156:VAL:HG11	3:A:180:THR:HG21	1.86	0.56
3:A:164:ASN:HB3	3:A:185:THR:HB	1.87	0.56
3:A:247:HIS:ND1	3:A:248:ILE:O	2.38	0.55
3:A:193:ASN:OD1	3:A:194:PHE:N	2.43	0.52
4:B:10:LEU:HD12	4:B:20:LEU:HG	1.92	0.52
3:A:132:LYS:O	4:B:122:PRO:HD2	2.11	0.50
2:H:38:TRP:CD1	2:H:82:LEU:HB2	2.48	0.49
3:A:151:PRO:HD2	3:A:200:HIS:CE1	2.49	0.48
3:A:272:LEU:HD21	3:A:275:GLU:HG3	1.95	0.47
4:B:122:PRO:HA	4:B:135:LEU:HD23	1.95	0.47
3:A:12:VAL:HG21	3:A:86:LEU:HD13	1.96	0.47
4:B:116:PRO:HB3	4:B:142:PHE:HB3	1.97	0.46
2:H:69:ILE:HG22	2:H:84:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ARG:HB2	1:L:76:ARG:O	2.16	0.45
2:H:131:PRO:HD3	2:H:216:LYS:HE2	1.98	0.45
2:H:92:THR:HG23	2:H:118:THR:HA	1.99	0.44
3:A:134:CYS:SG	4:B:211[B]:ARG:NH2	2.91	0.44
3:A:141:THR:HG21	4:B:119:THR:HG21	1.99	0.44
3:A:130:PRO:HD3	3:A:209:THR:HG21	1.99	0.44
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.53	0.44
3:A:170:PHE:CZ	4:B:138:THR:HB	2.53	0.44
1:L:113:PRO:HB3	1:L:139:PHE:HB3	2.00	0.43
3:A:53:PRO:HA	3:A:72:VAL:HG21	2.00	0.43
3:A:71:THR:HB	3:A:80:TYR:HB2	1.99	0.43
3:A:133:PRO:HB3	3:A:141:THR:O	2.20	0.42
1:L:61:ARG:NH2	1:L:81[B]:GLU:OE2	2.53	0.42
2:H:33:SER:HA	2:H:55:TYR:CE1	2.55	0.42
3:A:12:VAL:HG11	3:A:18:VAL:HB	2.02	0.42
4:B:34:TYR:O	4:B:36:ASN:ND2	2.53	0.42
4:B:35:ALA:N	4:B:52:GLY:O	2.53	0.41
2:H:152:GLY:HA2	2:H:182:LEU:HB3	2.02	0.41
1:L:115:VAL:HA	1:L:135:PHE:O	2.19	0.41
1:L:115:VAL:HG13	1:L:136:LEU:HD23	2.03	0.41
2:H:100:HIS:HB3	2:H:108:MET:SD	2.61	0.41
3:A:146:VAL:HG12	3:A:149:TYR:CD2	2.56	0.41
3:A:100:TRP:NE1	3:A:102:TYR:O	2.53	0.41
3:A:220:PRO:HD2	3:A:310:TYR:CZ	2.56	0.41
1:L:184:ASP:O	1:L:188:ARG:HG3	2.21	0.40
4:B:7:GLU:OE2	4:B:21:THR:OG1	2.26	0.40
4:B:17:THR:HG22	4:B:78:THR:HA	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	L	215/214 (100%)	211 (98%)	3 (1%)	1 (0%)	24	54
2	H	220/225 (98%)	216 (98%)	4 (2%)	0	100	100
3	A	306/321 (95%)	288 (94%)	16 (5%)	2 (1%)	18	48
4	B	210/215 (98%)	195 (93%)	14 (7%)	1 (0%)	24	54
All	All	951/975 (98%)	910 (96%)	37 (4%)	4 (0%)	30	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	151	PRO
4	B	95	SER
1	L	68	GLY
3	A	134	CYS

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	L	192/190 (101%)	190 (99%)	2 (1%)	68	89
2	H	194/197 (98%)	194 (100%)	0	100	100
3	A	272/286 (95%)	271 (100%)	1 (0%)	84	94
4	B	180/181 (99%)	180 (100%)	0	100	100
All	All	838/854 (98%)	835 (100%)	3 (0%)	84	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	116	SER
1	L	136	LEU
3	A	132	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
2	H	79	GLN
2	H	83	GLN
3	A	169	ASN
3	A	205	ASN
3	A	291	GLN
4	B	36	ASN
4	B	111	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 ⓘ

