



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 9, 2026 – 01:12 pm BST

PDB ID : 9TVT / pdb_00009tv
Title : CRYSTAL STRUCTURE OF SARS-COV-2 RECEPTOR BINDING DOMAIN (RBD-beta variant) in complex with 3D2 Fab and 1D1 Fab
Authors : Welin, M.; Cicek, H.; Focht, D.; Kimbung, Y.R.; Pisitkun, T.
Deposited on : 2026-01-13
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

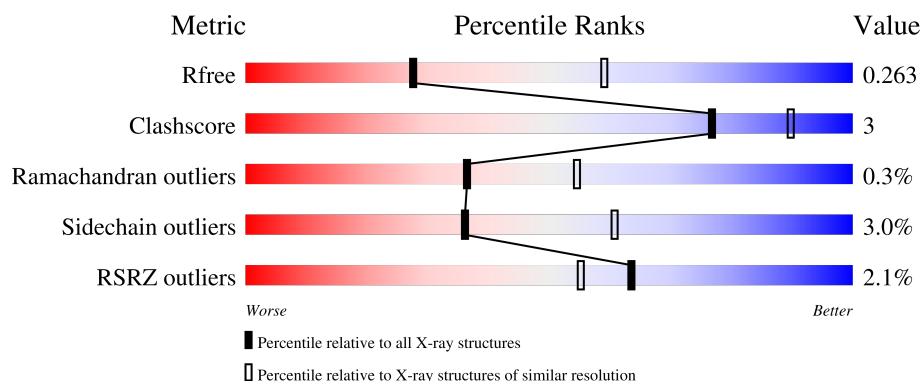
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	231	5% 73% 10% 16%
1	B	231	% 71% 11% 18%
2	C	221	% 83% 13% ..
2	H	221	% 88% 9% ..
3	D	214	% 92% 7%

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Mol	Chain	Length	Quality of chain
3	L	214	
4	E	231	
4	I	231	
5	F	216	
5	J	216	
6	M	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31593 atoms, of which 15575 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	A	193	Total	C	H	N	O	S	43	0	0
			2982	984	1450	255	285	8			
1	B	190	Total	C	H	N	O	S	41	0	0
			2935	969	1426	250	282	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	ASN	LYS	engineered mutation	UNP P0DTC2
A	484	LYS	GLU	engineered mutation	UNP P0DTC2
A	501	TYR	ASN	engineered mutation	UNP P0DTC2
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
B	417	ASN	LYS	engineered mutation	UNP P0DTC2
B	484	LYS	GLU	engineered mutation	UNP P0DTC2
B	501	TYR	ASN	engineered mutation	UNP P0DTC2
B	542	SER	-	expression tag	UNP P0DTC2
B	543	GLY	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 1D1 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	213	Total	C	H	N	O	S	63	0	0
			3154	1003	1571	263	311	6			
2	H	215	Total	C	H	N	O	S	64	0	0
			3172	1008	1579	265	314	6			

- Molecule 3 is a protein called 1D1 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	213	Total	C	H	N	O	S	60	0	0
			3236	1022	1596	276	337	5			
3	L	213	Total	C	H	N	O	S	60	0	0
			3236	1022	1596	276	337	5			

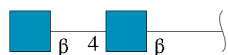
- Molecule 4 is a protein called 3D2 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	220	Total	C	H	N	O	S	70	0	0
			3279	1054	1625	272	322	6			
4	I	219	Total	C	H	N	O	S	70	0	0
			3272	1052	1622	271	321	6			

- Molecule 5 is a protein called 3D2 FAB LIGHT CHAIN.

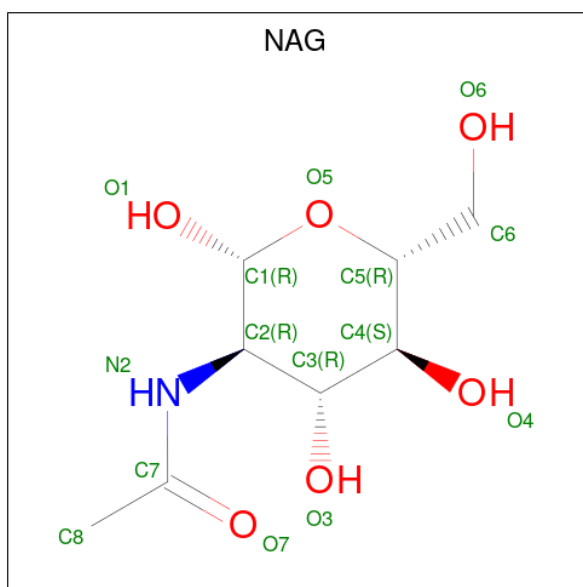
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	F	212	Total	C	H	N	O	S	66	0	0
			3113	990	1536	260	323	4			
5	J	210	Total	C	H	N	O	S	66	0	0
			3089	983	1525	257	320	4			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



