



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:48 AM UTC

PDB ID : 7PRY / pdb_00007pry
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 beta variant spike glycoprotein in complex with COVOX-45 and beta-6 Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-09-22
Resolution : 3.10 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

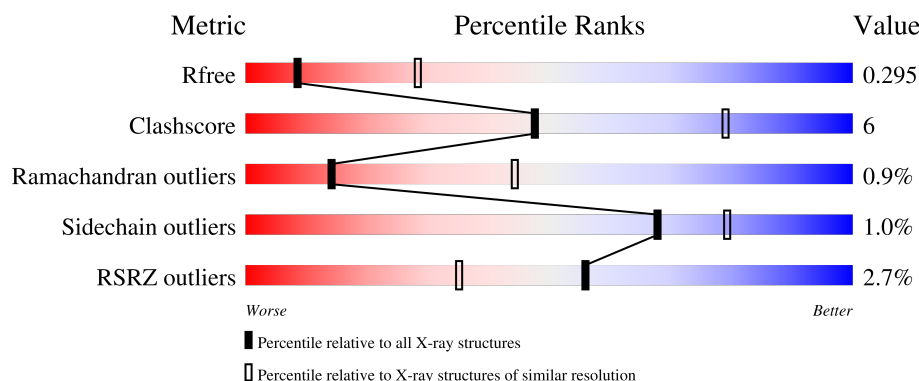
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	226	0% 83% 13% .
1	F	226	3% 79% 16% .
2	B	214	2% 87% 12%
2	G	214	2% 88% 11%
3	C	228	4% 80% 16% .

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Mol	Chain	Length	Quality of chain
3	H	228	75% 19%
4	D	215	5% 85% 14%
4	L	215	2% 82% 17%
5	E	210	4% 80% 12% 8%
5	I	210	3% 84% 8% 8%
6	J	3	67% 33%
6	K	3	67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16298 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 COVOX-45 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1631	1037	272	315	7			
1	F	216	Total	C	N	O	S	0	0	0
			1631	1037	272	315	7			

- Molecule 2 is a protein called COVOX-45 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1636	1023	271	338	4			
2	G	213	Total	C	N	O	S	0	0	0
			1636	1023	271	338	4			

- Molecule 3 is a protein called Beta-6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1644	1047	267	324	6			
3	C	220	Total	C	N	O	S	0	0	0
			1656	1053	269	327	7			

- Molecule 4 is a protein called Beta-6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	215	Total	C	N	O	S	0	0	0
			1662	1037	284	335	6			
4	D	215	Total	C	N	O	S	0	0	0
			1662	1037	284	335	6			

- Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	193	Total 1532	C 984	N 255	O 285	S 8	0	0	0
5	I	193	Total 1532	C 984	N 255	O 285	S 8	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

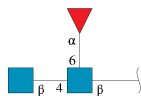
Chain	Residue	Modelled	Actual	Comment	Reference
E	319	MET	-	initiating methionine	UNP P0DTC2
E	320	GLY	-	expression tag	UNP P0DTC2
E	321	CYS	-	expression tag	UNP P0DTC2
E	322	VAL	-	expression tag	UNP P0DTC2
E	323	ALA	-	expression tag	UNP P0DTC2
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression 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	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2
I	319	MET	-	initiating methionine	UNP P0DTC2
I	320	GLY	-	expression tag	UNP P0DTC2
I	321	CYS	-	expression tag	UNP P0DTC2
I	322	VAL	-	expression tag	UNP P0DTC2
I	323	ALA	-	expression tag	UNP P0DTC2
I	324	GLU	-	expression tag	UNP P0DTC2
I	325	THR	-	expression tag	UNP P0DTC2
I	326	GLY	-	expression tag	UNP P0DTC2
I	327	HIS	-	expression tag	UNP P0DTC2
I	328	HIS	-	expression tag	UNP P0DTC2
I	329	HIS	-	expression tag	UNP P0DTC2
I	330	HIS	-	expression tag	UNP P0DTC2
I	331	HIS	-	expression tag	UNP P0DTC2
I	332	HIS	-	expression tag	UNP P0DTC2
I	417	ASN	LYS	variant	UNP P0DTC2
I	484	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	501	TYR	ASN	variant	UNP P0DTC2
I	527	LYS	-	expression tag	UNP P0DTC2
I	528	LYS	-	expression tag	UNP P0DTC2

- 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.