2 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	C	1	3,5	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	C	2	5	14,14,15	0.25	0	17,19,21	0.37	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	C	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

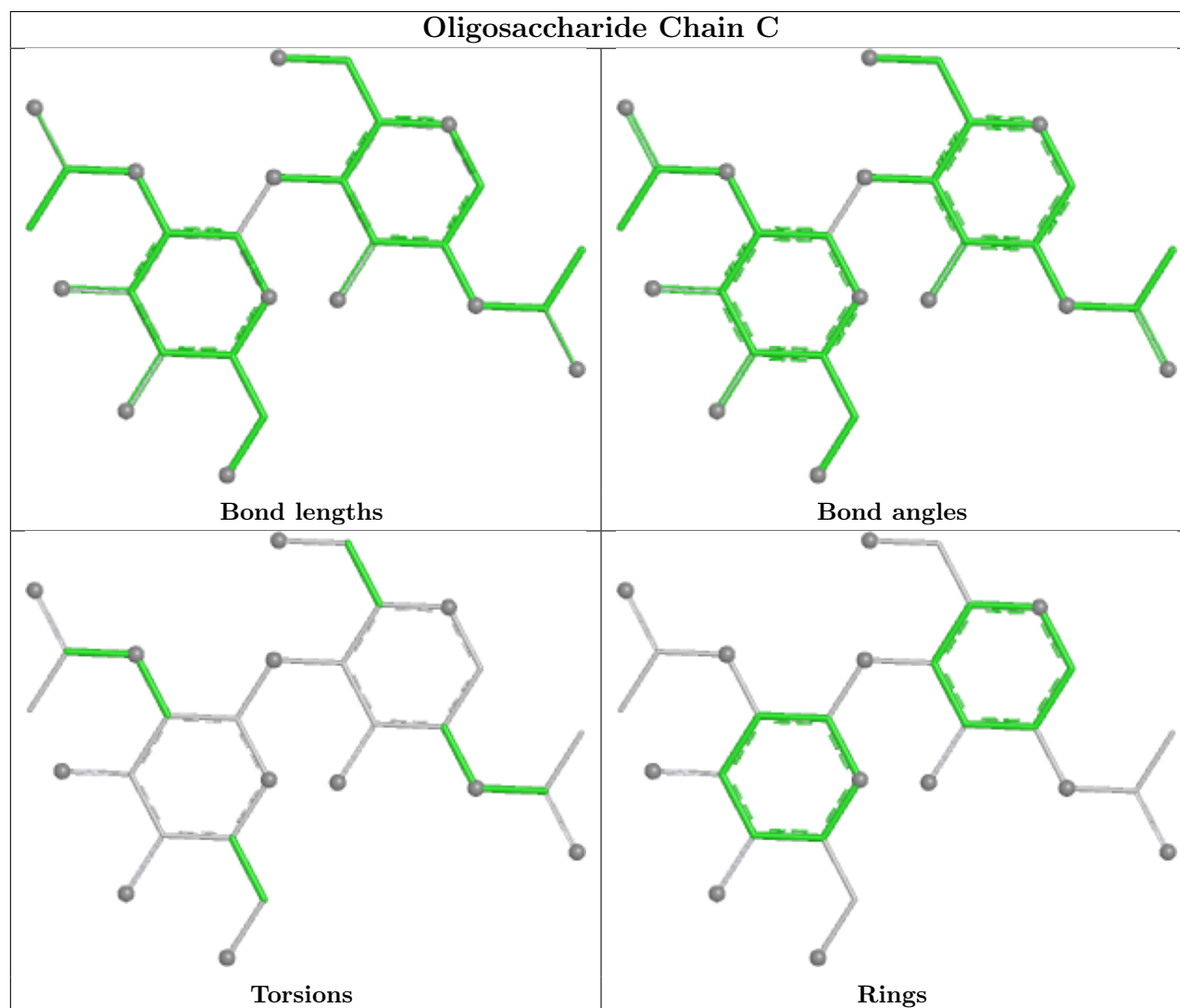
There are no chirality outliers.