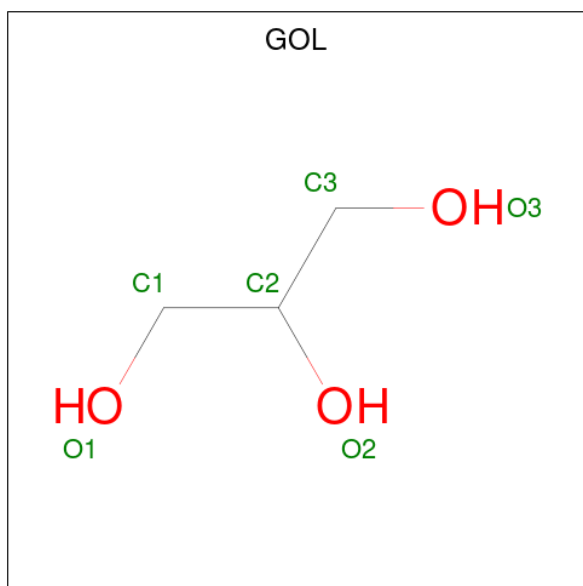
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	2	Total	C	H	N	O	11	0	0
			55	16	27	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	6	0
			28	8	14	1	5		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	J	1	Total	C	H	O	3	0
			14	3	8	3		

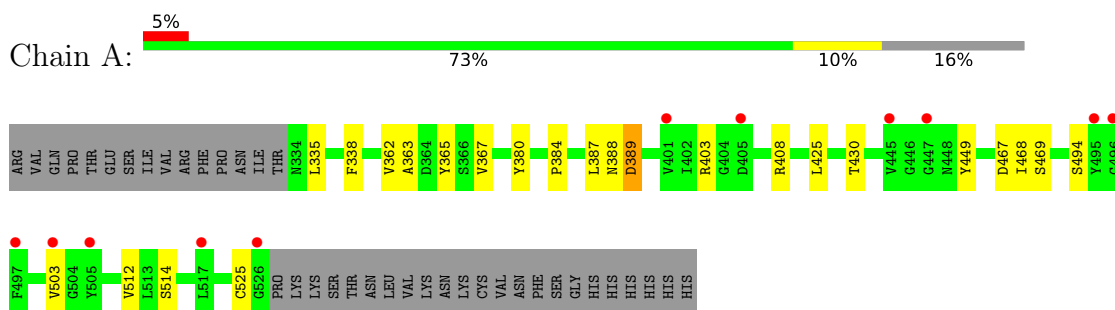
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total 4	O 4	0	0
9	B	5	Total 5	O 5	0	0
9	C	1	Total 1	O 1	0	0
9	D	2	Total 2	O 2	0	0
9	E	2	Total 2	O 2	0	0
9	F	1	Total 1	O 1	0	0
9	H	4	Total 4	O 4	0	0
9	I	3	Total 3	O 3	0	0
9	J	6	Total 6	O 6	0	0

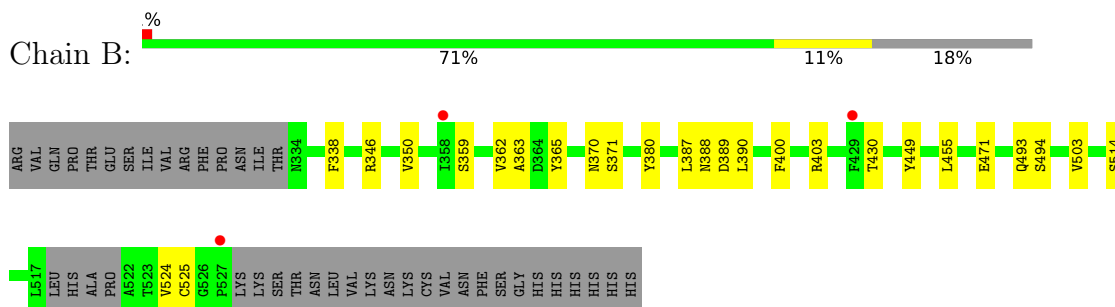
3 Residue-property plots [i](#)

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.

