



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 06:25 pm GMT

PDB ID : 7BEN
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 Spike glycoprotein in a ternary complex with COVOX-253 and COVOX-75 Fabs
Authors : Zhou, D.; Zhao, Y.; Ren, J.; Stuart, D.
Deposited on : 2020-12-24
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

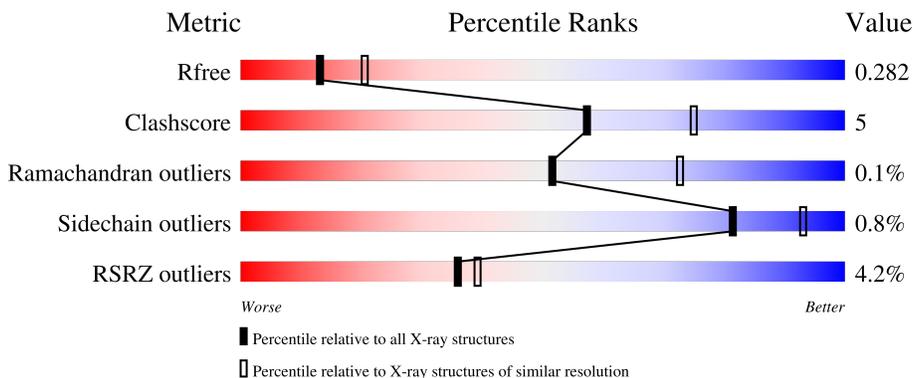
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	C	205	 9% (poor fit), 77% (0-1 outliers), 10% (2 outliers), 13% (3+ outliers or not modelled)
1	E	205	 7% (poor fit), 74% (0-1 outliers), 12% (2 outliers), 14% (3+ outliers or not modelled)
2	D	228	 8% (poor fit), 85% (0-1 outliers), 11% (2 outliers), . (3+ outliers or not modelled)
2	H	228	 6% (poor fit), 86% (0-1 outliers), 10% (2 outliers), . (3+ outliers or not modelled)
3	F	215	 3% (poor fit), 87% (0-1 outliers), 12% (2 outliers)

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Mol	Chain	Length	Quality of chain
3	L	215	 3% 87% 12%
4	A	232	 % 84% 11% ..
4	G	232	 87% 9% ..
5	B	214	 % 88% 12%
5	I	214	 % 89% 10%
6	J	3	 67% 33%
6	K	3	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BR	A	302	-	-	-	X
9	BR	G	307	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 16460 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	177	1416	908	235	267	6	0	0	0
1	C	178	1418	910	235	266	7	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	527	LYS	PRO	engineered mutation	UNP P0DTC2
C	324	GLU	-	expression tag	UNP P0DTC2
C	325	THR	-	expression tag	UNP P0DTC2
C	326	GLY	-	expression tag	UNP P0DTC2
C	327	HIS	-	expression tag	UNP P0DTC2
C	328	HIS	-	expression tag	UNP P0DTC2
C	329	HIS	-	expression tag	UNP P0DTC2
C	330	HIS	-	expression tag	UNP P0DTC2
C	331	HIS	-	expression tag	UNP P0DTC2
C	332	HIS	-	expression tag	UNP P0DTC2
C	527	LYS	PRO	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called COVOX-253 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1639	1031	276	323	9			
2	D	219	Total	C	N	O	S	0	1	0
			1646	1036	277	324	9			

- Molecule 3 is a protein called COVOX-253 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	2	0
			1631	1020	272	333	6			
3	F	214	Total	C	N	O	S	0	2	0
			1635	1022	272	335	6			

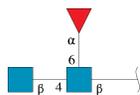
- Molecule 4 is a protein called COVOX-75 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	224	Total	C	N	O	S	0	1	0
			1694	1068	293	327	6			
4	G	224	Total	C	N	O	S	0	0	0
			1691	1066	293	326	6			

- Molecule 5 is a protein called COVOX-75 light chain.

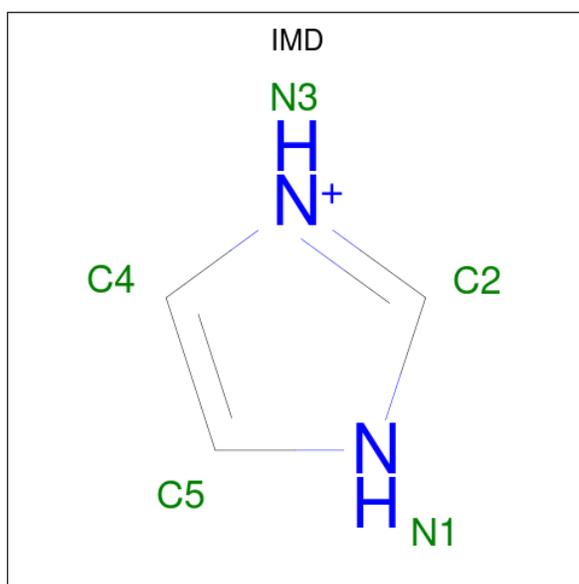
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	213	Total	C	N	O	S	0	1	0
			1633	1029	272	328	4			
5	I	213	Total	C	N	O	S	0	1	0
			1633	1029	272	328	4			

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



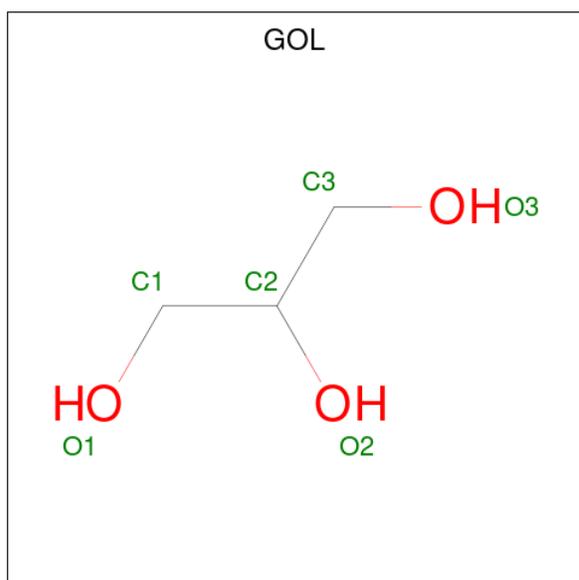
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	N	0	0
			5	3	2		
7	B	1	Total	C	N	0	0
			5	3	2		
7	F	1	Total	C	N	0	0
			5	3	2		
7	I	1	Total	C	N	0	0
			5	3	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

