



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 06:15 PM JST

PDB ID : 7FH0
Title : Crystallographic structure of two neutralizing nanobodies in complex with SARS-CoV-2 spike receptor-binding Domain (RBD)
Authors : Zheng, P.; Jin, J.
Deposited on : 2021-07-28
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : ?? (??), CSD ??CSD?? (????)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

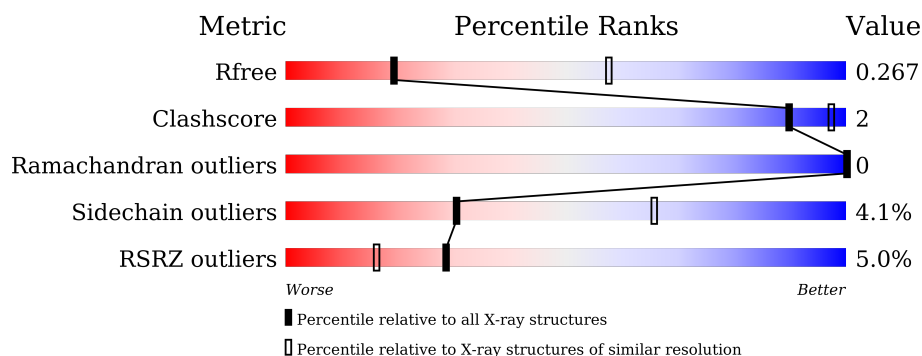
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	<div> <div>9%</div> <div>85%</div> <div>10%</div> </div>
2	B	261	<div> <div>2%</div> <div>88%</div> <div>5% • 6%</div> </div>
2	C	261	<div> <div>86%</div> <div>8% 6%</div> </div>
3	D	2	<div> <div>100%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	801	-	-	-	X
5	PEG	A	803	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7068 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 protein S1, Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3115	1998	521	580	16			

- Molecule 2 is a protein called nanobodies aRBD-2-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	0	0
			1911	1187	342	371	11			
2	C	246	Total	C	N	O	S	0	0	0
			1911	1187	342	371	11			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



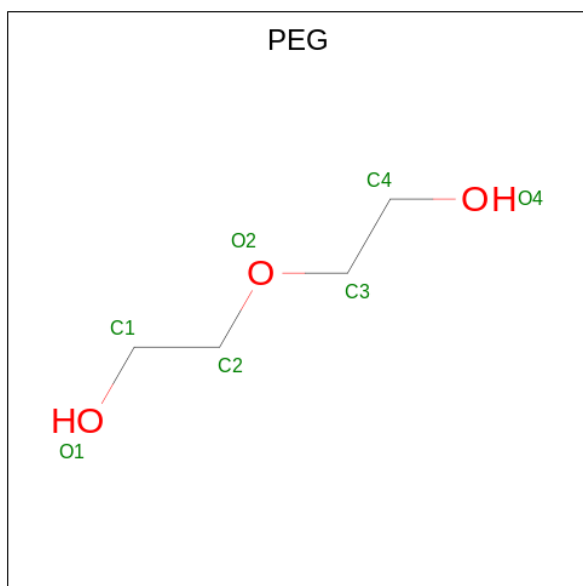
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



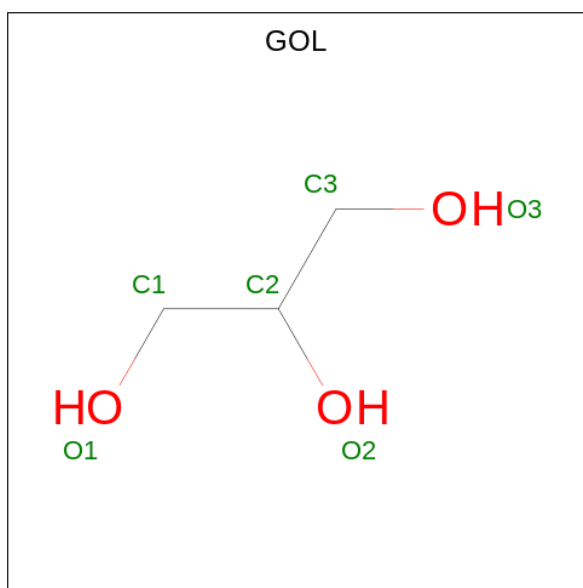
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