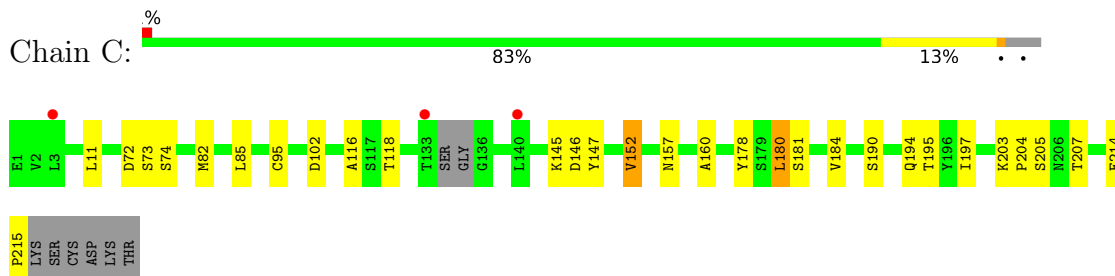
- Molecule 1: Spike protein S1



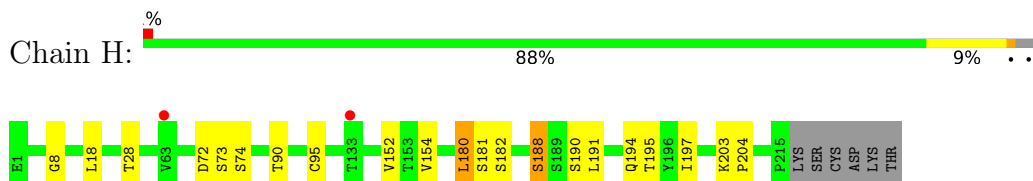
- Molecule 1: Spike protein S1



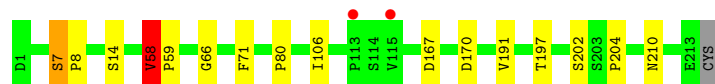
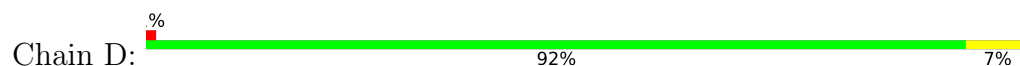
- Molecule 2: 1D1 FAB HEAVY CHAIN



- Molecule 2: 1D1 FAB HEAVY CHAIN



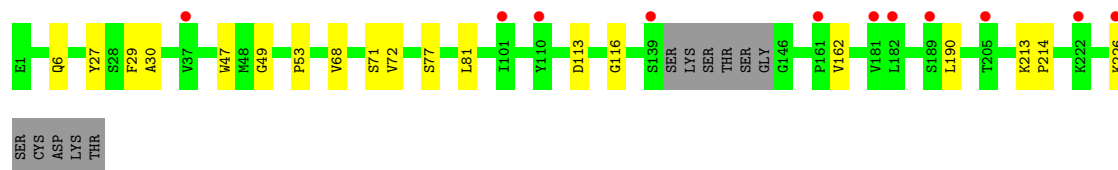
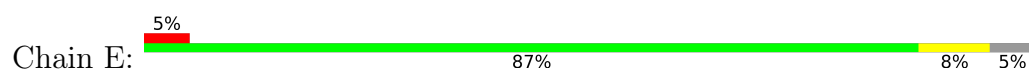
- Molecule 3: 1D1 FAB LIGHT CHAIN



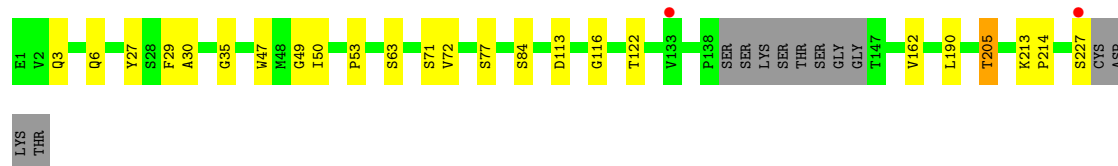
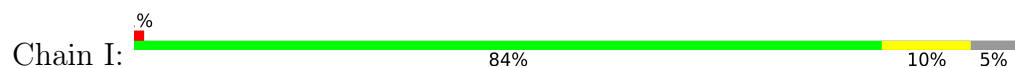
- Molecule 3: 1D1 FAB LIGHT CHAIN