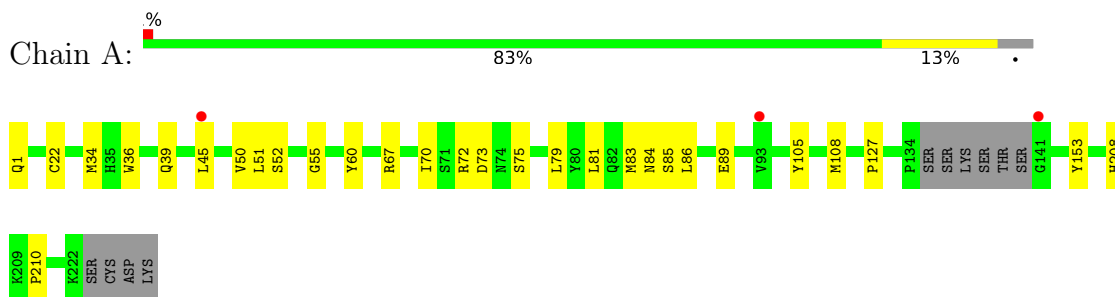


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

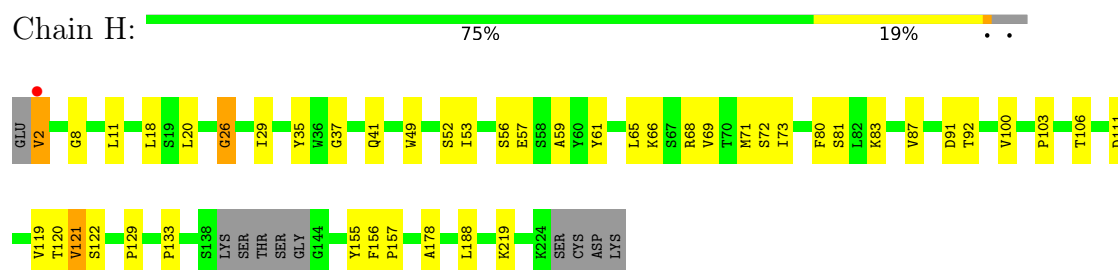
3 Residue-property plots [i](#)

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.