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](#)

10 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	EDO	H	301	-	3,3,3	0.42	0	2,2,2	0.39	0
7	BOG	H	305	-	20,20,20	1.30	2 (10%)	25,25,25	0.82	0
6	EDO	H	304	-	3,3,3	0.42	0	2,2,2	0.43	0
6	EDO	L	302	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	H	303	-	3,3,3	0.44	0	2,2,2	0.37	0
6	EDO	H	302	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	L	303	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	B	301	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	L	301	-	3,3,3	0.41	0	2,2,2	0.34	0
6	EDO	A	401	-	3,3,3	0.44	0	2,2,2	0.37	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
6	EDO	H	301	-	-	0/1/1/1	-
7	BOG	H	305	-	-	5/11/31/31	0/1/1/1
6	EDO	H	304	-	-	0/1/1/1	-
6	EDO	L	302	-	-	0/1/1/1	-
6	EDO	H	303	-	-	0/1/1/1	-
6	EDO	H	302	-	-	0/1/1/1	-
6	EDO	L	303	-	-	0/1/1/1	-
6	EDO	B	301	-	-	0/1/1/1	-
6	EDO	L	301	-	-	0/1/1/1	-
6	EDO	A	401	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	305	BOG	O5-C1	4.24	1.52	1.41
7	H	305	BOG	O1-C1	-2.33	1.36	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

