



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:24 AM UTC

PDB ID : 7WNB / pdb_00007wnb
Title : Crystal structure of SARS-CoV-2 spike receptor-binding domain (RBD) in complex with NCV2SG48 Fab
Authors : Yamamoto, A.; Higashiura, A.
Deposited on : 2022-01-18
Resolution : 2.18 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
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

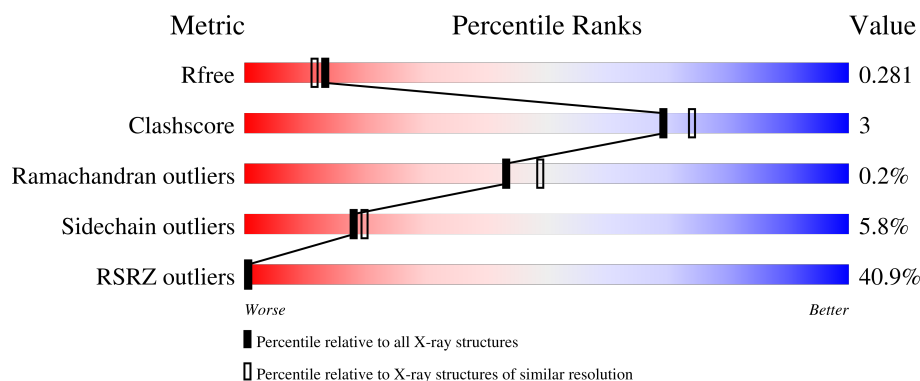
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	R	224	41% 74% 13% 12%
2	L	214	38% 90% 9%
3	H	230	35% 80% 11% 7%
4	B	2	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4990 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	197	Total	C	N	O	S	0	0	0
			1560	1000	261	291	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	537	THR	-	expression tag	UNP P0DTC2
R	538	GLY	-	expression tag	UNP P0DTC2
R	539	HIS	-	expression tag	UNP P0DTC2
R	540	HIS	-	expression tag	UNP P0DTC2
R	541	HIS	-	expression tag	UNP P0DTC2
R	542	HIS	-	expression tag	UNP P0DTC2
R	543	HIS	-	expression tag	UNP P0DTC2
R	544	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1630	1019	279	328	4			

- Molecule 3 is a protein called Fab Heavy chain.

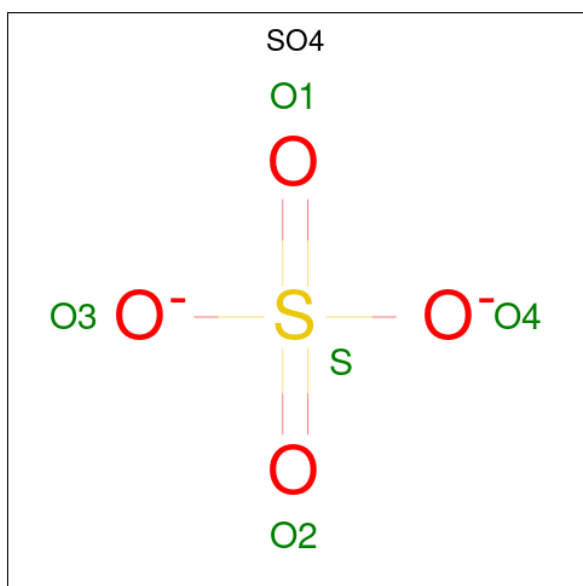
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	213	Total	C	N	O	S	0	0	0
			1594	1009	269	310	6			

- Molecule 4 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
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	O	S	0	0
			5	4	1		