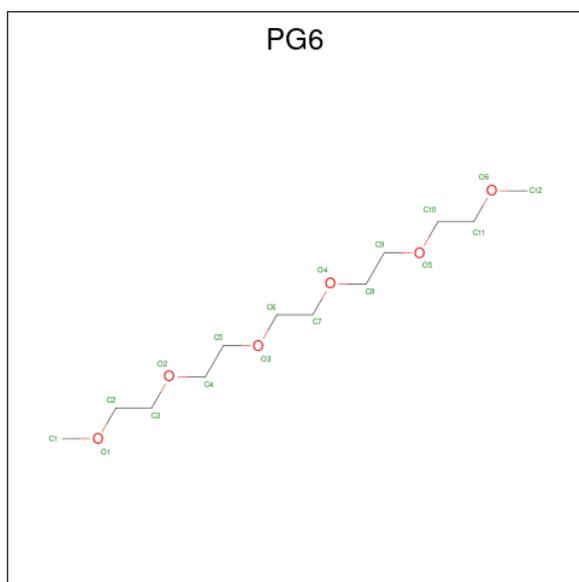


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	2	Total	Br	0	0
			2	2		
9	A	2	Total	Br	0	0
			2	2		
9	B	2	Total	Br	0	0
			2	2		
9	D	1	Total	Br	0	0
			1	1		
9	G	5	Total	Br	0	0
			5	5		
9	I	2	Total	Br	0	0
			2	2		

- Molecule 10 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	G	1	Total	C O	0	0
			7	4 3		

- Molecule 12 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	G	1	Total	I	0	0
			1	1		

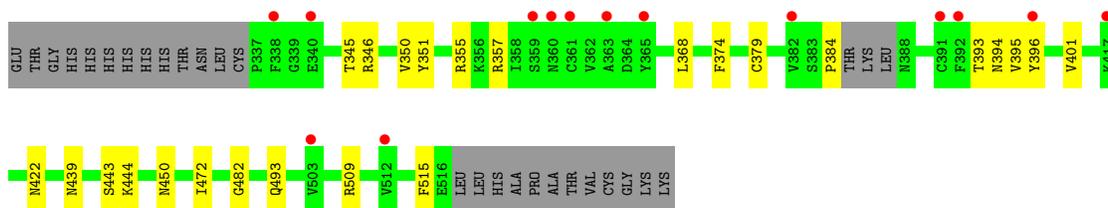
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	E	16	Total	O	0	0
			16	16		
13	H	15	Total	O	0	0
			15	15		
13	L	29	Total	O	0	0
			29	29		
13	A	35	Total	O	0	0
			35	35		
13	B	26	Total	O	0	0
			26	26		
13	C	12	Total	O	0	0
			12	12		
13	D	21	Total	O	0	0
			21	21		
13	F	23	Total	O	0	0
			23	23		
13	G	33	Total	O	0	0
			33	33		
13	I	23	Total	O	0	0
			23	23		

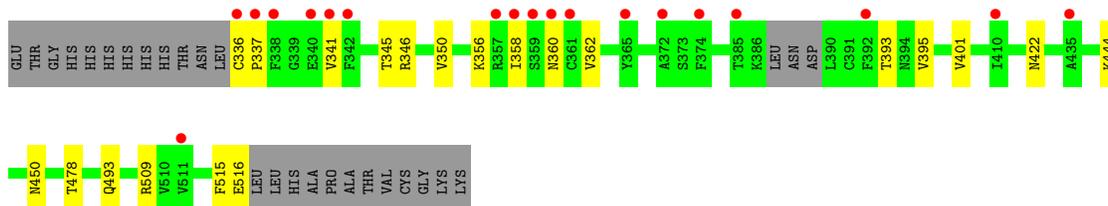
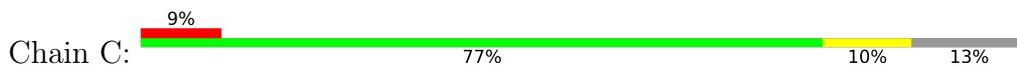
3 Residue-property plots [i](#)

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.

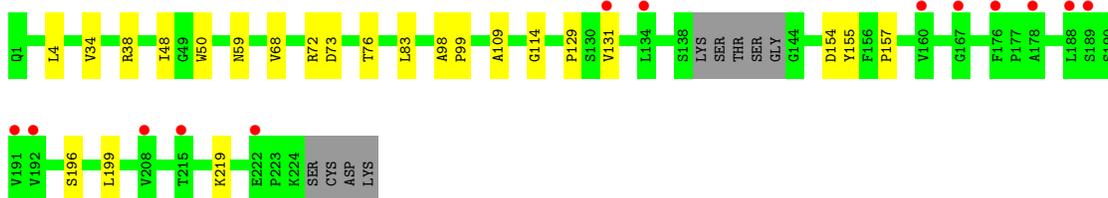
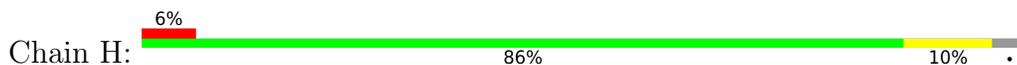
- Molecule 1: Spike glycoprotein