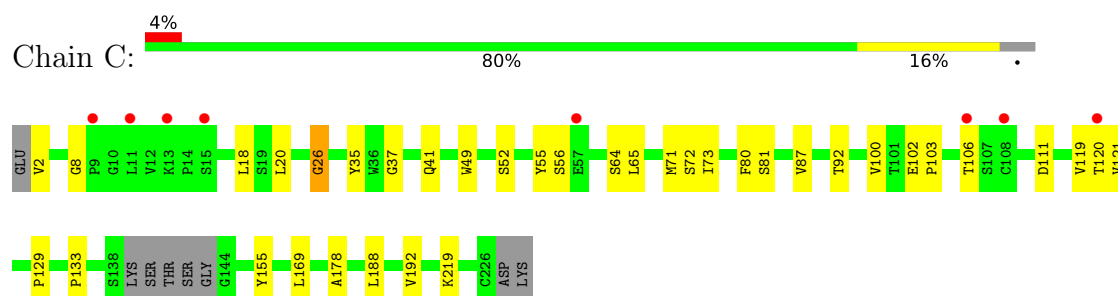
- Molecule 1: COVOX-45 Fab heavy chain



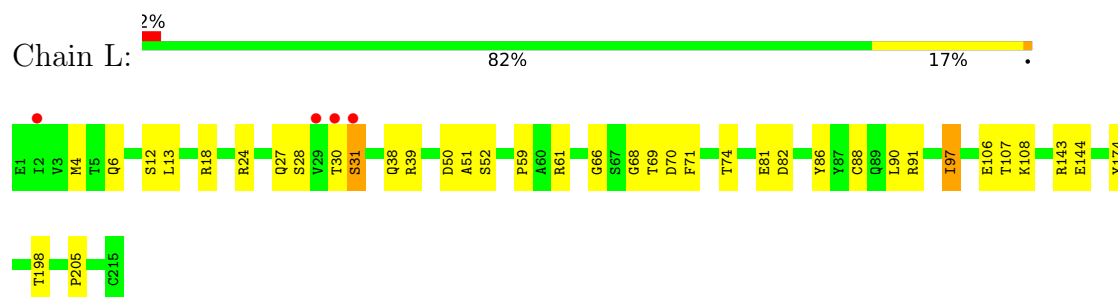
- Molecule 3: Beta-6 Fab heavy chain



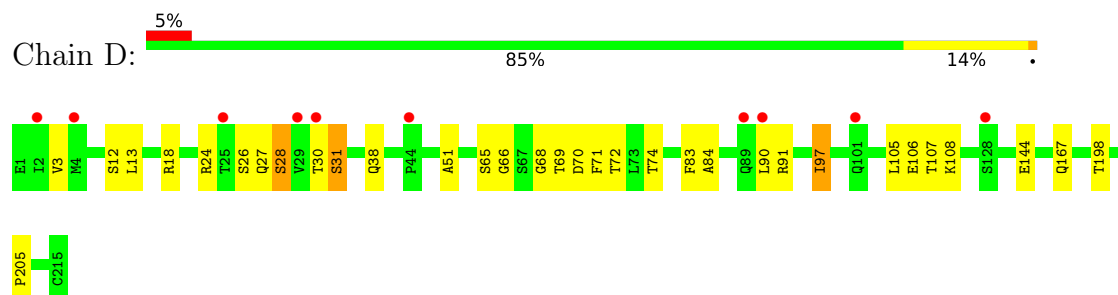
- Molecule 3: Beta-6 Fab heavy chain



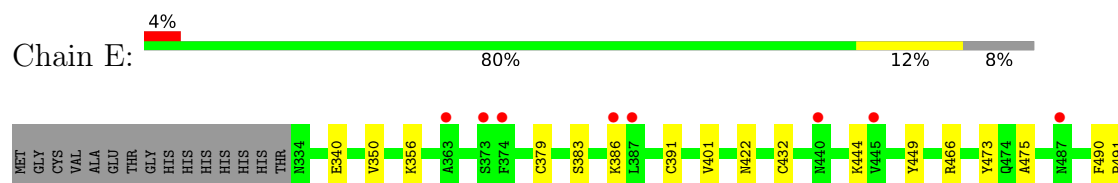
- Molecule 4: Beta-6 Fab light chain



- Molecule 4: Beta-6 Fab light chain

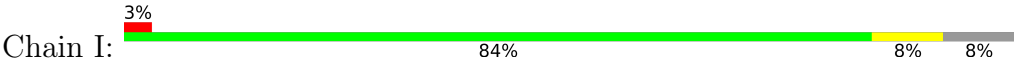


- Molecule 5: Spike protein S1





● Molecule 5: Spike protein S1



● 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.39Å 166.78Å 120.18Å 90.00° 108.52° 90.00°	Depositor
Resolution (Å)	58.32 – 3.10 58.32 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (58.32-3.10) 99.8 (58.32-3.10)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.244 , 0.291 0.246 , 0.295	Depositor DCC
R_{free} test set	2723 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16298	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.05% 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: NAG, FUC

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	0.13	0/1672	0.30	0/2276
1	F	0.12	0/1672	0.26	0/2276
2	B	0.13	0/1670	0.31	0/2271
2	G	0.12	0/1670	0.29	0/2271
3	C	0.14	0/1701	0.31	0/2326
3	H	0.16	0/1689	0.34	0/2310
4	D	0.12	0/1699	0.28	0/2312
4	L	0.12	0/1699	0.29	0/2312
5	E	0.11	0/1576	0.27	0/2145
5	I	0.12	0/1576	0.27	0/2145
All	All	0.13	0/16624	0.29	0/22644

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	A	1631	0	1596	18	0
1	F	1631	0	1596	24	0
2	B	1636	0	1581	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1636	0	1581	13	0
3	C	1656	0	1618	22	0
3	H	1644	0	1609	29	0
4	D	1662	0	1610	22	0
4	L	1662	0	1611	24	0
5	E	1532	0	1448	15	0
5	I	1532	0	1448	10	0
6	J	38	0	34	0	0
6	K	38	0	34	0	0
All	All	16298	0	15766	178	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 6.