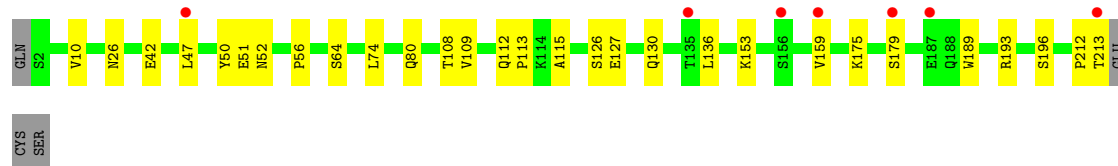
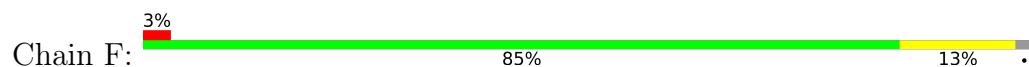
- Molecule 4: 3D2 FAB HEAVY CHAIN



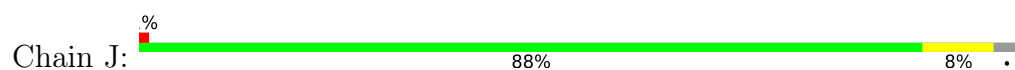
- Molecule 4: 3D2 FAB HEAVY CHAIN



- Molecule 5: 3D2 FAB LIGHT CHAIN



- Molecule 5: 3D2 FAB LIGHT CHAIN



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.17Å 65.20Å 204.02Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	49.95 – 2.85 49.95 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.95-2.85) 99.9 (49.95-2.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.126)	Depositor
R, R_{free}	0.206 , 0.262 0.209 , 0.263	Depositor DCC
R_{free} test set	3386 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31593	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	A	0.50	0/1576	0.89	1/2145 (0.0%)
1	B	0.51	0/1551	0.91	1/2109 (0.0%)
2	C	0.52	0/1619	0.94	1/2204 (0.0%)
2	H	0.53	0/1630	0.91	1/2220 (0.0%)
3	D	0.52	0/1674	0.94	2/2276 (0.1%)
3	L	0.53	0/1674	0.97	2/2276 (0.1%)
4	E	0.51	0/1700	0.88	1/2317 (0.0%)
4	I	0.51	0/1696	0.88	2/2312 (0.1%)
5	F	0.52	0/1616	0.86	0/2212
5	J	0.52	0/1602	0.89	1/2191 (0.0%)
All	All	0.52	0/16338	0.91	12/22262 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
5	J	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	20	THR	CA-CB-OG1	-8.07	97.49	109.60
4	E	113	ASP	CA-CB-CG	7.62	120.22	112.60
4	I	205	THR	CA-CB-OG1	-6.29	100.16	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ARG	CB-CA-C	-6.14	99.09	109.83
1	B	403	ARG	CB-CA-C	-5.79	99.71	109.83

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	ARG	Sidechain
1	B	346	ARG	Sidechain
5	J	62	ARG	Sidechain

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	1532	1450	1448	9	0
1	B	1509	1426	1424	11	0
2	C	1583	1571	1568	14	0
2	H	1593	1579	1577	10	0
3	D	1640	1596	1594	7	0
3	L	1640	1596	1594	6	1
4	E	1654	1625	1620	9	0
4	I	1650	1622	1617	9	0
5	F	1577	1536	1533	10	1
5	J	1564	1525	1522	7	0
6	M	28	27	25	0	0
7	B	14	14	13	0	0
8	J	6	8	8	0	0
9	A	4	0	0	0	0
9	B	5	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
9	E	2	0	0	0	0
9	F	1	0	0	0	0
9	H	4	0	0	0	0
9	I	3	0	0	0	0
9	J	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16018	15575	15543	92	1

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.