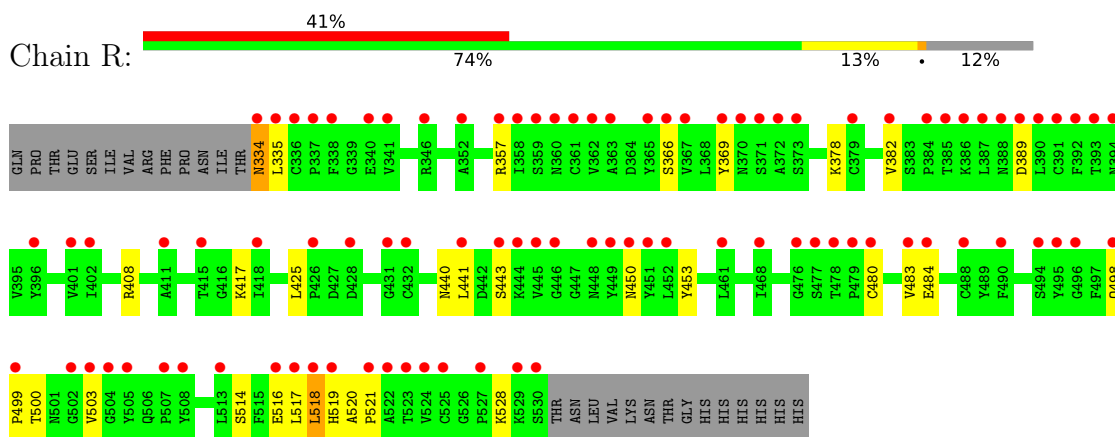
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	32	Total	O	0	0
			32	32		
6	L	81	Total	O	0	0
			81	81		
6	H	60	Total	O	0	0
			60	60		

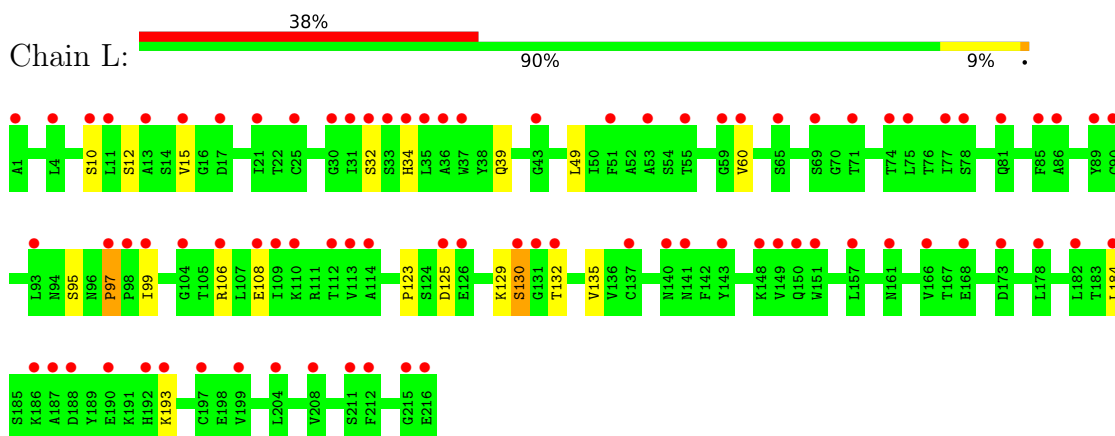
3 Residue-property plots [i](#)

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.

