

Full wwPDB X-ray Structure Validation Report (i)

Jul 22, 2024 – 06:12 PM JST

PDB ID : 8XX0

Title: Crystal structure of anti-IgE antibody HMK-12 Fab complexed with IgE

F(ab')2

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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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.37.1

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

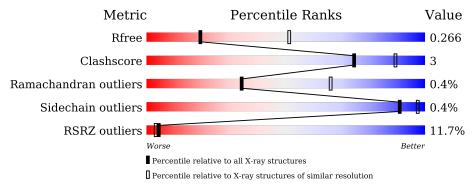
Validation Pipeline (wwPDB-VP) : 2.37.1

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 2.90 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	93%	7%
2	Н	225	91%	8% •
3	A	321	26%	12% • •
4	В	215	12%	8% •
5	С	2	100%	370



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 1667	C 1036	N 284	O 341	S 6	0	4	0

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

\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Н	222	Total 1694	C 1076	N 279	O 332	S 7	0	0	0

• 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	С	N	О	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	В	211	Total 1601	C 1002	N 270	O 323	S 6	0	2	0

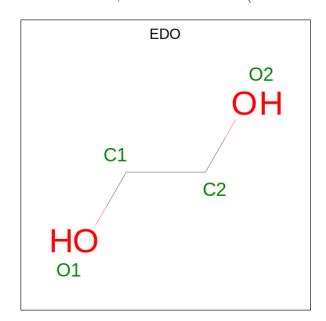
• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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



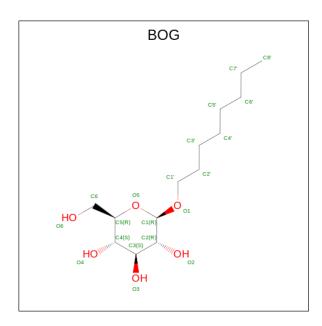
 \bullet Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



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
		1	4 2 2		
6	L	1	Total C O	0	0
0	П	1	4 2 2	U	0
6	Н	1	Total C O	0	0
0	П	1	4 2 2	0	U
6	Н	1	Total C O	0	0
0	П	1	4 2 2	0	0
6	Н	1	Total C O	0	0
0	П	1	4 2 2	U	U
6	Н	1	Total C O	0	0
0	П	1	4 2 2	0	U
6	A	1	Total C O	0	0
0	A	1	4 2 2	0	0
6	В	1	Total C O	0	0
0	Б		4 2 2	0	U

 \bullet Molecule 7 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $\mathrm{C}_{14}\mathrm{H}_{28}\mathrm{O}_6).$





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

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	28	Total O 28 28	0	0
8	Н	22	Total O 22 22	0	0
8	A	19	Total O 19 19	0	0
8	В	7	Total O 7 7	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: anti-IgE antibody HMK-12 Fab light chain







 \bullet 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 (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	282.05Å 86.09Å 56.06Å	Donositor
a, b, c, α , β , γ	90.00° 97.19° 90.00°	Depositor
Resolution (Å)	49.60 - 2.90	Depositor
Resolution (A)	49.60 - 2.90	EDS
% Data completeness	99.9 (49.60-2.90)	Depositor
(in resolution range)	99.9 (49.60-2.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.23 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.225 , 0.267	Depositor
R, R_{free}	0.227 , 0.266	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 $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 51.0	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.

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



¹Intensities estimated from amplitudes.

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	L	0.25	0/1714	0.50	0/2320	
2	Н	0.26	0/1742	0.53	0/2383	
3	A	0.25	0/2503	0.50	0/3409	
4	В	0.25	0/1642	0.50	0/2242	
All	All	0.25	0/7601	0.51	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 maintenain 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	Н	1694	0	1646	9	0
3	A	2436	0	2336	23	0
4	В	1601	0	1561	11	0
5	С	28	0	25	0	0
6	A	4	0	6	0	0
6	В	4	0	6	0	0
6	Н	16	0	24	0	0
6	L	12	0	18	1	0
7	Н	20	0	28	0	0
8	A	19	0	0	0	0
8	В	7	0	0	0	0
8	Н	22	0	0	0	0
8	L	28	0	0	0	0
All	All	7558	0	7258	47	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	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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A J		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	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 (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	Perce	entiles
1	L	$215/214\ (100\%)$	211 (98%)	3 (1%)	1 (0%)	29	61
2	Н	$220/225\ (98\%)$	216 (98%)	4 (2%)	0	100	100
3	A	306/321 (95%)	288 (94%)	16 (5%)	2 (1%)	22	54
4	В	$210/215\ (98\%)$	195 (93%)	14 (7%)	1 (0%)	29	61
All	All	951/975~(98%)	910 (96%)	37 (4%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