The worst 5 of 92 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:PRO:HA	3:D:106:ILE:CD1	2.21	0.71
5:F:126:SER:O	5:F:130:GLN:HG2	1.93	0.66
2:C:145:LYS:HG2	2:C:146:ASP:OD1	1.97	0.64
2:H:188:SER:HA	2:H:191:LEU:HD23	1.80	0.64
4:I:53:PRO:HA	4:I:72:VAL:HG11	1.80	0.64

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:213:THR:O	3:L:3:GLN:NE2[4_456]	2.12	0.08

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	A	191/231 (83%)	180 (94%)	9 (5%)	2 (1%)	12	25
1	B	186/231 (80%)	175 (94%)	11 (6%)	0	100	100
2	C	209/221 (95%)	197 (94%)	11 (5%)	1 (0%)	24	42
2	H	213/221 (96%)	206 (97%)	7 (3%)	0	100	100
3	D	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	24	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	24	42
4	E	216/231 (94%)	205 (95%)	11 (5%)	0	100	100
4	I	215/231 (93%)	204 (95%)	11 (5%)	0	100	100
5	F	210/216 (97%)	198 (94%)	10 (5%)	2 (1%)	12	25
5	J	206/216 (95%)	197 (96%)	9 (4%)	0	100	100
All	All	2068/2226 (93%)	1960 (95%)	101 (5%)	7 (0%)	36	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ASP
1	A	388	ASN
5	F	212	PRO
5	F	56	PRO
2	C	184	VAL

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	166/203 (82%)	161 (97%)	5 (3%)	36	61
1	B	164/203 (81%)	159 (97%)	5 (3%)	36	61
2	C	178/185 (96%)	173 (97%)	5 (3%)	38	62
2	H	179/185 (97%)	174 (97%)	5 (3%)	38	62
3	D	189/190 (100%)	185 (98%)	4 (2%)	47	70
3	L	189/190 (100%)	185 (98%)	4 (2%)	47	70
4	E	186/196 (95%)	183 (98%)	3 (2%)	55	76
4	I	186/196 (95%)	178 (96%)	8 (4%)	26	50
5	F	178/182 (98%)	170 (96%)	8 (4%)	24	48
5	J	177/182 (97%)	171 (97%)	6 (3%)	32	58
All	All	1792/1912 (94%)	1739 (97%)	53 (3%)	36	61

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	179	SER
4	I	3	GLN
3	L	7	SER
5	F	193	ARG
2	H	95	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	112	GLN
2	H	81	GLN
5	J	174	ASN
2	H	83	ASN
3	D	152	ASN

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	$\# Z > 2$
6	NAG	M	1	1,6	14,14,15	0.40	0	17,19,21	0.85	1 (5%)
6	NAG	M	2	6	14,14,15	0.34	0	17,19,21	1.29	2 (11%)

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	M	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	M	2	6	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	2	NAG	C1-C2-N2	3.58	116.61	110.49
6	M	2	NAG	C2-N2-C7	2.80	126.89	122.90
6	M	1	NAG	C1-C2-N2	2.28	114.39	110.49

There are no chirality outliers.