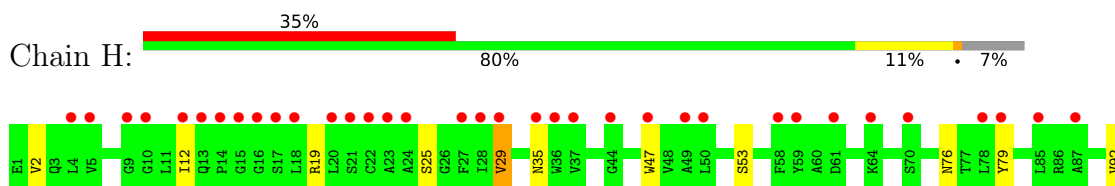
- Molecule 1: Spike protein S1

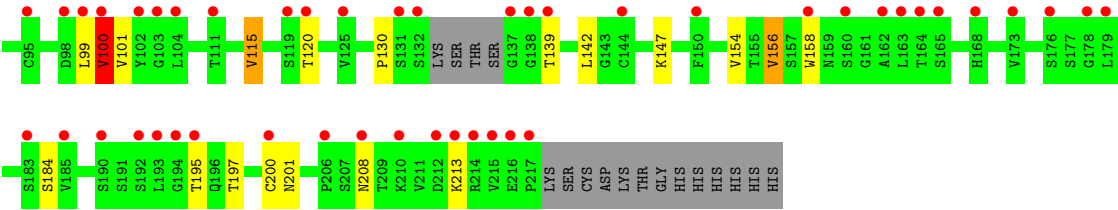


- Molecule 2: Fab Light chain



- Molecule 3: Fab Heavy chain





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.30Å 102.94Å 114.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.65 – 2.18 43.65 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.65-2.18) 98.7 (43.65-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.245 , 0.281 0.246 , 0.281	Depositor DCC
R_{free} test set	2725 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: SO4, 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	R	0.33	0/1604	0.50	0/2181
2	L	0.34	0/1665	0.57	1/2262 (0.0%)
3	H	0.36	0/1630	0.58	1/2221 (0.0%)
All	All	0.35	0/4899	0.55	2/6664 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	100	VAL	N-CA-CB	-5.44	102.26	111.23
2	L	97	PRO	N-CA-C	5.30	117.17	110.70

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	R	1560	0	1483	12	0
2	L	1630	0	1597	11	0
3	H	1594	0	1569	11	0
4	B	28	0	25	0	0
5	L	5	0	0	0	0
6	H	60	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	81	0	0	1	0
6	R	32	0	0	0	0
All	All	4990	0	4674	33	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 (33) 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)
2:L:193:LYS:NZ	6:L:402:HOH:O	2.27	0.65
2:L:97:PRO:O	2:L:99:ILE:N	2.29	0.65
2:L:39:GLN:HB2	2:L:49:LEU:HD11	1.81	0.63
2:L:10:SER:OG	2:L:106:ARG:NH2	2.38	0.56
1:R:480:CYS:O	1:R:483:VAL:HG12	2.05	0.55
2:L:123:PRO:HD3	2:L:135:VAL:HG22	1.89	0.55
1:R:357:ARG:HH11	1:R:357:ARG:HB3	1.74	0.53
1:R:335:LEU:HD12	1:R:335:LEU:H	1.74	0.52
3:H:99:LEU:O	3:H:101:VAL:N	2.44	0.51
1:R:366:SER:HA	1:R:369:TYR:CZ	2.47	0.50
1:R:440:ASN:OD1	1:R:441:LEU:HD12	2.11	0.50
1:R:516:GLU:HG2	1:R:518:LEU:HD23	1.94	0.49
1:R:417:LYS:HE3	1:R:453:TYR:CD2	2.49	0.48
3:H:12:ILE:O	3:H:115:VAL:HA	2.13	0.48
1:R:389:ASP:OD2	1:R:528:LYS:HD2	2.14	0.47
3:H:158:TRP:CH2	3:H:200:CYS:HB3	2.49	0.47
1:R:520:ALA:HB1	1:R:521:PRO:HD2	1.97	0.46
2:L:12:SER:HA	2:L:108:GLU:O	2.16	0.46
3:H:29:VAL:HG13	3:H:76:ASN:OD1	2.15	0.46
3:H:35:ASN:HD22	3:H:47:TRP:CD1	2.34	0.46
1:R:443:SER:HB3	1:R:499:PRO:HD3	1.98	0.45
3:H:156:VAL:HA	3:H:201:ASN:O	2.17	0.45
2:L:32:SER:C	2:L:34:HIS:H	2.26	0.43
2:L:125:ASP:O	2:L:129:LYS:HG3	2.19	0.42
3:H:156:VAL:HG21	3:H:184:SER:CB	2.49	0.42
1:R:334:ASN:N	1:R:334:ASN:HD22	2.18	0.42
3:H:130:PRO:HB3	3:H:142:LEU:HB3	2.01	0.42
1:R:357:ARG:HB3	1:R:357:ARG:NH1	2.35	0.41
2:L:130:SER:OG	2:L:132:THR:HG22	2.21	0.41
2:L:49:LEU:HA	2:L:60:VAL:HG21	2.03	0.41
3:H:19:ARG:HD3	3:H:79:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:213:LYS:HD2	3:H:213:LYS:HA	1.80	0.41
2:L:95:SER:HA	3:H:100:VAL:CG1	2.51	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	Percentiles	
1	R	195/224 (87%)	187 (96%)	8 (4%)	0	100	100
2	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
3	H	209/230 (91%)	203 (97%)	5 (2%)	1 (0%)	24	25
All	All	616/668 (92%)	595 (97%)	20 (3%)	1 (0%)	43	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	100	VAL