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

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	Perce	ntiles
1	L	192/190 (101%)	190 (99%)	2 (1%)	76	92
2	Н	194/197 (98%)	194 (100%)	0	100	100
3	A	$272/286\ (95\%)$	271 (100%)	1 (0%)	91	97
4	В	180/181 (99%)	180 (100%)	0	100	100
All	All	838/854 (98%)	835 (100%)	3 (0%)	91	97

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 (2) such sidechains are listed below:



Mol	Chain	Res	Type
3	A	291	GLN
4	В	36	ASN

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)

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).

Mal	Trunc	e Chain Res Lir		T inle	Bond lengths			Bond angles		
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	NAG	С	1	3,5	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	С	2	5	14,14,15	0.25	0	17,19,21	0.35	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	С	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	С	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.

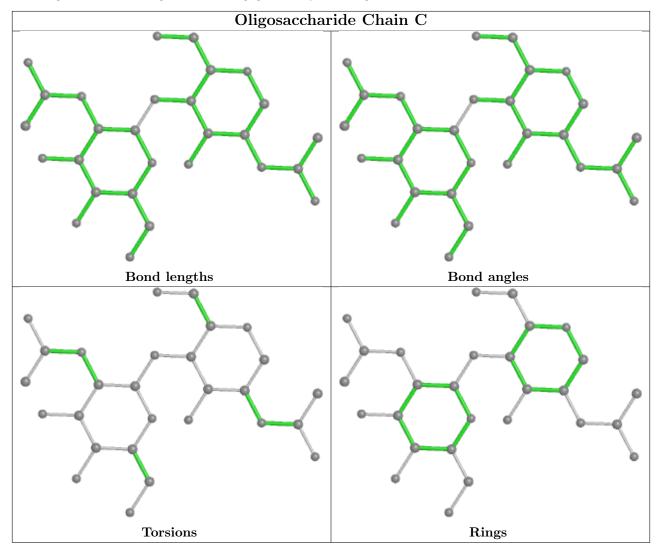
There are no torsion outliers.



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	Tuna	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	eles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	Н	303	-	3,3,3	0.47	0	2,2,2	0.33	0
6	EDO	В	301	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	Н	302	_	3,3,3	0.47	0	2,2,2	0.31	0
6	EDO	Н	304	_	3,3,3	0.45	0	2,2,2	0.39	0
6	EDO	L	303	_	3,3,3	0.47	0	2,2,2	0.31	0
6	EDO	L	302	_	3,3,3	0.46	0	2,2,2	0.32	0
7	BOG	Н	305	_	20,20,20	1.29	2 (10%)	25,25,25	0.82	0
6	EDO	L	301	-	3,3,3	0.45	0	2,2,2	0.30	0
6	EDO	A	401	-	3,3,3	0.47	0	2,2,2	0.33	0
6	EDO	Н	301	-	3,3,3	0.45	0	2,2,2	0.35	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	Н	303	-	-	0/1/1/1	-
6	EDO	В	301	-	-	0/1/1/1	-
6	EDO	Н	302	-	-	0/1/1/1	-
6	EDO	Н	304	ı	-	0/1/1/1	-
6	EDO	L	303	-	-	0/1/1/1	-
6	EDO	L	302	-	-	0/1/1/1	-
7	BOG	Н	305	-	-	5/11/31/31	0/1/1/1
6	EDO	L	301	-	-	0/1/1/1	-
6	EDO	A	401	-	-	0/1/1/1	-
6	EDO	Н	301	_	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
7	Н	305	BOG	O5-C1	4.29	1.52	1.41
7	Н	305	BOG	O1-C1	-2.26	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	Н	305	BOG	C2-C1-O1-C1'
7	Н	305	BOG	O5-C1-O1-C1'