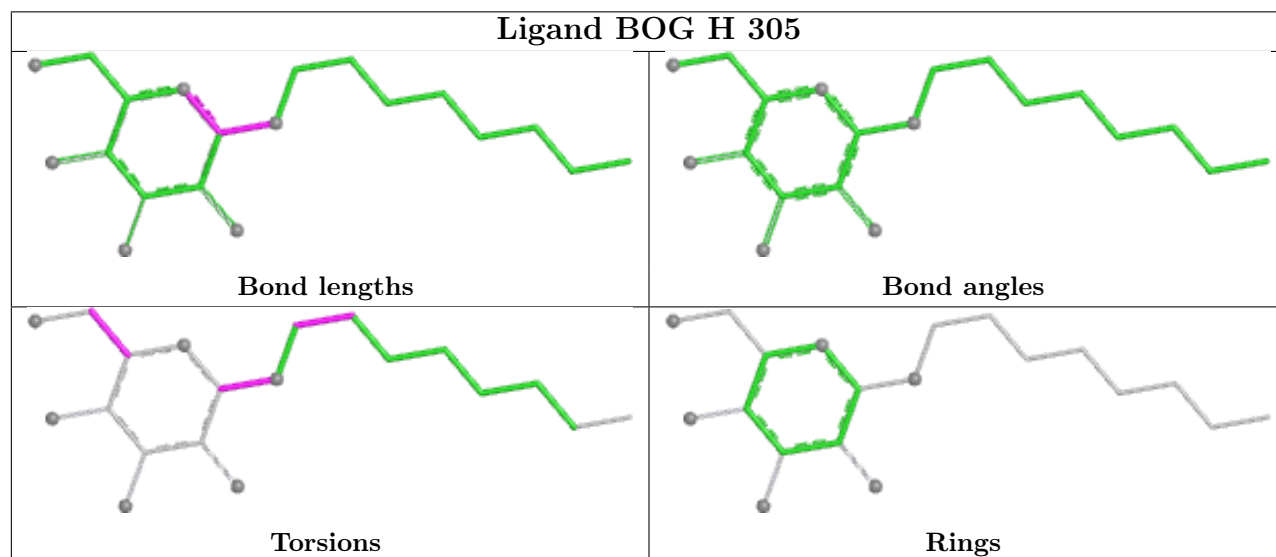
Mol	Chain	Res	Type	Atoms
7	H	305	BOG	C2-C1-O1-C1'
7	H	305	BOG	O5-C1-O1-C1'
7	H	305	BOG	O5-C5-C6-O6
7	H	305	BOG	C4-C5-C6-O6
7	H	305	BOG	O1-C1'-C2'-C3'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	303	EDO	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	L	213/214 (99%)	0.17	8 (3%)	44	36	22, 42, 87, 123	4 (1%)
2	H	222/225 (98%)	0.11	7 (3%)	50	41	24, 42, 62, 101	0
3	A	311/321 (96%)	1.38	104 (33%)	1	1	26, 88, 141, 170	1 (0%)
4	B	211/215 (98%)	0.88	35 (16%)	4	3	41, 65, 143, 178	2 (0%)
All	All	957/975 (98%)	0.71	154 (16%)	4	4	22, 54, 131, 178	7 (0%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	152	GLY	5.3
3	A	49	GLY	5.3
4	B	156	THR	4.8
3	A	72	VAL	4.8
4	B	158	VAL	4.7
3	A	204	PHE	4.5
3	A	198	VAL	4.3
3	A	25	SER	4.2
3	A	151	PRO	4.2
3	A	212	VAL	4.2
1	L	135	PHE	4.2
3	A	153	PRO	4.1
4	B	1	GLN	4.0
3	A	137	THR	4.0
3	A	71	THR	4.0
3	A	159	TYR	3.9
3	A	53	PRO	3.9
3	A	57	GLY	3.9
3	A	150	PHE	3.8
3	A	207	SER	3.7
4	B	155	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
3	A	181	THR	3.7
4	B	211[A]	ARG	3.7
3	A	122	SER	3.6
3	A	56	GLY	3.6
4	B	96	ASN	3.6
3	A	155	THR	3.6
3	A	199	THR	3.6
3	A	213	ARG	3.5
4	B	164	THR	3.5
3	A	55	GLY	3.5
3	A	75	PRO	3.5
3	A	126	PRO	3.5
3	A	173	LEU	3.5
3	A	104	THR	3.4
3	A	180	THR	3.4
3	A	177	LEU	3.4
4	B	154	ASP	3.3
3	A	147	LYS	3.3
3	A	105	TYR	3.2
3	A	51	ILE	3.2
3	A	215	VAL	3.2
4	B	98[A]	LEU	3.2
3	A	41	PRO	3.2
3	A	276	GLU	3.1
3	A	31	SER	3.1
3	A	172	ALA	3.1
3	A	203	SER	3.1
3	A	201	PRO	3.1
3	A	146	VAL	3.0
4	B	210	SER	3.0
3	A	26	GLY	3.0
3	A	210	ILE	3.0
3	A	202	PRO	3.0
3	A	191	ALA	3.0
2	H	222	GLY	3.0
3	A	163	LEU	3.0
3	A	102	TYR	2.9
3	A	171	PRO	2.9
3	A	136	GLY	2.9
3	A	5	GLN	2.9
3	A	178	LYS	2.9
3	A	209	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	34	MET	2.8
3	A	32	TYR	2.8
4	B	36	ASN	2.8
4	B	95	SER	2.8
3	A	132	LYS	2.8
2	H	1	ASP	2.8
3	A	42	GLY	2.8
1	L	212	ASN	2.8
4	B	195	SER	2.8
1	L	184	ASP	2.7
3	A	69	THR	2.7
3	A	101	TYR	2.7
3	A	226	HIS	2.7
2	H	200	THR	2.7
3	A	43	ARG	2.7
3	A	174	GLY	2.7
3	A	124	ARG	2.7
4	B	99	VAL	2.6
4	B	133	ALA	2.6
3	A	30	THR	2.6
3	A	142	LEU	2.6
1	L	195	GLU	2.6
1	L	153	SER	2.6
3	A	47	TRP	2.6
1	L	205	ILE	2.6
3	A	140	MET	2.6
4	B	32	SER	2.5
3	A	28	THR	2.5
3	A	2	VAL	2.5
3	A	184	VAL	2.5
4	B	153	VAL	2.5
4	B	30	THR	2.5
3	A	165	MET	2.4
3	A	149	TYR	2.4
3	A	200	HIS	2.4
3	A	77	SER	2.4
3	A	211	LEU	2.4
3	A	123	ILE	2.4
4	B	53	THR	2.4
2	H	45	ASN	2.4
3	A	59	LYS	2.4
3	A	134	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	54	ASN	2.3
1	L	126	THR	2.3
3	A	133	PRO	2.3
4	B	160	GLN	2.3
3	A	70	LEU	2.3
4	B	181	LEU	2.3
3	A	130	PRO	2.3
3	A	214	PRO	2.3
3	A	176	GLU	2.3
3	A	67	LYS	2.3
4	B	132	LYS	2.3
4	B	152	LYS	2.3
4	B	130	THR	2.3
3	A	129	TYR	2.3
3	A	196	CYS	2.2
3	A	52	ASP	2.2
3	A	235	HIS	2.2
4	B	182	THR	2.2
4	B	188	TRP	2.2
4	B	128	LEU	2.2
3	A	58	THR	2.2
3	A	21	SER	2.2
3	A	175	SER	2.2
1	L	213	GLU	2.2
4	B	206	GLU	2.2
3	A	164	ASN	2.2
4	B	191	HIS	2.2
3	A	62	GLU	2.2
3	A	50	ARG	2.1
3	A	141	THR	2.1
4	B	31	THR	2.1
4	B	134	THR	2.1
3	A	107	PHE	2.1
4	B	209	LEU	2.1
4	B	34	TYR	2.1
3	A	76	SER	2.1
3	A	144	CYS	2.1
4	B	110	GLY	2.1
3	A	24	ALA	2.1
2	H	17	SER	2.1
2	H	33	SER	2.1
3	A	10	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	145	LEU	2.1
2	H	69	ILE	2.1
4	B	97	HIS	2.0
3	A	162	SER	2.0
3	A	205	ASN	2.0
3	A	29	PHE	2.0
3	A	60	TYR	2.0