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	R	170/196 (87%)	156 (92%)	14 (8%)	10	10
2	L	186/186 (100%)	183 (98%)	3 (2%)	55	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	177/193 (92%)	163 (92%)	14 (8%)	11	11
All	All	533/575 (93%)	502 (94%)	31 (6%)	18	20

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	334	ASN
1	R	378	LYS
1	R	382	VAL
1	R	408	ARG
1	R	425	LEU
1	R	450	ASN
1	R	484	GLU
1	R	498	GLN
1	R	500	THR
1	R	503	VAL
1	R	514	SER
1	R	517	LEU
1	R	518	LEU
1	R	519	HIS
2	L	15	VAL
2	L	130	SER
2	L	184	LEU
3	H	2	VAL
3	H	25	SER
3	H	29	VAL
3	H	53	SER
3	H	92	VAL
3	H	115	VAL
3	H	120	THR
3	H	139	THR
3	H	147	LYS
3	H	154	VAL
3	H	156	VAL
3	H	195	THR
3	H	197	THR
3	H	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	414	GLN
1	R	460	ASN
1	R	493	GLN
1	R	519	HIS
2	L	3	GLN
2	L	150	GLN
2	L	192	HIS

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	$\# Z > 2$
4	NAG	B	1	1,4	14,14,15	0.36	0	17,19,21	0.96	1 (5%)
4	NAG	B	2	4	14,14,15	0.28	0	17,19,21	0.45	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
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	1	NAG	C1-O5-C5	3.18	116.45	112.19

There are no chirality outliers.