All (178) 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)
4:L:51:ALA:HB1	4:L:66:GLY:HA3	1.69	0.74
1:A:51:LEU:HD22	1:A:55:GLY:HA2	1.73	0.70
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.75	0.68
1:A:50:VAL:HG21	1:A:105:TYR:HB3	1.76	0.67
4:L:68:GLY:O	4:L:70:ASP:N	2.28	0.67
4:D:51:ALA:HB1	4:D:66:GLY:HA3	1.77	0.66
1:F:50:VAL:HG21	1:F:105:TYR:HB3	1.76	0.66
1:F:51:LEU:HD22	1:F:55:GLY:HA2	1.77	0.65
4:D:18:ARG:HH21	4:D:74:THR:HG21	1.61	0.64
3:C:35:TYR:HB2	3:C:100:VAL:HB	1.81	0.63
5:I:340:GLU:OE1	5:I:356:LYS:NZ	2.31	0.63
1:F:22:CYS:HB3	1:F:79:LEU:HB3	1.82	0.62
4:D:30:THR:HG21	4:D:68:GLY:HA2	1.81	0.62
3:H:35:TYR:HB2	3:H:100:VAL:HB	1.82	0.62
4:L:18:ARG:HH21	4:L:74:THR:HG21	1.64	0.62
5:E:466:ARG:NH2	1:F:104:TYR:OH	2.29	0.62
3:C:2:VAL:HA	3:C:26:GLY:HA3	1.81	0.61
1:A:52:SER:O	1:A:72:ARG:NH1	2.33	0.61
3:H:92:THR:HG23	3:H:120:THR:HA	1.83	0.61
5:I:383:SER:HB2	5:I:386:LYS:HG2	1.82	0.60
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.83	0.60
1:A:22:CYS:HB3	1:A:79:LEU:HB3	1.83	0.60
5:E:383:SER:HB2	5:E:386:LYS:HG2	1.84	0.59
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:105:ASP:OD1	2:G:106:ILE:N	2.35	0.59
4:L:30:THR:HG21	4:L:68:GLY:HA2	1.84	0.59
3:H:41:GLN:NE2	4:L:38:GLN:OE1	2.33	0.58
1:F:83:MET:HB3	1:F:86:LEU:HD21	1.85	0.58
1:A:67:ARG:NH1	1:A:85:SER:O	2.33	0.58
4:D:12:SER:HB3	4:D:108:LYS:HB2	1.86	0.58
4:D:68:GLY:O	4:D:70:ASP:N	2.36	0.58
1:F:52:SER:O	1:F:72:ARG:NH1	2.35	0.57
3:H:18:LEU:HB2	3:H:87:VAL:HG21	1.86	0.57
4:D:107:THR:O	4:D:167:GLN:NE2	2.32	0.56
2:G:93:ASN:OD1	2:G:94:LEU:N	2.39	0.56
4:L:144:GLU:N	4:L:144:GLU:OE1	2.38	0.56
3:H:72:SER:OG	3:H:81:SER:OG	2.24	0.55
1:F:35:HIS:HB2	1:F:97:ALA:HB3	1.87	0.55
1:A:108:MET:HE3	2:B:96:LEU:HD12	1.88	0.55
1:A:51:LEU:HD13	1:A:72:ARG:HD2	1.88	0.55
1:A:89:GLU:OE1	1:A:89:GLU:N	2.35	0.55
3:H:87:VAL:HG12	3:H:121:VAL:HG21	1.89	0.55
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.38	0.55
3:C:102:GLU:OE1	5:I:498:GLN:NE2	2.36	0.55
5:E:340:GLU:OE1	5:E:356:LYS:NZ	2.39	0.55
1:F:108:MET:HE3	2:G:96:LEU:HD12	1.88	0.55
3:H:68:ARG:HH22	3:H:91:ASP:CG	2.15	0.55
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.90	0.54
3:C:18:LEU:HB2	3:C:87:VAL:HG21	1.90	0.54
3:C:41:GLN:NE2	4:D:38:GLN:OE1	2.39	0.54
2:G:35:TRP:CE2	2:G:73:PHE:HB2	2.43	0.53
4:D:13:LEU:O	4:D:107:THR:HA	2.08	0.53
3:H:18:LEU:HD11	3:H:119:VAL:HG21	1.89	0.53
4:D:144:GLU:N	4:D:144:GLU:OE1	2.39	0.53
1:F:89:GLU:OE1	1:F:89:GLU:N	2.39	0.53
1:F:34:MET:HB3	1:F:79:LEU:HD22	1.90	0.53
2:G:187:GLU:OE1	2:G:211:ARG:NH1	2.42	0.53
1:F:127:PRO:HB3	1:F:153:TYR:HB3	1.91	0.53
2:B:93:ASN:OD1	2:B:94:LEU:N	2.41	0.52
4:D:24:ARG:HA	4:D:70:ASP:HA	1.90	0.52
3:H:129:PRO:HB3	3:H:155:TYR:HB3	1.91	0.52
5:E:401:VAL:HG22	5:E:509:ARG:HG2	1.92	0.52
3:C:106:THR:HG21	4:D:31:SER:OG	2.09	0.52