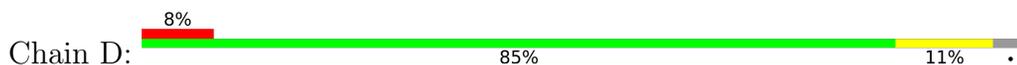
- Molecule 1: Spike glycoprotein

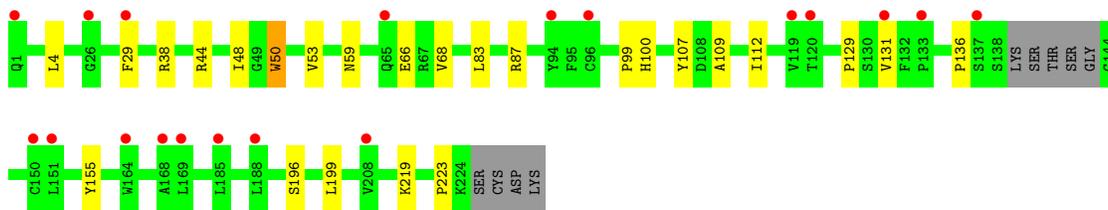


- Molecule 2: COVOX-253 heavy chain

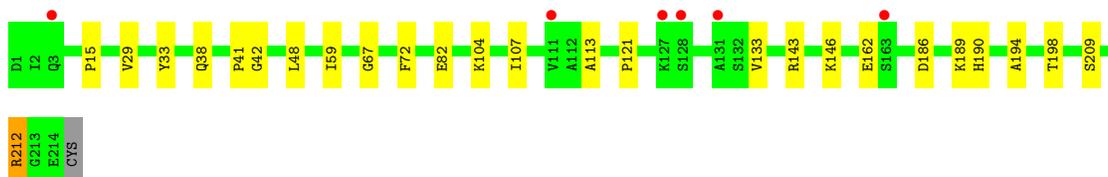
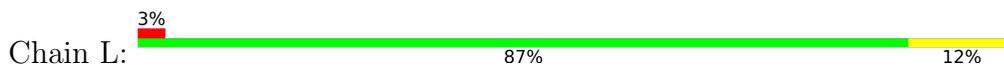


- Molecule 2: COVOX-253 heavy chain

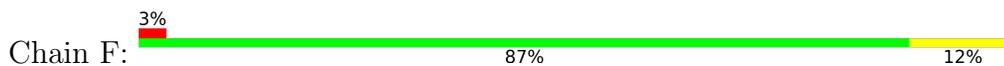




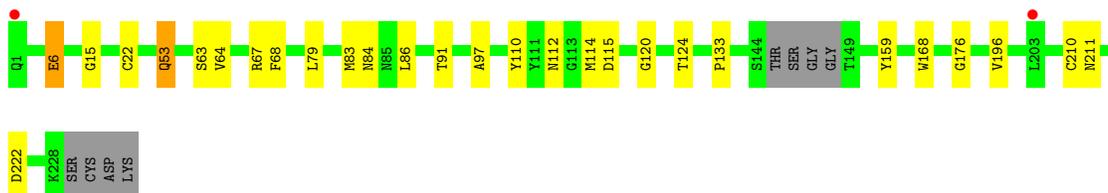
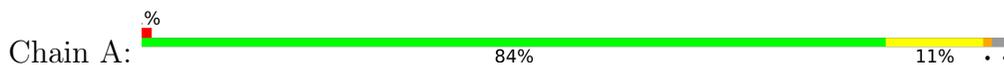
- Molecule 3: COVOX-253 light chain



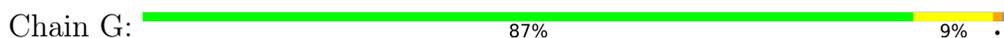
- Molecule 3: COVOX-253 light chain



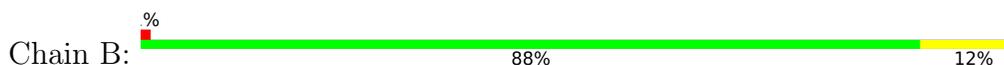
- Molecule 4: COVOX-75 heavy chain



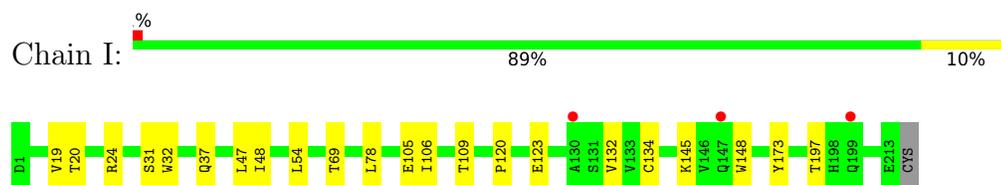
- Molecule 4: COVOX-75 heavy chain



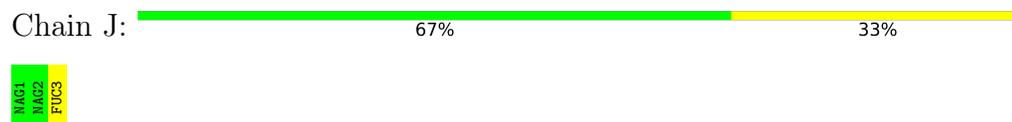
- Molecule 5: COVOX-75 light chain



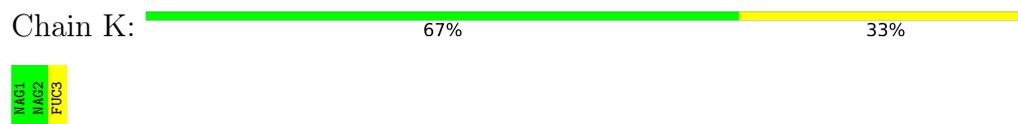
- Molecule 5: COVOX-75 light chain



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.19Å 149.79Å 229.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.38 – 2.50 59.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (58.38-2.50) 99.5 (59.07-2.50)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.240 , 0.282 0.240 , 0.282	Depositor DCC
R_{free} test set	5594 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtrriage
Anisotropy	0.209	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16460	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8665e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PG6, IOD, IMD, GOL, NAG, PEG, FUC, BR

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	C	0.27	0/1458	0.44	0/1981
1	E	0.26	0/1456	0.44	0/1977
2	D	0.26	0/1687	0.48	0/2301
2	H	0.25	0/1677	0.49	0/2289
3	F	0.26	0/1677	0.49	0/2277
3	L	0.25	0/1673	0.47	0/2272
4	A	0.27	0/1737	0.49	0/2370
4	G	0.26	0/1731	0.49	0/2362
5	B	0.26	0/1673	0.46	0/2273
5	I	0.26	0/1673	0.46	0/2273
All	All	0.26	0/16442	0.47	0/22375

There are no bond length outliers.

There are no bond angle outliers.