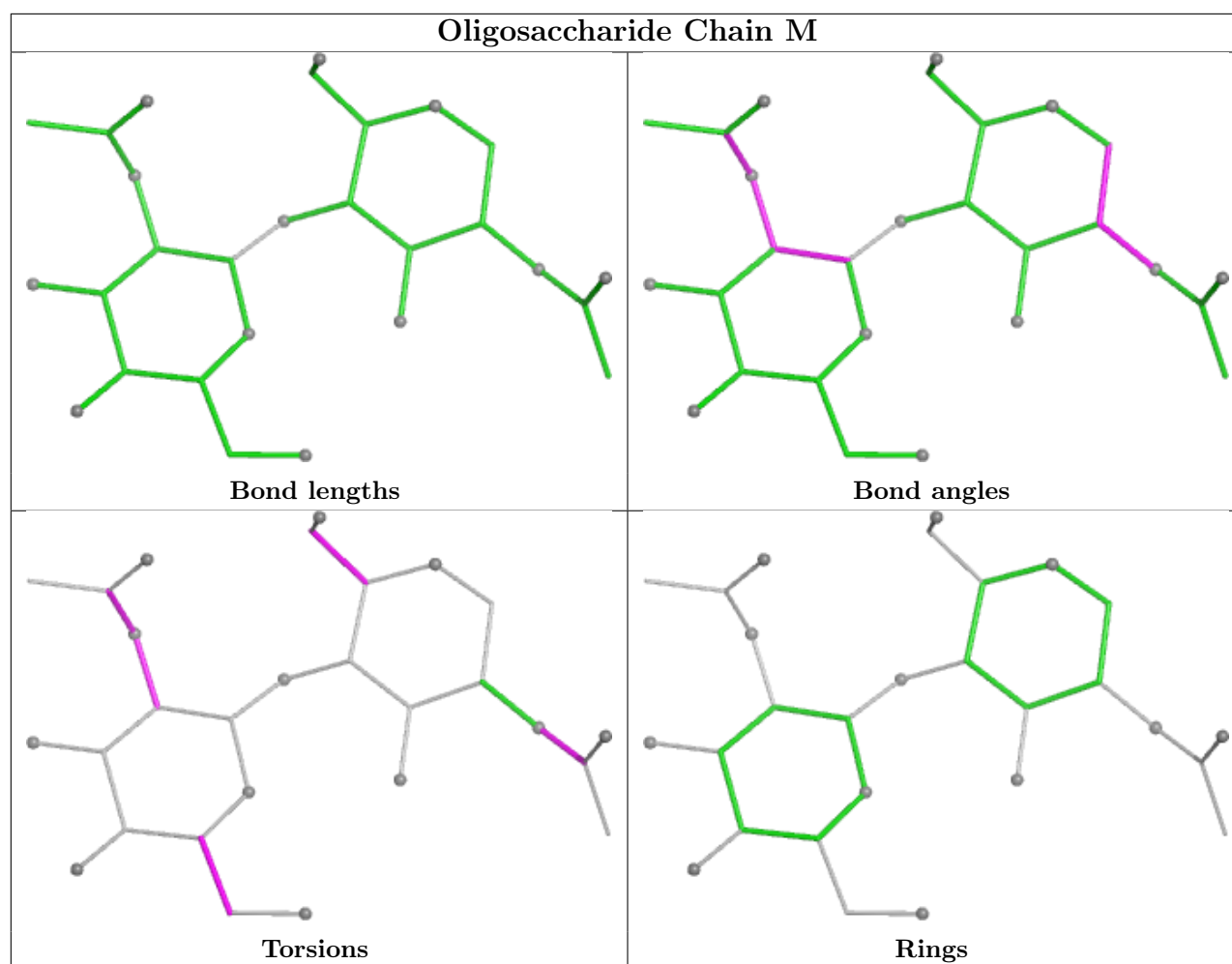
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
6	M	1	NAG	C8-C7-N2-C2
6	M	1	NAG	O7-C7-N2-C2
6	M	2	NAG	C3-C2-N2-C7

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GOL	J	301	-	5,5,5	0.10	0	5,5,5	0.27	0
7	NAG	B	601	1	14,14,15	0.45	0	17,19,21	1.47	2 (11%)

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
8	GOL	J	301	-	-	0/4/4/4	-
7	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	601	NAG	C2-N2-C7	3.74	128.22	122.90
7	B	601	NAG	C1-C2-N2	3.20	115.95	110.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	NAG	C8-C7-N2-C2
7	B	601	NAG	O7-C7-N2-C2

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 [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	A	193/231 (83%)	0.06	11 (5%) 29 22	51, 72, 125, 158	0
1	B	190/231 (82%)	-0.05	3 (1%) 70 64	57, 83, 139, 162	0
2	C	213/221 (96%)	0.17	3 (1%) 73 67	65, 93, 136, 174	0
2	H	215/221 (97%)	-0.39	2 (0%) 81 76	54, 74, 106, 147	0
3	D	213/214 (99%)	-0.30	2 (0%) 81 76	58, 82, 107, 125	0
3	L	213/214 (99%)	-0.27	2 (0%) 81 76	49, 75, 105, 119	0
4	E	220/231 (95%)	0.20	11 (5%) 34 27	63, 103, 141, 166	0
4	I	219/231 (94%)	-0.36	2 (0%) 81 76	55, 84, 107, 141	0
5	F	212/216 (98%)	0.04	7 (3%) 49 40	60, 102, 137, 169	0
5	J	210/216 (97%)	-0.25	2 (0%) 79 74	53, 87, 143, 155	0
All	All	2098/2226 (94%)	-0.12	45 (2%) 63 55	49, 85, 133, 174	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	113	PRO	3.9
1	A	526	GLY	3.7
5	F	47	LEU	3.6
1	A	503	VAL	3.4
4	E	101	ILE	3.3