5:I:498:GLN:HB2	5:I:501:TYR:CE1	2.45	0.52
4:L:12:SER:HB3	4:L:108:LYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:ALA:HB2	3:C:188:LEU:HD23	1.91	0.51
2:G:35:TRP:HB2	2:G:48:ILE:HB	1.92	0.51
3:C:129:PRO:HB3	3:C:155:TYR:HB3	1.92	0.51
3:C:49:TRP:CE2	4:D:97:ILE:HD12	2.45	0.51
2:B:193:ALA:HB2	2:B:208:SER:HB3	1.91	0.51
1:F:7:SER:OG	1:F:21:SER:OG	2.28	0.51
1:A:1:GLN:N	5:I:519:HIS:O	2.39	0.51
1:F:35:HIS:NE2	1:F:105:TYR:O	2.43	0.50
1:F:67:ARG:NH1	1:F:85:SER:O	2.40	0.50
2:G:61:ARG:NH1	2:G:82:ASP:OD2	2.35	0.50
2:B:21:ILE:HG21	2:B:102:THR:HG21	1.94	0.50
3:C:72:SER:OG	3:C:81:SER:OG	2.29	0.50
4:L:24:ARG:HA	4:L:70:ASP:HA	1.92	0.50
2:B:136:LEU:HB2	2:B:175:LEU:HB3	1.93	0.50
4:D:38:GLN:O	4:D:84:ALA:HB1	2.13	0.49
3:H:106:THR:HG21	4:L:31:SER:OG	2.12	0.49
5:E:490:PHE:CD1	5:E:491:PRO:HD2	2.49	0.48
2:G:145:LYS:HB3	2:G:197:THR:OG1	2.12	0.48
3:C:178:ALA:HA	3:C:188:LEU:HB3	1.94	0.48
3:H:73:ILE:HG13	3:H:80:PHE:HB3	1.95	0.48
1:F:108:MET:HB3	1:F:111:TRP:HE1	1.79	0.48
3:H:49:TRP:CE2	4:L:97:ILE:HD12	2.49	0.48
5:I:401:VAL:HG22	5:I:509:ARG:HG2	1.96	0.48
1:A:127:PRO:HB3	1:A:153:TYR:HB3	1.95	0.48
5:I:490:PHE:CD1	5:I:491:PRO:HD2	2.49	0.48
1:A:67:ARG:HG2	1:A:84:ASN:O	2.14	0.47
3:H:178:ALA:HB2	3:H:188:LEU:HD23	1.96	0.47
1:F:73:ASP:OD1	1:F:75:SER:OG	2.29	0.47
1:F:60:TYR:CE2	1:F:70:ILE:HG22	2.49	0.47
3:H:8:GLY:HA3	3:H:20:LEU:HD23	1.96	0.47
4:L:90:LEU:O	4:L:97:ILE:HA	2.15	0.47
1:F:51:LEU:HD21	1:F:58:LYS:HG2	1.97	0.47
4:L:13:LEU:O	4:L:107:THR:HA	2.15	0.47
3:C:92:THR:HG23	3:C:120:THR:HA	1.96	0.47
1:F:173:THR:HG23	1:F:188:SER:HB2	1.97	0.47
3:H:66:LYS:HA	3:H:69:VAL:HG12	1.96	0.46
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.31	0.46
3:C:73:ILE:HG13	3:C:80:PHE:HB3	1.97	0.46
5:E:498:GLN:HB2	5:E:501:TYR:CE1	2.50	0.46
2:B:33:LEU:HD11	2:B:88:CYS:HB2	1.98	0.46
3:H:53:ILE:HD13	3:H:73:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.97	0.46
3:H:122:SER:HB3	3:H:156:PHE:CZ	2.51	0.46
2:B:47:LEU:HA	2:B:58:VAL:HG21	1.99	0.45
4:D:198:THR:HG22	4:D:205:PRO:HB3	1.99	0.45
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.52	0.45
4:L:198:THR:HG22	4:L:205:PRO:HB3	1.98	0.45
2:G:108:ARG:HD3	2:G:109:THR:O	2.17	0.45
1:F:67:ARG:HG2	1:F:84:ASN:O	2.17	0.45
1:F:127:PRO:HD2	1:F:213:THR:HG21	1.98	0.45
4:D:90:LEU:O	4:D:97:ILE:HA	2.17	0.45
4:D:65:SER:HB3	4:D:72:THR:HB	1.97	0.45
5:I:444:LYS:O	5:I:498:GLN:HG2	2.17	0.45
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.99	0.44
3:H:53:ILE:HB	3:H:71:MET:HE2	2.00	0.44
3:H:106:THR:HG23	4:L:91:ARG:O	2.18	0.44
3:C:8:GLY:HA3	3:C:20:LEU:HD23	1.98	0.44
4:D:66:GLY:HA2	4:D:71:PHE:CD2	2.52	0.44
4:L:6:GLN:OE1	4:L:88:CYS:N	2.42	0.44
4:L:143:ARG:HB3	4:L:174:TYR:CD1	2.52	0.44
2:G:136:LEU:HB2	2:G:175:LEU:HB3	1.99	0.44
3:H:11:LEU:HD21	3:H:157:PRO:HG3	2.00	0.44