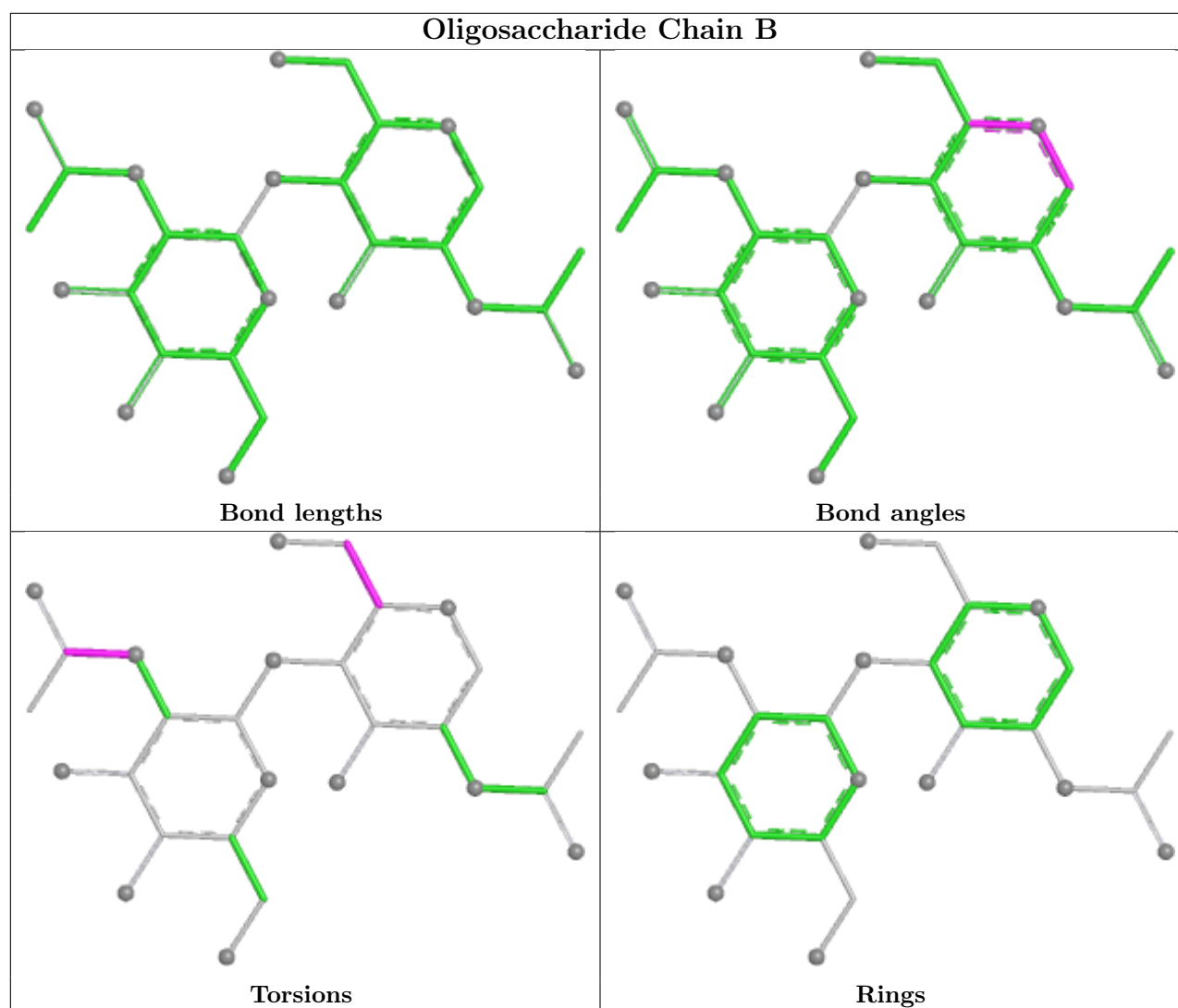
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2

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](#)

1 ligand is 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	SO4	L	301	-	4,4,4	0.26	0	6,6,6	0.11	0