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

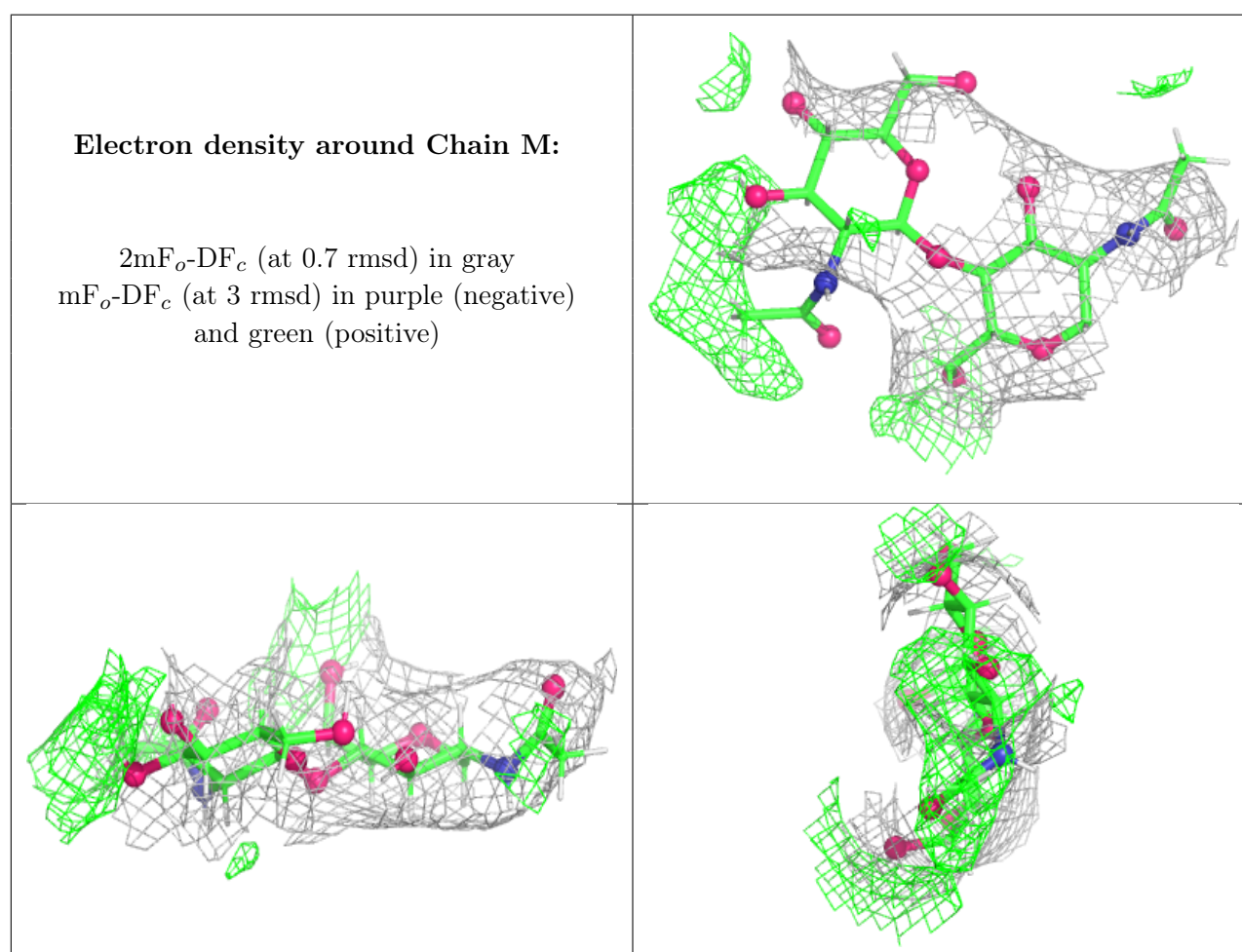
There are no non-standard protein/DNA/RNA residues in this entry.

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	M	1	14/15	-	-	93,102,111,130	5
6	NAG	M	2	14/15	-	-	129,151,181,202	6

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	601	14/15	0.84	0.11	78,92,97,99	6
8	GOL	J	301	6/6	0.90	0.12	80,84,95,97	3

6.5 Other polymers [i](#)

There are no such residues in this entry.