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

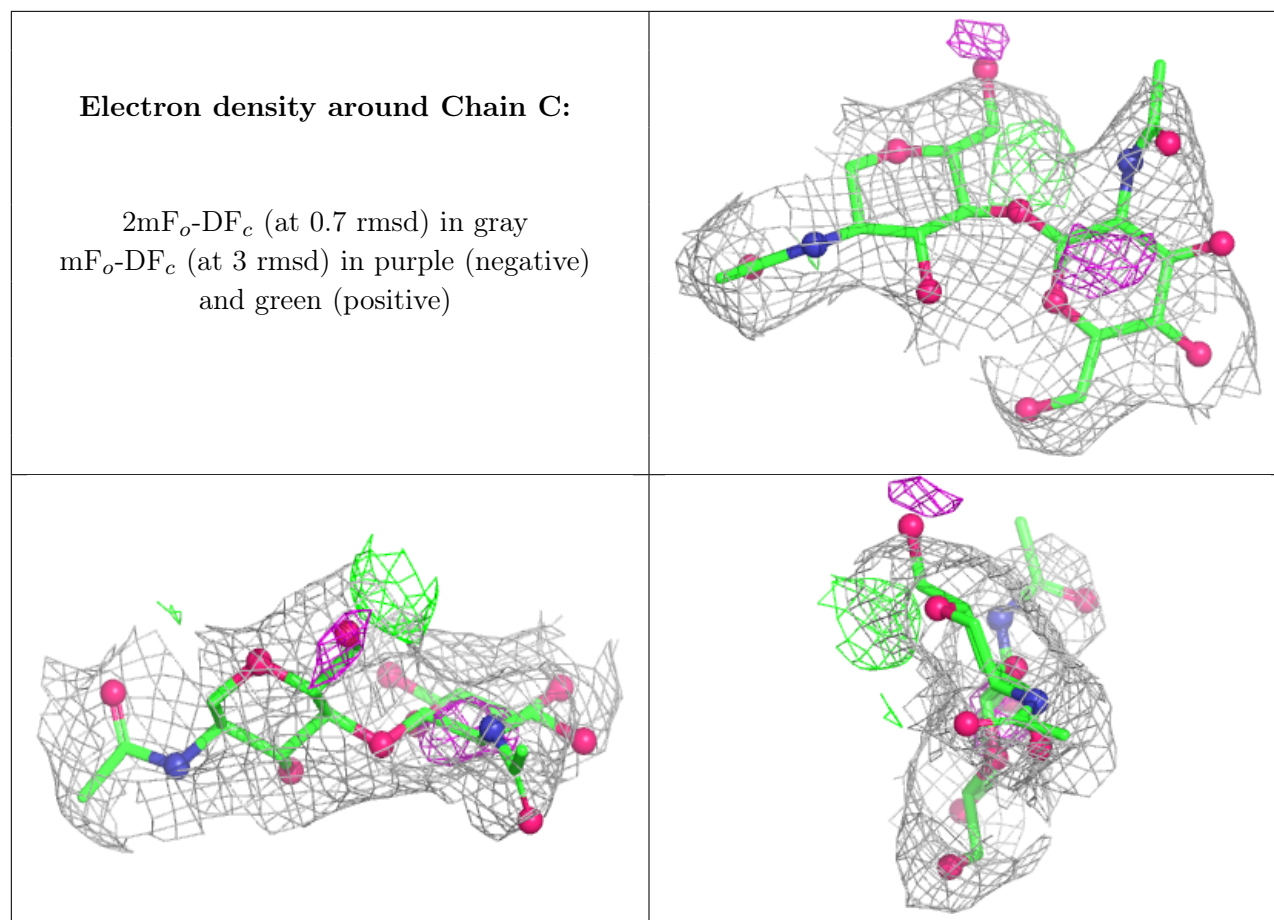
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	1	14/15	-	-	48,56,63,69	0
5	NAG	C	2	14/15	-	-	50,59,63,66	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.