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	C	1418	0	1328	14	0
1	E	1416	0	1327	17	0
2	D	1646	0	1611	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1639	0	1595	12	0
3	F	1635	0	1579	18	0
3	L	1631	0	1575	19	0
4	A	1694	0	1662	17	0
4	G	1691	0	1657	17	0
5	B	1633	0	1601	15	0
5	I	1633	0	1601	13	0
6	J	38	0	34	0	0
6	K	38	0	34	1	0
7	B	5	0	5	0	0
7	E	5	0	5	1	0
7	F	5	0	5	2	0
7	I	5	0	5	1	0
8	B	12	0	16	0	0
8	E	12	0	16	2	0
8	F	6	0	8	0	0
9	A	2	0	0	1	0
9	B	2	0	0	0	0
9	D	1	0	0	0	0
9	G	5	0	0	4	0
9	H	2	0	0	0	0
9	I	2	0	0	0	0
10	F	18	0	26	1	0
10	L	18	0	26	4	0
11	G	14	0	20	0	0
12	G	1	0	0	0	0
13	A	35	0	0	5	0
13	B	26	0	0	4	0
13	C	12	0	0	2	0
13	D	21	0	0	3	0
13	E	16	0	0	3	0
13	F	23	0	0	2	0
13	G	33	0	0	2	0
13	H	15	0	0	2	0
13	I	23	0	0	1	0
13	L	29	0	0	5	0
All	All	16460	0	15736	155	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 5.

The worst 5 of 155 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)
13:D:413:HOH:O	9:G:307:BR:BR	2.43	0.91
1:E:346:ARG:HH22	1:E:450:ASN:HB3	1.35	0.90
3:L:113:ALA:O	13:L:401:HOH:O	1.89	0.90
13:D:407:HOH:O	9:G:307:BR:BR	2.46	0.88
2:D:66:GLU:HA	4:G:30:ASN:HD21	1.42	0.85

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	C	174/205 (85%)	162 (93%)	11 (6%)	1 (1%)	25	43
1	E	173/205 (84%)	161 (93%)	12 (7%)	0	100	100
2	D	216/228 (95%)	205 (95%)	11 (5%)	0	100	100
2	H	215/228 (94%)	203 (94%)	12 (6%)	0	100	100
3	F	214/215 (100%)	206 (96%)	8 (4%)	0	100	100
3	L	214/215 (100%)	205 (96%)	8 (4%)	1 (0%)	29	48
4	A	221/232 (95%)	217 (98%)	4 (2%)	0	100	100
4	G	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
5	B	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
5	I	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	2071/2188 (95%)	1983 (96%)	86 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	360	ASN
3	L	212	ARG

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	C	153/177 (86%)	152 (99%)	1 (1%)	84	94
1	E	153/177 (86%)	152 (99%)	1 (1%)	84	94
2	D	188/196 (96%)	186 (99%)	2 (1%)	73	89
2	H	186/196 (95%)	185 (100%)	1 (0%)	88	96
3	F	185/184 (100%)	185 (100%)	0	100	100
3	L	184/184 (100%)	184 (100%)	0	100	100
4	A	190/196 (97%)	188 (99%)	2 (1%)	73	89
4	G	189/196 (96%)	187 (99%)	2 (1%)	73	89
5	B	187/187 (100%)	183 (98%)	4 (2%)	53	78
5	I	187/187 (100%)	186 (100%)	1 (0%)	88	96
All	All	1802/1880 (96%)	1788 (99%)	14 (1%)	81	93

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	207	LYS
1	C	345	THR
5	I	109	THR
4	G	13	GLN
4	G	53	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	30	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](#)

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
6	NAG	J	1	6,2	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	J	2	6	14,14,15	0.28	0	17,19,21	0.44	0
6	FUC	J	3	6	10,10,11	0.95	1 (10%)	14,14,16	0.77	0
6	NAG	K	1	6,2	14,14,15	0.31	0	17,19,21	0.47	0
6	NAG	K	2	6	14,14,15	0.25	0	17,19,21	0.42	0
6	FUC	K	3	6	10,10,11	0.88	0	14,14,16	0.80	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	NAG	J	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	FUC	J	3	6	-	-	0/1/1/1
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	FUC	K	3	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	3	FUC	O5-C1	-2.16	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

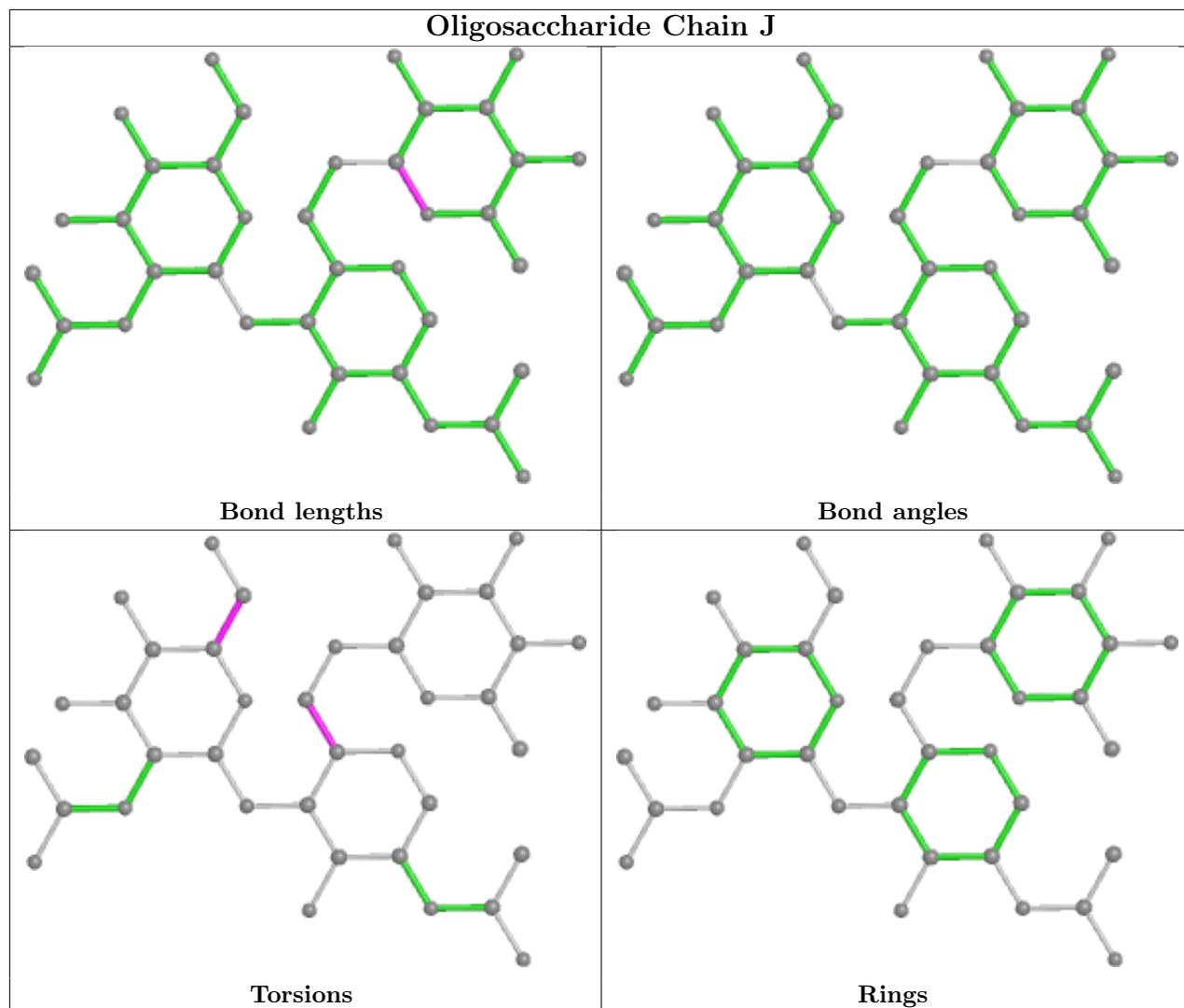
Mol	Chain	Res	Type	Atoms
6	K	2	NAG	C4-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6