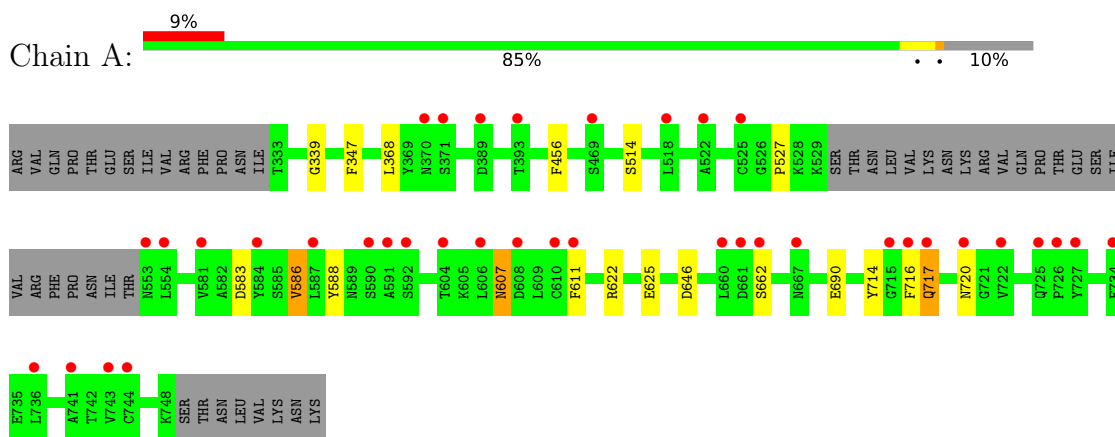
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	25	Total	O	0	0
			25	25		
7	B	16	Total	O	0	0
			16	16		
7	C	15	Total	O	0	0
			15	15		

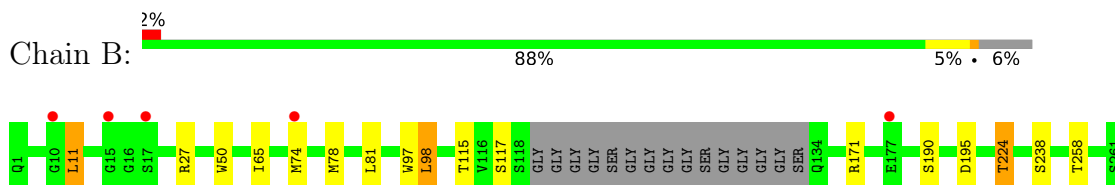
3 Residue-property plots

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.

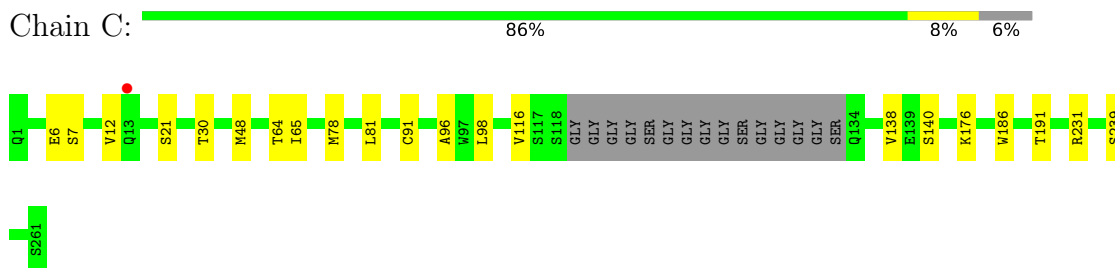
- Molecule 1: Spike protein S1,Spike protein S1



- Molecule 2: nanobodies aRBD-2-7



- Molecule 2: nanobodies aRBD-2-7



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.46Å 154.46Å 257.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.50 – 3.20 49.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.50-3.20) 99.9 (49.50-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.263 0.212 , 0.267	Depositor DCC
R_{free} test set	1554 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7068	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: NAG, GOL, PEG

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	0.46	1/3203 (0.0%)	0.64	0/4356
2	B	0.42	0/1954	0.69	0/2643
2	C	0.43	0/1954	0.68	0/2643
All	All	0.44	1/7111 (0.0%)	0.66	0/9642

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	GLN	C-N	8.55	1.50	1.34

There are no bond angle outliers.