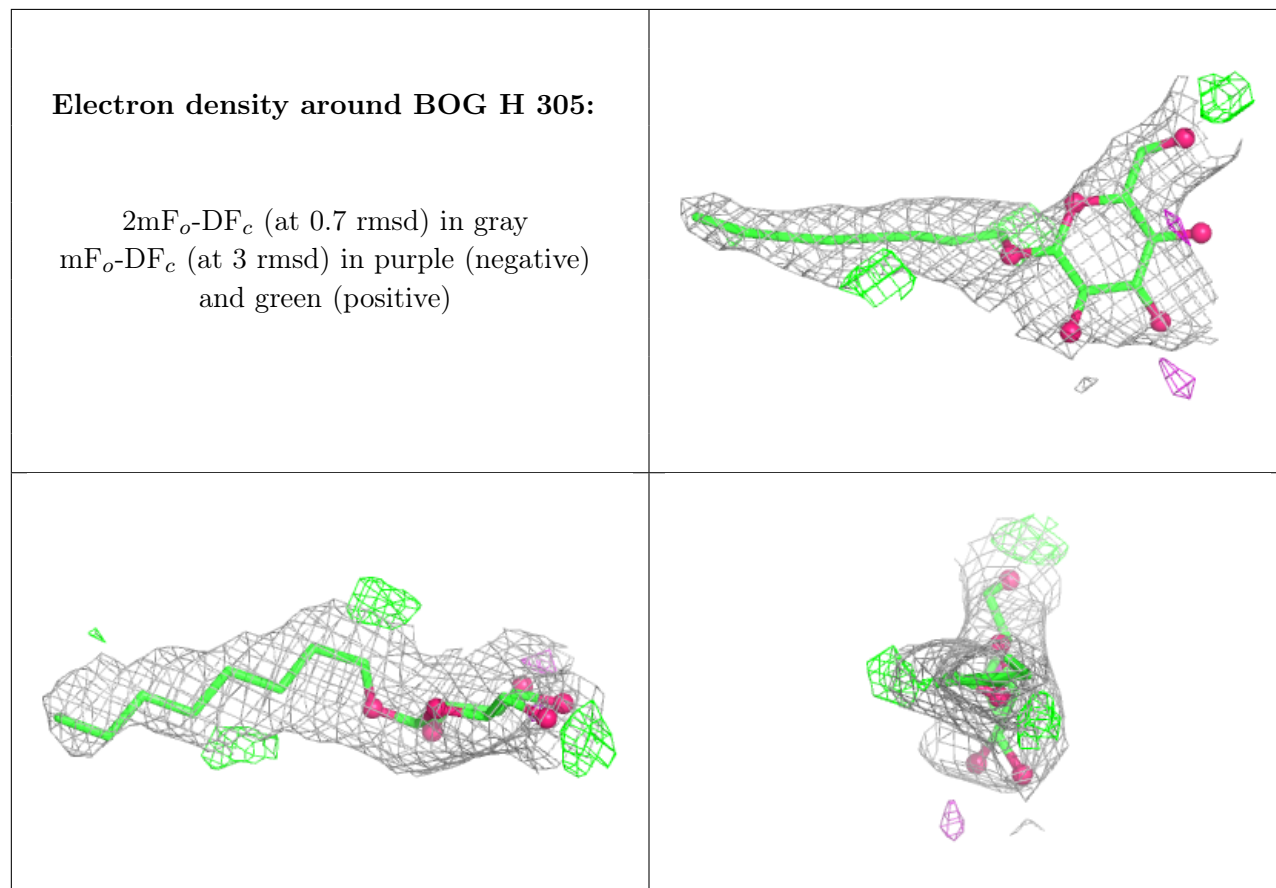
6.4 Ligands [i](#)

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
7	BOG	H	305	20/20	0.67	0.17	44,61,71,75	0
6	EDO	B	301	4/4	0.71	0.21	70,73,76,82	0
6	EDO	A	401	4/4	0.77	0.16	44,46,56,57	0
6	EDO	L	303	4/4	0.78	0.15	38,40,41,43	0
6	EDO	H	301	4/4	0.81	0.28	46,50,51,53	0
6	EDO	H	303	4/4	0.90	0.15	44,44,53,54	0
6	EDO	L	301	4/4	0.90	0.15	33,33,35,37	0
6	EDO	H	304	4/4	0.91	0.13	27,32,32,39	0
6	EDO	H	302	4/4	0.91	0.12	53,57,57,61	0
6	EDO	L	302	4/4	0.93	0.11	30,32,38,42	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 ⓘ

There are no such residues in this entry.