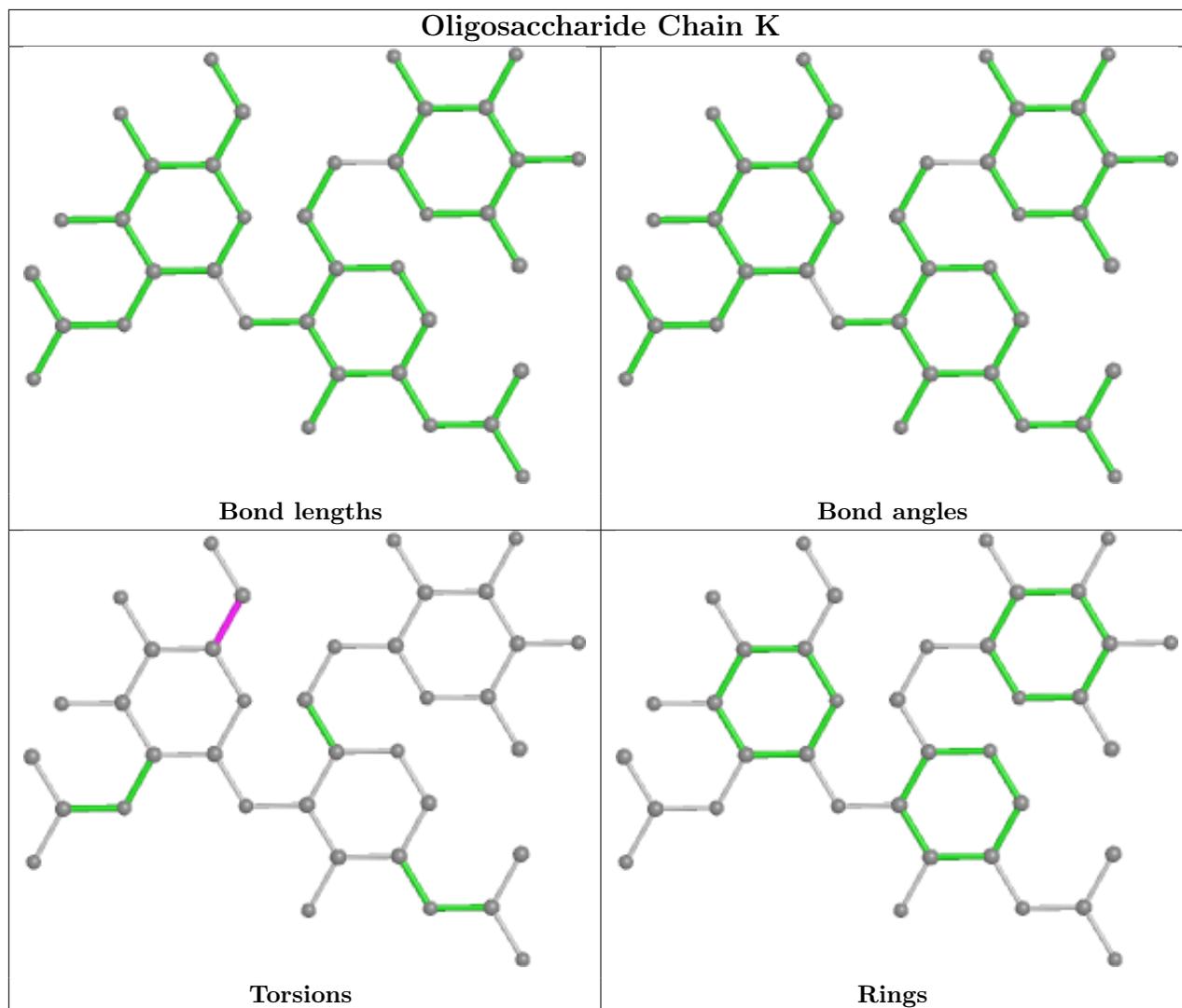
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	3	FUC	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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 15 are monoatomic - leaving 13 for Mogul analysis.