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	3115	0	2963	11	0
2	B	1911	0	1791	7	0
2	C	1911	0	1791	5	0
3	D	28	0	25	5	0
4	A	14	0	13	0	0
5	A	14	0	20	0	0
5	B	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	8	0	0
6	C	6	0	8	0	0
7	A	25	0	0	0	0
7	B	16	0	0	0	0
7	C	15	0	0	0	0
All	All	7068	0	6629	25	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 (25) 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:714:TYR:HB3	1:A:716:PHE:CE1	2.17	0.79
1:A:714:TYR:HB3	1:A:716:PHE:CZ	2.22	0.74
1:A:339:GLY:HA2	3:D:1:NAG:O7	1.97	0.65
1:A:622:ARG:HB2	1:A:625:GLU:HG3	1.80	0.62
1:A:456:PHE:CE1	2:B:98:LEU:HG	2.37	0.60
3:D:2:NAG:O4	3:D:2:NAG:H83	2.03	0.59
1:A:662:SER:HB2	1:A:716:PHE:O	2.03	0.58
1:A:527:PRO:HD3	1:A:607:ASN:HB3	1.90	0.53
2:B:97:TRP:HA	2:B:97:TRP:CE3	2.44	0.53
2:B:224:THR:OG1	2:B:258:THR:HA	2.10	0.51
2:C:30:THR:HG21	2:C:96:ALA:O	2.12	0.50
2:C:48:MET:HB2	2:C:65:ILE:HD12	1.93	0.50
2:B:65:ILE:HD11	2:B:74:MET:HE1	1.93	0.49
1:A:714:TYR:CB	1:A:716:PHE:CZ	2.95	0.49
2:C:6:GLU:HG2	2:C:91:CYS:SG	2.54	0.46
2:B:97:TRP:HA	2:B:97:TRP:HE3	1.80	0.46
3:D:2:NAG:O7	3:D:2:NAG:H3	2.13	0.45
2:C:12:VAL:O	2:C:116:VAL:HA	2.16	0.45
1:A:717:GLN:O	1:A:720:ASN:OD1	2.35	0.45
3:D:1:NAG:H4	3:D:2:NAG:H2	1.44	0.43
2:B:11:LEU:HD22	2:B:115:THR:HB	2.00	0.43
1:A:339:GLY:CA	3:D:1:NAG:O7	2.67	0.42
2:C:78:MET:HB3	2:C:81:LEU:HD21	2.01	0.42
2:B:78:MET:HB3	2:B:81:LEU:HD21	2.03	0.41
1:A:583:ASP:HB2	1:A:586:VAL:HG22	2.04	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	A	389/438 (89%)	370 (95%)	19 (5%)	0	100	100
2	B	242/261 (93%)	235 (97%)	7 (3%)	0	100	100
2	C	242/261 (93%)	233 (96%)	9 (4%)	0	100	100
All	All	873/960 (91%)	838 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/384 (88%)	330 (97%)	9 (3%)	44	75
2	B	193/196 (98%)	183 (95%)	10 (5%)	23	59
2	C	193/196 (98%)	182 (94%)	11 (6%)	20	56
All	All	725/776 (93%)	695 (96%)	30 (4%)	30	66

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	PHE
1	A	368	LEU
1	A	514	SER
1	A	586	VAL
1	A	588	TYR

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Mol	Chain	Res	Type
1	A	607	ASN
1	A	611	PHE
1	A	646	ASP
1	A	690	GLU
2	B	11	LEU
2	B	27	ARG
2	B	50	TRP
2	B	98	LEU
2	B	117	SER
2	B	171	ARG
2	B	190	SER
2	B	195	ASP
2	B	224	THR
2	B	238	SER
2	C	7	SER
2	C	21	SER
2	C	64	THR
2	C	98	LEU
2	C	138	VAL
2	C	140	SER
2	C	176	LYS
2	C	186	TRP
2	C	191	THR
2	C	231	ARG
2	C	239	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	607	ASN
2	B	104	HIS
2	C	136	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.

There are no bond length outliers.

There are no bond angle outliers.