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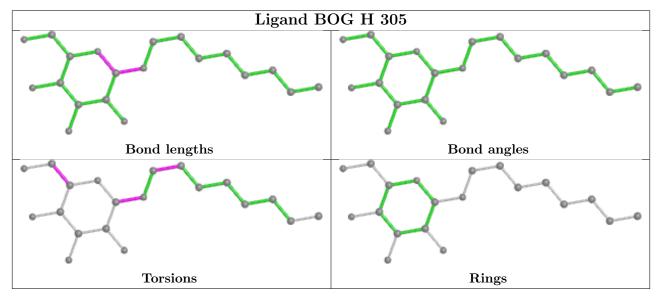
Mol	Chain	Res	Type	Atoms
7	Н	305	BOG	O5-C5-C6-O6
7	Н	305	BOG	C4-C5-C6-O6
7	Н	305	BOG	O1-C1'-C2'-C3'

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 then 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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	L	213/214 (99%)	0.04	4 (1%) 66 65	23, 42, 87, 123	0
2	Н	222/225 (98%)	-0.07	0 100 100	24, 42, 62, 101	0
3	A	311/321 (96%)	1.22	83 (26%) 0 0	26, 88, 141, 170	0
4	В	211/215 (98%)	0.61	25 (11%) 4 3	41, 65, 143, 178	0
All	All	957/975 (98%)	0.52	112 (11%) 4 3	23, 55, 131, 178	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	207	SER	7.0
3	A	198	VAL	6.1
3	A	213	ARG	6.1
3	A	177	LEU	5.1
3	A	71	THR	5.0
3	A	49	GLY	4.9
3	A	209	THR	4.8
3	A	174	GLY	4.8
4	В	181	LEU	4.7
3	A	25	SER	4.6
3	A	72	VAL	4.5
3	A	180	THR	4.5
3	A	77	SER	4.4
3	A	181	THR	4.4
3	A	130	PRO	4.3
3	A	147	LYS	4.3
3	A	215	VAL	4.3
3	A	211	LEU	4.1
3	A	136	GLY	4.1
3	A	54	ASN	4.1
3	A	212	VAL	4.1

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Mol	Chain	Res	Type	RSRZ			
3	A	124	ARG	4.0			
3	A	132	LYS	3.9			
3	A	152	GLY	3.9			
3	A	53	PRO	3.8			
4	В	133	ALA	3.7			
4	В	194	TYR	3.7			
4	В	190	ARG	3.7			
4	В	125	SER	3.7			
3	A	196	CYS	3.6			
3	A	158	TRP	3.6			
3	A	104	THR	3.6			
3	A	276	GLU	3.6			
3	A	204	PHE	3.6			
3	A	143	GLY	3.6			
3	A	184	VAL	3.5			
3	A	159	TYR	3.5			
3	A	173	LEU	3.5			
3	A	185	THR	3.5			
4	В	159	THR	3.4			
3	A	26	GLY	3.4			
4	В	129	GLU	3.4			
3	A	162	SER	3.4			
4	В	160	GLN	3.4			
4	В	158	VAL	3.3			
4	В	195	SER	3.3			
3	A	134	CYS	3.3			
4	В	183	LEU	3.3			
3	A	161	ASP	3.3			
3	A	122	SER	3.3			
3	A	164	ASN	3.3			
3	A	5	GLN	3.2			
3	A	142	LEU	3.2			
1	L	135	PHE	3.2			
3	A	140	MET	3.2			
3	A	160	SER	3.1			
4	В	124	SER	3.1			
3	A	57	GLY	3.1			
3	A	194	PHE	3.1			
4	В	209	LEU	3.1			
4	В	1	GLN	3.0			
3	A	28	THR	3.0			
3	A	193	ASN	3.0			