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	$\# Z > 2$
10	PG6	L	301	-	17,17,17	0.52	0	16,16,16	0.17	0
8	GOL	E	603	-	5,5,5	0.89	0	5,5,5	1.00	0
7	IMD	I	301	-	3,5,5	0.41	0	4,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	B	303	-	5,5,5	0.96	0	5,5,5	0.98	0
7	IMD	F	403	-	3,5,5	0.38	0	4,5,5	0.58	0
8	GOL	F	401	-	5,5,5	0.92	0	5,5,5	0.98	0
8	GOL	B	301	-	5,5,5	0.85	0	5,5,5	1.05	0
8	GOL	E	602	-	5,5,5	0.90	0	5,5,5	1.02	0
7	IMD	B	302	-	3,5,5	0.42	0	4,5,5	0.57	0
10	PG6	F	402	-	17,17,17	0.53	0	16,16,16	0.18	0
11	PEG	G	301	-	6,6,6	0.49	0	5,5,5	0.28	0
11	PEG	G	302	-	6,6,6	0.48	0	5,5,5	0.28	0
7	IMD	E	601	-	3,5,5	0.41	0	4,5,5	0.58	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
10	PG6	L	301	-	-	8/15/15/15	-
8	GOL	E	603	-	-	1/4/4/4	-
8	GOL	B	303	-	-	2/4/4/4	-
7	IMD	I	301	-	-	-	0/1/1/1
7	IMD	F	403	-	-	-	0/1/1/1
8	GOL	F	401	-	-	2/4/4/4	-
8	GOL	B	301	-	-	2/4/4/4	-
8	GOL	E	602	-	-	0/4/4/4	-
10	PG6	F	402	-	-	10/15/15/15	-
7	IMD	B	302	-	-	-	0/1/1/1
11	PEG	G	301	-	-	2/4/4/4	-
11	PEG	G	302	-	-	4/4/4/4	-
7	IMD	E	601	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	303	GOL	O1-C1-C2-C3
11	G	301	PEG	O1-C1-C2-O2

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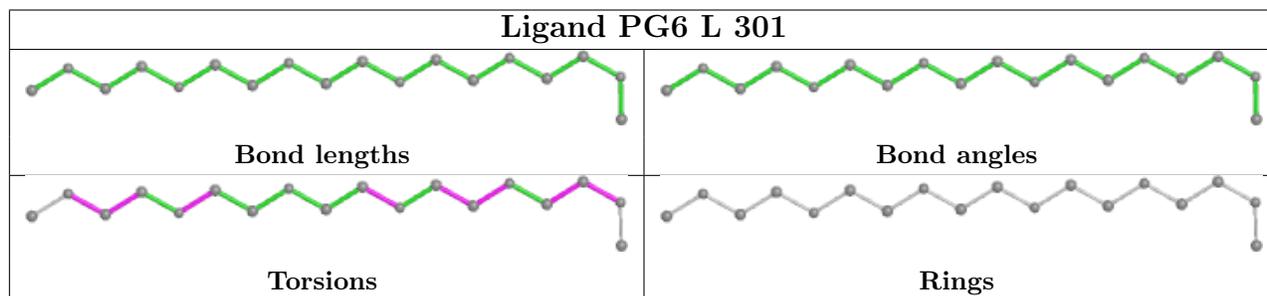
Mol	Chain	Res	Type	Atoms
10	L	301	PG6	O2-C4-C5-O3
11	G	301	PEG	O2-C3-C4-O4
10	F	402	PG6	O4-C8-C9-O5

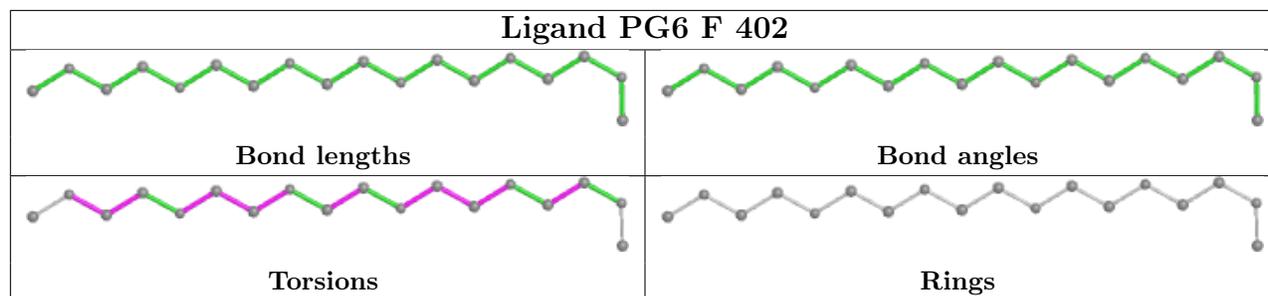
There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	301	PG6	4	0
8	E	603	GOL	1	0
7	I	301	IMD	1	0
7	F	403	IMD	2	0
8	E	602	GOL	1	0
10	F	402	PG6	1	0
7	E	601	IMD	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 [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, 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	C	178/205 (86%)	0.88	19 (10%) 6 5	53, 74, 136, 218	0
1	E	177/205 (86%)	0.78	14 (7%) 12 12	53, 74, 131, 205	0
2	D	219/228 (96%)	0.69	19 (8%) 10 10	54, 76, 102, 116	0
2	H	219/228 (96%)	0.66	13 (5%) 22 23	53, 76, 96, 110	0
3	F	214/215 (99%)	0.57	7 (3%) 46 50	50, 72, 94, 147	0
3	L	214/215 (99%)	0.52	6 (2%) 53 56	49, 70, 92, 148	0
4	A	224/232 (96%)	0.43	2 (0%) 84 86	41, 58, 90, 115	0
4	G	224/232 (96%)	0.45	1 (0%) 92 93	40, 57, 95, 118	0
5	B	213/214 (99%)	0.39	3 (1%) 75 77	47, 69, 88, 103	0
5	I	213/214 (99%)	0.32	3 (1%) 75 77	47, 71, 91, 107	0
All	All	2095/2188 (95%)	0.56	87 (4%) 36 39	40, 70, 101, 218	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	PRO	8.5
1	C	361	CYS	6.2
1	E	338	PHE	5.4
1	E	360	ASN	5.3
1	C	365	TYR	4.9

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](#)