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 [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	R	197/224 (87%)	2.23	92 (46%) 0 0	27, 43, 70, 100	0
2	L	214/214 (100%)	1.86	82 (38%) 1 1	28, 39, 52, 58	0
3	H	213/230 (92%)	1.85	81 (38%) 1 1	29, 38, 55, 74	0
All	All	624/668 (93%)	1.97	255 (40%) 0 0	27, 40, 62, 100	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	517	LEU	7.1
1	R	336	CYS	7.0
1	R	369	TYR	6.8
2	L	97	PRO	6.8
1	R	372	ALA	6.7
1	R	385	THR	6.6
1	R	499	PRO	5.6
1	R	518	LEU	5.5
1	R	370	ASN	5.4
2	L	32	SER	4.9
1	R	389	ASP	4.9
1	R	391	CYS	4.7
1	R	363	ALA	4.6
3	H	137	GLY	4.6
2	L	197	CYS	4.5
1	R	445	VAL	4.4
2	L	151	TRP	4.3
3	H	131	SER	4.3
3	H	138	GLY	4.3
3	H	194	GLY	4.3
3	H	212	ASP	4.2
1	R	392	PHE	4.2
1	R	516	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	R	504	GLY	4.1
1	R	523	THR	4.1
1	R	525	CYS	4.1
3	H	99	LEU	4.1
3	H	132	SER	4.1
1	R	365	TYR	4.0
3	H	216	GLU	4.0
2	L	1	ALA	4.0
3	H	9	GLY	4.0
3	H	16	GLY	4.0
3	H	78	LEU	4.0
1	R	362	VAL	4.0
3	H	5	VAL	4.0
1	R	361	CYS	4.0
1	R	432	CYS	3.9
1	R	524	VAL	3.9
2	L	98	PRO	3.9
2	L	157	LEU	3.9
3	H	103	GLY	3.8
1	R	358	ILE	3.8
2	L	99	ILE	3.8
1	R	379	CYS	3.7
3	H	120	THR	3.7
1	R	446	GLY	3.7
2	L	30	GLY	3.7
2	L	109	ILE	3.7
3	H	36	TRP	3.7
1	R	488	CYS	3.6
1	R	521	PRO	3.6
3	H	200	CYS	3.6
1	R	519	HIS	3.6
2	L	132	THR	3.6
3	H	59	TYR	3.6
2	L	93	LEU	3.5
1	R	335	LEU	3.4
2	L	173	ASP	3.4
2	L	74	THR	3.4
2	L	108	GLU	3.4
1	R	505	TYR	3.4
3	H	178	GLY	3.4
1	R	449	TYR	3.3
2	L	31	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	R	367	VAL	3.3
1	R	396	TYR	3.3
1	R	480	CYS	3.3
1	R	394	ASN	3.3
3	H	13	GLN	3.3
2	L	65	SER	3.2
2	L	106	ARG	3.2
1	R	522	ALA	3.2
1	R	384	PRO	3.2
1	R	401	VAL	3.2
2	L	89	TYR	3.2
1	R	357	ARG	3.1
2	L	51	PHE	3.1
3	H	158	TRP	3.1
1	R	508	TYR	3.1
1	R	478	THR	3.1
1	R	338	PHE	3.1
1	R	337	PRO	3.1
1	R	366	SER	3.1
3	H	47	TRP	3.0
1	R	402	ILE	3.0
1	R	530	SER	3.0
3	H	12	ILE	3.0
3	H	29	VAL	3.0
3	H	37	VAL	3.0
3	H	165	SER	3.0
1	R	476	GLY	3.0
1	R	477	SER	3.0
2	L	208	VAL	3.0
3	H	213	LYS	3.0
3	H	27	PHE	3.0
3	H	58	PHE	3.0
2	L	13	ALA	2.9
3	H	139	THR	2.9
2	L	33	SER	2.9
2	L	78	SER	2.9
2	L	11	LEU	2.9
3	H	185	VAL	2.9
1	R	441	LEU	2.9
2	L	25	CYS	2.9
1	R	346	ARG	2.9
2	L	126	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	R	448	ASN	2.9
2	L	140	ASN	2.9
1	R	411	ALA	2.9
3	H	100	VAL	2.8
2	L	215	GLY	2.8
3	H	18	LEU	2.8
2	L	90	CYS	2.8
3	H	87	ALA	2.8