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Mol	nued fron Chain	Res	Type	RSRZ
3	A	123	ILE	3.0
3	A	129	TYR	3.0
4	В	191	HIS	2.9
3	A	165	MET	2.9
4	В	154	ASP	2.8
3	A	144	CYS	2.8
4	В	156	THR	2.8
3	A	203	SER	2.8
4	В	134	THR	2.8
3	A	195	THR	2.7
3	A	145	LEU	2.7
3	A	279	LEU	2.7
3	A	32	TYR	2.7
3	A	133	PRO	2.7
3	A	34	MET	2.7
3	A	148	ASP	2.6
3	A	178	LYS	2.6
3	A	199	THR	2.6
3	A	128	LEU	2.6
3	A	201	PRO	2.5
3	A	55	GLY	2.5
3	A	210	ILE	2.5
3	A	126	PRO	2.4
4	В	210	SER	2.4
3	A	200	HIS	2.4
3	A	249	LEU	2.4
4	В	128	LEU	2.4
3	A	3	GLN	2.3
3	A	191	ALA	2.3
3	A	52	ASP	2.3
3	A	156	VAL	2.2
3	A	175	SER	2.2
4	В	135	LEU	2.2
4	В	123	PRO	2.2
4	В	122	PRO	2.2
3	A	214	PRO	2.2
4	В	188	TRP	2.1
3	A	69	THR	2.1
3	A	127	GLN	2.1
1	L	24	LYS	2.1
3	A	172	ALA	2.1
3	A	27	TYR	2.1



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Mol	Chain	Res	Type	RSRZ
3	A	155	THR	2.1
1	L	205	ILE	2.1
3	A	146	VAL	2.1
3	A	141	THR	2.0
3	A	135	LYS	2.0
1	L	184	ASP	2.0
4	В	155	GLY	2.0

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

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

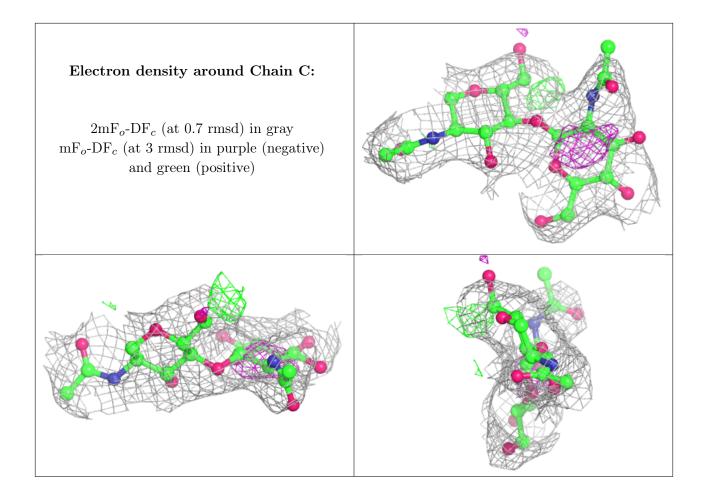
6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	NAG	С	2	14/15	0.81	0.30	50,59,63,66	0
5	NAG	С	1	14/15	0.85	0.16	48,56,63,69	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)

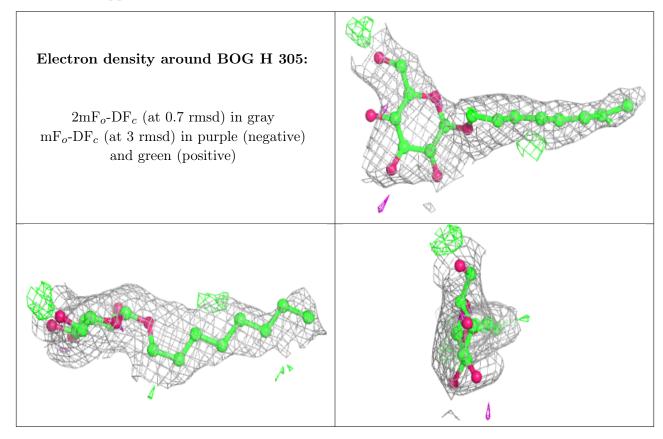
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
7	BOG	Н	305	20/20	0.74	0.29	44,61,71,75	0
6	EDO	В	301	4/4	0.81	0.34	70,73,76,82	0
6	EDO	Н	301	4/4	0.87	0.54	46,50,51,53	0
6	EDO	L	303	4/4	0.88	0.23	38,40,41,43	0
6	EDO	A	401	4/4	0.89	0.18	44,46,56,57	0
6	EDO	Н	304	4/4	0.90	0.22	27,32,32,39	0
6	EDO	L	301	4/4	0.90	0.38	33,33,35,37	0
6	EDO	Н	302	4/4	0.91	0.23	53,57,57,61	0
6	EDO	Н	303	4/4	0.91	0.33	44,44,53,54	0
6	EDO	L	302	4/4	0.94	0.19	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 (i)

There are no such residues in this entry.