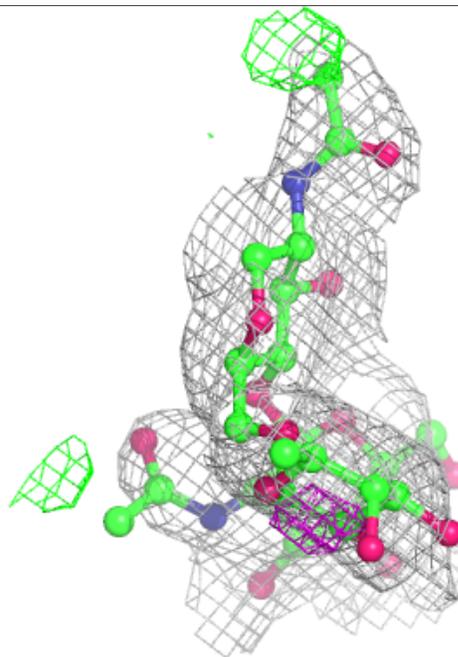
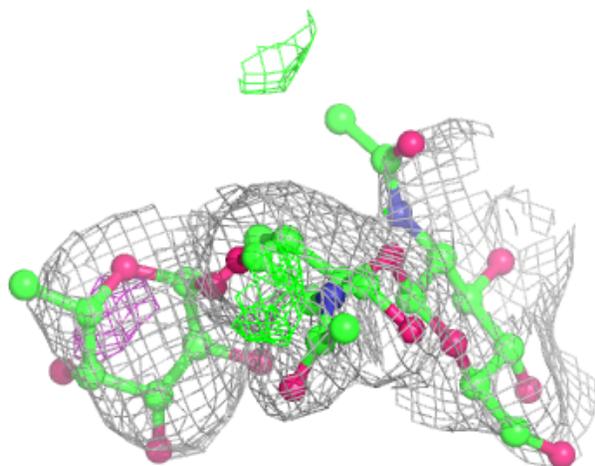
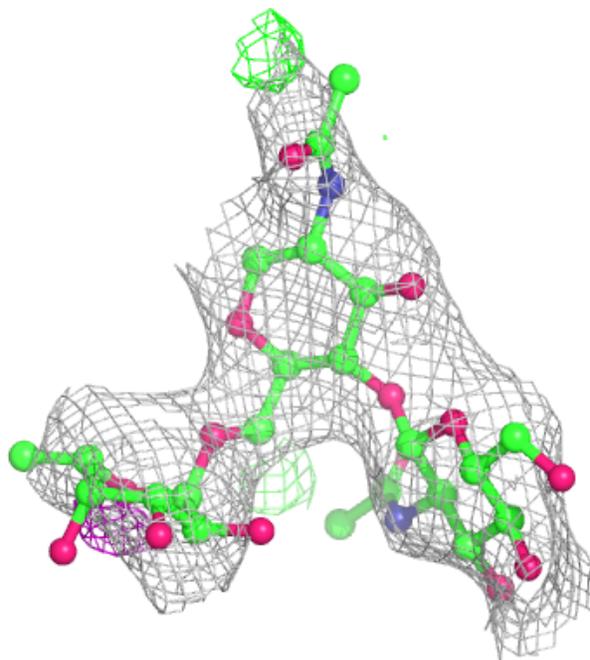
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

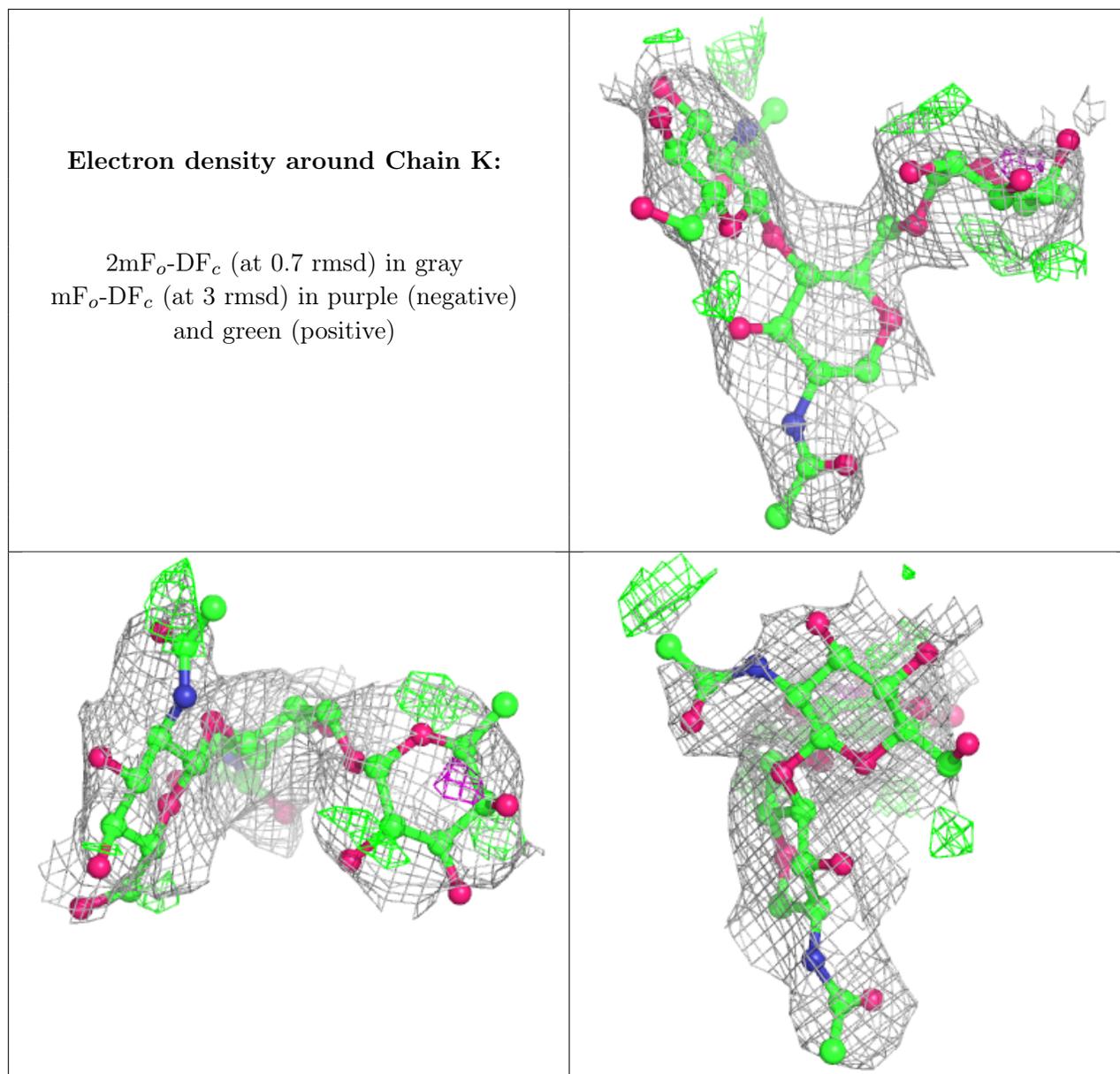
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	K	2	14/15	0.78	0.24	107,117,128,129	0
6	FUC	J	3	10/11	0.79	0.31	91,106,116,119	0
6	NAG	J	2	14/15	0.81	0.26	105,117,121,123	0
6	FUC	K	3	10/11	0.82	0.26	99,110,116,121	0
6	NAG	K	1	14/15	0.87	0.18	84,94,107,115	0
6	NAG	J	1	14/15	0.88	0.15	82,95,102,115	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 J:

$2mF_o-DF_c$ (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
9	BR	I	303	1/1	0.60	0.11	174,174,174,174	0
11	PEG	G	301	7/7	0.68	0.18	72,89,99,100	0
9	BR	G	303	1/1	0.69	0.10	136,136,136,136	0
7	IMD	I	301	5/5	0.72	0.22	92,94,100,103	0

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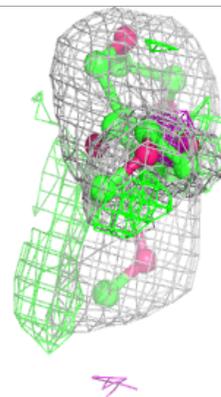
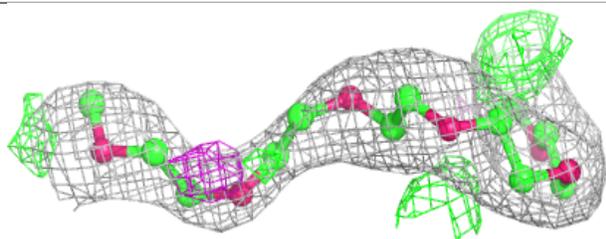
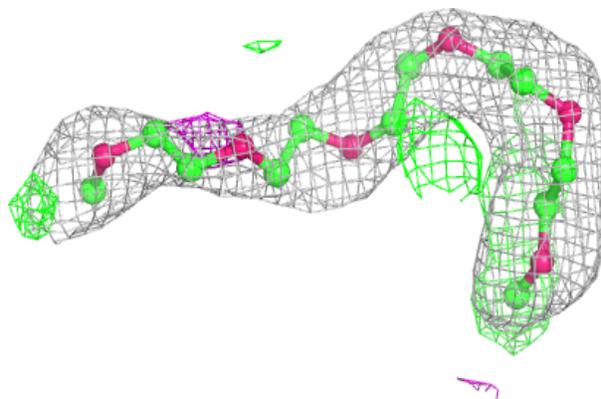
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	BR	G	305	1/1	0.77	0.12	141,141,141,141	0
8	GOL	B	303	6/6	0.78	0.22	65,68,76,82	0
9	BR	H	301	1/1	0.80	0.09	141,141,141,141	0
9	BR	A	302	1/1	0.80	0.43	238,238,238,238	0
11	PEG	G	302	7/7	0.80	0.13	80,84,93,95	0
7	IMD	E	601	5/5	0.81	0.18	92,92,95,96	0
9	BR	G	307	1/1	0.82	0.08	149,149,149,149	0
7	IMD	F	403	5/5	0.83	0.32	114,114,126,137	0
12	IOD	G	308	1/1	0.83	0.36	254,254,254,254	0
10	PG6	F	402	18/18	0.84	0.25	49,69,83,91	0
9	BR	G	304	1/1	0.84	0.10	112,112,112,112	0
10	PG6	L	301	18/18	0.85	0.25	55,71,90,92	0
8	GOL	E	602	6/6	0.86	0.15	80,86,89,93	0
8	GOL	F	401	6/6	0.86	0.21	71,75,84,87	0
8	GOL	E	603	6/6	0.87	0.19	73,79,83,85	0
9	BR	G	306	1/1	0.87	0.08	128,128,128,128	0
8	GOL	B	301	6/6	0.87	0.19	61,72,73,73	0
9	BR	A	301	1/1	0.88	0.10	132,132,132,132	0
9	BR	I	302	1/1	0.90	0.12	123,123,123,123	0
7	IMD	B	302	5/5	0.92	0.21	70,72,84,88	0
9	BR	B	305	1/1	0.93	0.52	256,256,256,256	0
9	BR	B	304	1/1	0.94	0.10	93,93,93,93	0
9	BR	H	302	1/1	0.97	0.09	78,78,78,78	0
9	BR	D	301	1/1	0.99	0.16	78,78,78,78	0

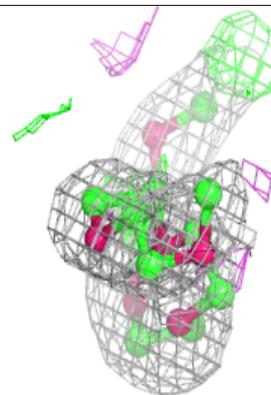
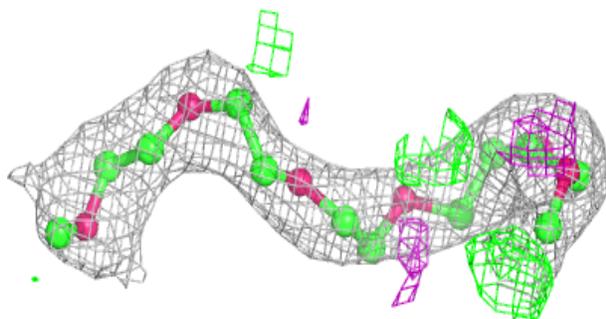
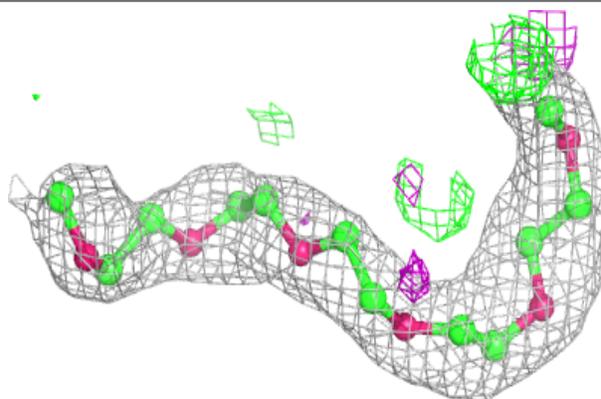
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PG6 F 402:

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

**Electron density around PG6 L 301:**

$2mF_o-DF_c$ (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.