1	R	387	LEU	2.8
3	H	4	LEU	2.8
3	H	50	LEU	2.8
1	R	388	ASN	2.8
1	R	484	GLU	2.8
1	R	444	LYS	2.8
1	R	341	VAL	2.8
3	H	144	CYS	2.8
1	R	360	ASN	2.7
3	H	28	ILE	2.7
2	L	34	HIS	2.7
2	L	216	GLU	2.7
3	H	183	SER	2.7
3	H	190	SER	2.7
3	H	44	GLY	2.7
2	L	182	LEU	2.7
2	L	17	ASP	2.7
2	L	35	LEU	2.6
2	L	178	LEU	2.6
3	H	20	LEU	2.6
2	L	125	ASP	2.6
3	H	195	THR	2.6
3	H	163	LEU	2.6
3	H	61	ASP	2.6
1	R	483	VAL	2.6
2	L	21	ILE	2.6
3	H	10	GLY	2.6
3	H	35	ASN	2.6
2	L	85	PHE	2.5
1	R	503	VAL	2.5
2	L	166	VAL	2.5
3	H	215	VAL	2.5
3	H	79	TYR	2.5
3	H	102	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	148	LYS	2.5
2	L	71	THR	2.5
3	H	98	ASP	2.5
1	R	382	VAL	2.5
2	L	188	ASP	2.5
2	L	114	ALA	2.5
3	H	160	SER	2.5
3	H	162	ALA	2.5
1	R	386	LYS	2.5
1	R	450	ASN	2.5
2	L	69	SER	2.5
2	L	86	ALA	2.5
3	H	206	PRO	2.5
3	H	193	LEU	2.5
2	L	110	LYS	2.5
1	R	468	ILE	2.5
2	L	199	VAL	2.4
1	R	393	THR	2.4
3	H	119	SER	2.4
2	L	36	ALA	2.4
3	H	24	ALA	2.4
3	H	49	ALA	2.4
2	L	75	LEU	2.4
2	L	184	LEU	2.4
3	H	64	LYS	2.4
1	R	502	GLY	2.4
2	L	141	ASN	2.4
3	H	125	VAL	2.4
1	R	359	SER	2.4
2	L	4	LEU	2.4
2	L	43	GLY	2.4
3	H	22	CYS	2.4
3	H	210	LYS	2.4
1	R	451	TYR	2.4
1	R	452	LEU	2.4
1	R	340	GLU	2.4
3	H	208	ASN	2.4
1	R	371	SER	2.4
1	R	373	SER	2.4
2	L	130	SER	2.4
2	L	212	PHE	2.3
2	L	15	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	H	14	PRO	2.3
3	H	164	THR	2.3
2	L	161	ASN	2.3
1	R	479	PRO	2.3
2	L	187	ALA	2.3
1	R	496	GLY	2.3
2	L	104	GLY	2.3
3	H	179	LEU	2.3
2	L	59	GLY	2.3
1	R	390	LEU	2.3
1	R	461	LEU	2.3
2	L	168	GLU	2.2
1	R	494	SER	2.2
1	R	418	ILE	2.2
2	L	149	VAL	2.2
3	H	173	VAL	2.2
1	R	428	ASP	2.2
1	R	513	LEU	2.2
1	R	495	TYR	2.2
1	R	490	PHE	2.2
1	R	334	ASN	2.2
2	L	113	VAL	2.2
3	H	217	PRO	2.2
3	H	23	ALA	2.2
2	L	137	CYS	2.2
1	R	443	SER	2.2
2	L	10	SER	2.2
3	H	21	SER	2.2
3	H	192	SER	2.2
2	L	186	LYS	2.2
3	H	150	PHE	2.2
2	L	150	GLN	2.2
3	H	85	LEU	2.2
2	L	211	SER	2.2
2	L	143	TYR	2.2
2	L	112	THR	2.2
2	L	77	ILE	2.1
3	H	168	HIS	2.1
1	R	426	PRO	2.1
3	H	111	THR	2.1
2	L	60	VAL	2.1
2	L	53	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	17	SER	2.1
1	R	498	GLN	2.1
2	L	81	GLN	2.1
1	R	431	GLY	2.1
3	H	15	GLY	2.1
3	H	214	ARG	2.1
2	L	37	TRP	2.1
1	R	507	PRO	2.1
2	L	131	GLY	2.1
1	R	529	LYS	2.1
1	R	352	ALA	2.1
2	L	190	GLU	2.0
2	L	204	LEU	2.0
3	H	95	CYS	2.0
2	L	192	HIS	2.0
1	R	415	THR	2.0
2	L	55	THR	2.0
3	H	70	SER	2.0
3	H	176	SER	2.0
3	H	104	LEU	2.0
2	L	193	LYS	2.0
1	R	527	PRO	2.0