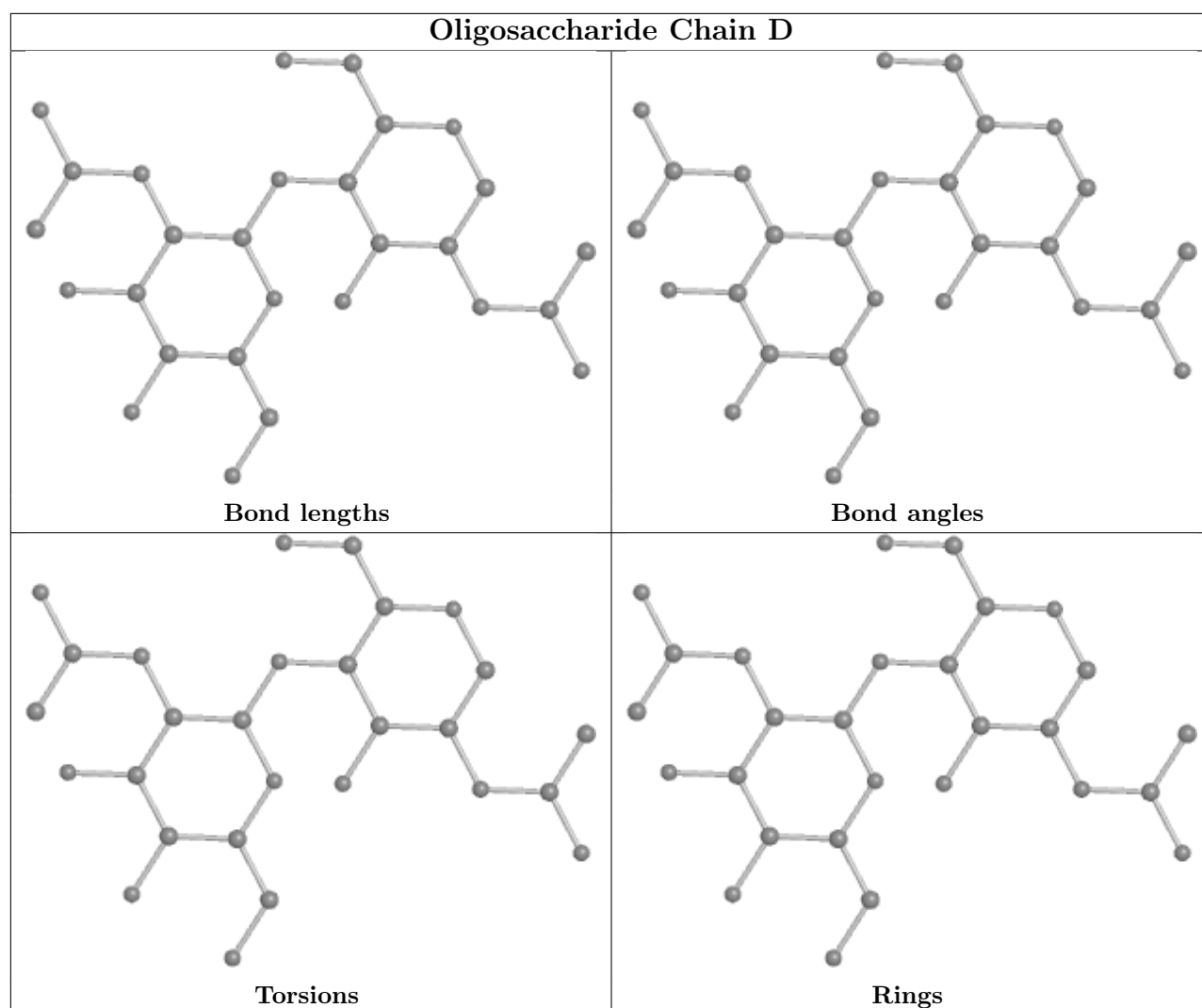
There are no chirality outliers.

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](#)

6 ligands are modelled in this entry.

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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/438 (89%)	0.63	38 (9%) 7 4	61, 103, 159, 182	0
2	B	246/261 (94%)	0.42	5 (2%) 65 51	62, 91, 135, 164	0
2	C	246/261 (94%)	0.28	1 (0%) 92 89	60, 84, 130, 168	0
All	All	885/960 (92%)	0.47	44 (4%) 28 16	60, 92, 148, 182	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	SER	4.6
1	A	716	PHE	4.6
1	A	608	ASP	4.5
1	A	715	GLY	3.7
1	A	610	CYS	3.2
1	A	667	ASN	3.2
1	A	370	ASN	3.1
1	A	606	LEU	3.1
1	A	592	SER	3.1
1	A	727	TYR	3.0
1	A	581	VAL	2.9
2	B	10	GLY	2.9
1	A	591	ALA	2.9
1	A	726	PRO	2.8
1	A	722	VAL	2.8
1	A	743	VAL	2.7
1	A	661	ASP	2.7
1	A	717	GLN	2.7
2	B	15	GLY	2.7
1	A	590	SER	2.6
1	A	725	GLN	2.6
1	A	734	PHE	2.6
1	A	611	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	393	THR	2.5
1	A	604	THR	2.5
1	A	741	ALA	2.4
1	A	720	ASN	2.4
1	A	584	TYR	2.3
1	A	525	CYS	2.2
2	B	17	SER	2.2
1	A	389	ASP	2.2
1	A	744	CYS	2.2
1	A	554	LEU	2.2
1	A	587	LEU	2.2
2	C	13	GLN	2.2
2	B	177	GLU	2.2
1	A	518	LEU	2.2
1	A	553	ASN	2.1
2	B	74	MET	2.1
1	A	660	LEU	2.1
1	A	469	SER	2.1
1	A	522	ALA	2.1
1	A	662	SER	2.0
1	A	736	LEU	2.0