3:H:178:ALA:HA	3:H:188:LEU:HB3	1.99	0.44
1:F:208:HIS:CD2	1:F:210:PRO:HD2	2.53	0.44
3:C:18:LEU:HD11	3:C:119:VAL:HG21	1.99	0.44
2:B:103:LYS:HZ3	2:B:142:ARG:HD2	1.83	0.44
5:I:393:THR:HA	5:I:522:ALA:HA	2.00	0.44
1:A:60:TYR:CE2	1:A:70:ILE:HG22	2.53	0.43
1:A:208:HIS:CD2	1:A:210:PRO:HD2	2.52	0.43
3:C:55:TYR:HA	3:C:73:ILE:HD13	1.99	0.43
4:D:26:SER:O	4:D:28:SER:N	2.51	0.43
3:H:61:TYR:HE2	3:H:71:MET:HG3	1.82	0.43
5:E:473:TYR:CE2	5:E:475:ALA:HB2	2.54	0.43
2:B:50:ASP:O	2:B:52:SER:N	2.49	0.43
2:G:108:ARG:NH1	2:G:109:THR:O	2.50	0.43
4:D:30:THR:CG2	4:D:68:GLY:HA2	2.48	0.43
1:A:73:ASP:OD1	1:A:75:SER:OG	2.27	0.43
4:L:30:THR:CG2	4:L:68:GLY:HA2	2.49	0.43
4:L:66:GLY:HA2	4:L:71:PHE:CD2	2.53	0.43
3:C:71:MET:HE2	3:C:71:MET:HB3	1.80	0.43
3:C:133:PRO:HD3	3:C:219:LYS:HE2	2.01	0.43
3:H:37:GLY:HA2	3:H:52:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:133:PRO:HD3	3:H:219:LYS:HE2	2.01	0.43
4:L:91:ARG:HG2	4:L:97:ILE:HG12	2.00	0.42
1:F:36:TRP:CG	1:F:81:LEU:HD22	2.53	0.42
2:G:89:GLN:HB2	2:G:98:PHE:CD2	2.54	0.42
3:H:53:ILE:HG13	3:H:59:ALA:HB2	2.02	0.42
5:E:525:CYS:HB3	5:E:526:GLY:H	1.68	0.42
2:B:35:TRP:CE2	2:B:73:PHE:HB2	2.55	0.42
5:E:444:LYS:O	5:E:498:GLN:HG2	2.19	0.42
4:L:50:ASP:O	4:L:52:SER:N	2.49	0.42
4:D:83:PHE:CD2	4:D:105:LEU:HG	2.55	0.42
5:E:519:HIS:O	1:F:1:GLN:N	2.52	0.42
5:E:497:PHE:N	5:E:501:TYR:HE2	2.18	0.41
4:L:39:ARG:NH2	4:L:81:GLU:O	2.53	0.41
2:G:6:GLN:NE2	2:G:102:THR:OG1	2.52	0.41
3:H:68:ARG:NH2	3:H:91:ASP:OD1	2.48	0.41
4:D:3:VAL:H	4:D:26:SER:HB3	1.85	0.41
3:H:29:ILE:CG2	3:H:73:ILE:HD11	2.51	0.41
2:B:115:VAL:HG21	2:B:196:VAL:HG11	2.03	0.41
4:L:4:MET:HE2	4:L:4:MET:HB2	1.71	0.41
3:C:106:THR:HG23	4:D:91:ARG:O	2.20	0.41
5:I:498:GLN:HB2	5:I:501:TYR:CZ	2.55	0.41
5:E:350:VAL:HG22	5:E:422:ASN:HB3	2.02	0.41
5:E:391:CYS:HA	5:E:525:CYS:HA	2.02	0.40
3:C:35:TYR:CB	3:C:100:VAL:HB	2.50	0.40
3:C:37:GLY:HA2	3:C:52:SER:HA	2.03	0.40
4:L:59:PRO:HB2	4:L:61:ARG:HG2	2.04	0.40
5:E:379:CYS:HA	5:E:432:CYS:HA	2.03	0.40
3:H:87:VAL:HG13	3:H:91:ASP:HB2	2.04	0.40
4:L:82:ASP:O	4:L:86:TYR:OH	2.34	0.40
3:C:169:LEU:HD21	3:C:192:VAL:HG21	2.04	0.40
5:E:502:GLY:O	5:E:506:GLN:HG3	2.22	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	212/226 (94%)	203 (96%)	9 (4%)	0	100	100
1	F	212/226 (94%)	203 (96%)	9 (4%)	0	100	100
2	B	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	G	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
3	C	216/228 (95%)	198 (92%)	14 (6%)	4 (2%)	6	27
3	H	214/228 (94%)	194 (91%)	16 (8%)	4 (2%)	6	27
4	D	213/215 (99%)	194 (91%)	14 (7%)	5 (2%)	5	23
4	L	213/215 (99%)	194 (91%)	14 (7%)	5 (2%)	5	23
5	E	191/210 (91%)	178 (93%)	13 (7%)	0	100	100
5	I	191/210 (91%)	177 (93%)	14 (7%)	0	100	100
All	All	2084/2186 (95%)	1949 (94%)	117 (6%)	18 (1%)	14	44