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

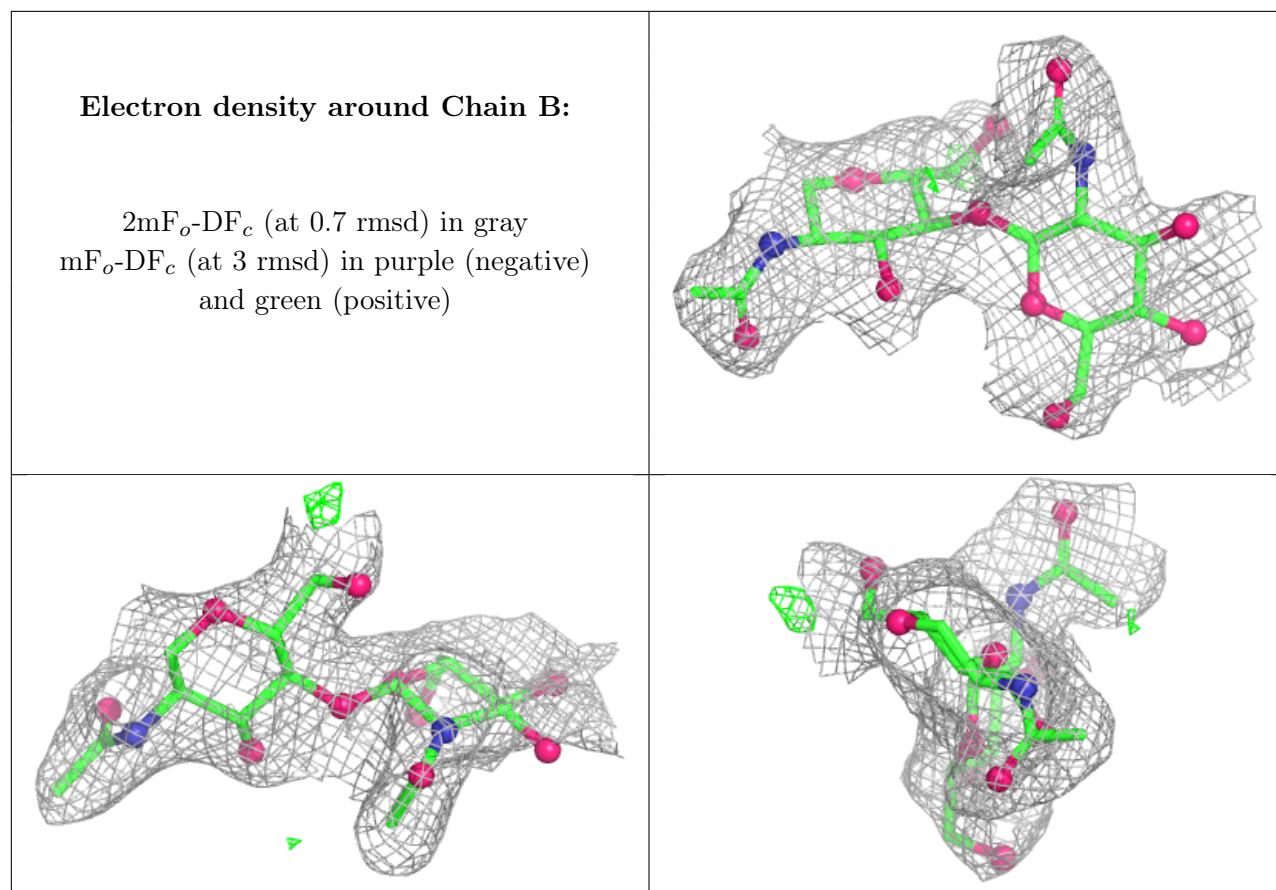
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	B	1	14/15	-	-	51,68,79,81	0
4	NAG	B	2	14/15	-	-	77,83,85,88	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
5	SO4	L	301	5/5	0.87	0.09	53,58,70,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.