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

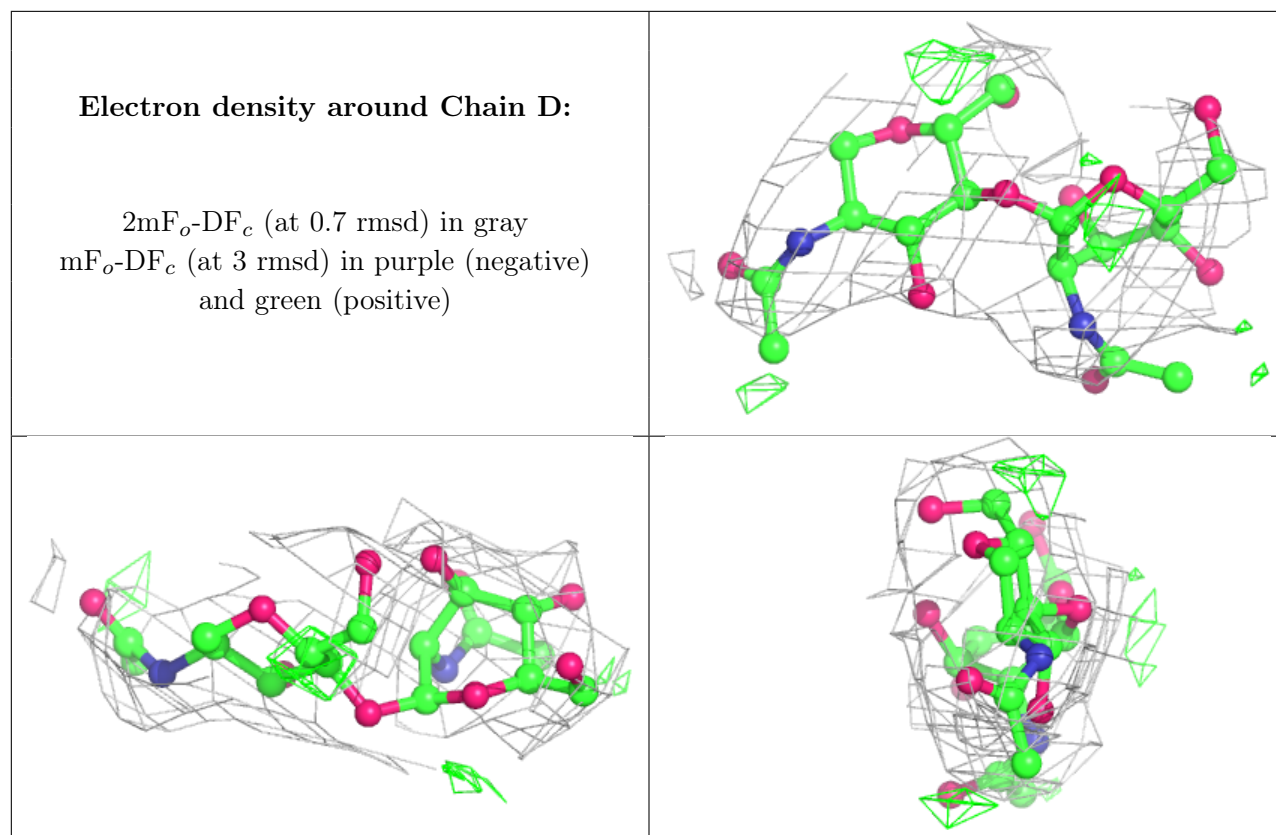
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
3	NAG	D	2	14/15	0.87	0.24	142,156,162,162	0
3	NAG	D	1	14/15	0.88	0.19	131,135,143,151	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(Å ²)	Q<0.9
5	PEG	A	802	7/7	0.64	0.27	118,126,130,131	0
4	NAG	A	801	14/15	0.71	0.42	143,169,176,177	0
5	PEG	A	803	7/7	0.77	0.63	115,128,134,138	0
5	PEG	B	301	7/7	0.78	0.34	82,101,107,108	0
6	GOL	B	302	6/6	0.80	0.41	105,112,117,119	0
6	GOL	C	301	6/6	0.86	0.38	102,105,107,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.