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	69	THR
4	D	69	THR
3	H	56	SER
4	L	27	GLN
4	L	31	SER
3	C	56	SER
4	D	27	GLN
4	D	31	SER
3	H	111	ASP
4	L	28	SER
4	D	28	SER
3	H	26	GLY
3	C	26	GLY
3	C	111	ASP
3	H	103	PRO
3	C	103	PRO
4	L	97	ILE
4	D	97	ILE

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	179/189 (95%)	179 (100%)	0	100	100
1	F	179/189 (95%)	177 (99%)	2 (1%)	65	78
2	B	187/188 (100%)	185 (99%)	2 (1%)	65	78
2	G	187/188 (100%)	185 (99%)	2 (1%)	65	78
3	C	192/199 (96%)	189 (98%)	3 (2%)	55	75
3	H	190/199 (96%)	185 (97%)	5 (3%)	40	68
4	D	188/188 (100%)	187 (100%)	1 (0%)	81	85
4	L	188/188 (100%)	187 (100%)	1 (0%)	81	85
5	E	166/180 (92%)	165 (99%)	1 (1%)	78	83
5	I	166/180 (92%)	164 (99%)	2 (1%)	63	78
All	All	1822/1888 (96%)	1803 (99%)	19 (1%)	68	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	LEU
2	B	105	ASP
3	H	2	VAL
3	H	57	GLU
3	H	65	LEU
3	H	83	LYS
3	H	121	VAL
4	L	106	GLU
5	E	449	TYR
1	F	105	TYR
1	F	125	LYS
2	G	195	GLU
2	G	196	VAL
3	C	64	SER
3	C	65	LEU
3	C	121	VAL

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Mol	Chain	Res	Type
4	D	106	GLU
5	I	430	THR
5	I	449	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	79	GLN
2	B	160	GLN
2	B	210	ASN
3	H	78	ASN
4	L	93	ASN
4	L	200	GLN
5	E	414	GLN
5	E	498	GLN
1	F	172	HIS
2	G	6	GLN
2	G	53	ASN
2	G	138	ASN
4	D	200	GLN
5	I	354	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	6,5	14,14,15	0.34	0	17,19,21	0.65	1 (5%)
6	NAG	J	2	6	14,14,15	0.18	0	17,19,21	0.36	0
6	FUC	J	3	6	10,10,11	0.65	0	14,14,16	0.69	0
6	NAG	K	1	6,5	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
6	NAG	K	2	6	14,14,15	0.23	0	17,19,21	0.38	0
6	FUC	K	3	6	10,10,11	0.71	0	14,14,16	0.70	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	6,5	-	0/6/23/26	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	6,5	-	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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	C1-O5-C5	2.08	114.97	112.19
6	J	1	NAG	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

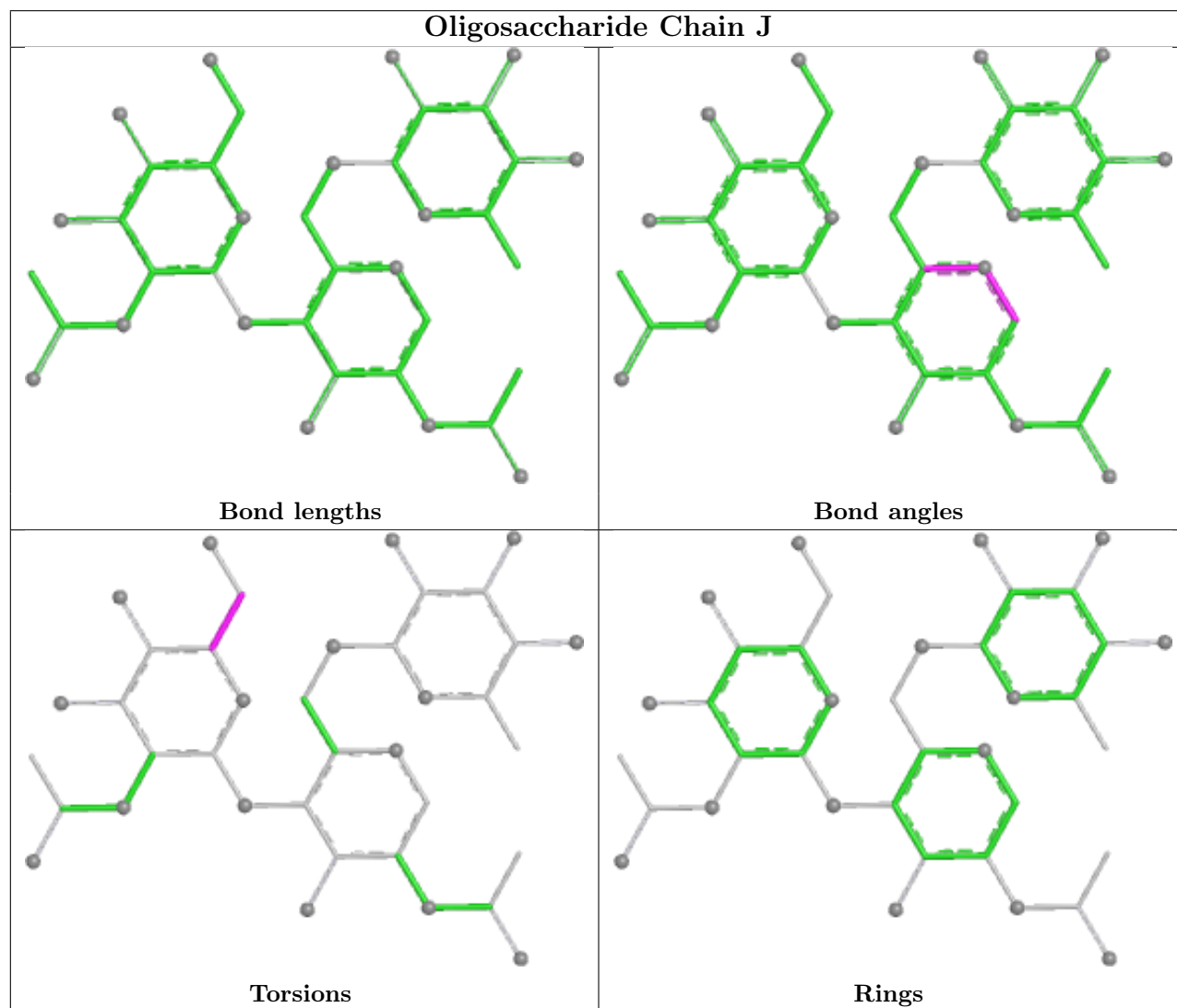
All (4) torsion outliers are listed below:

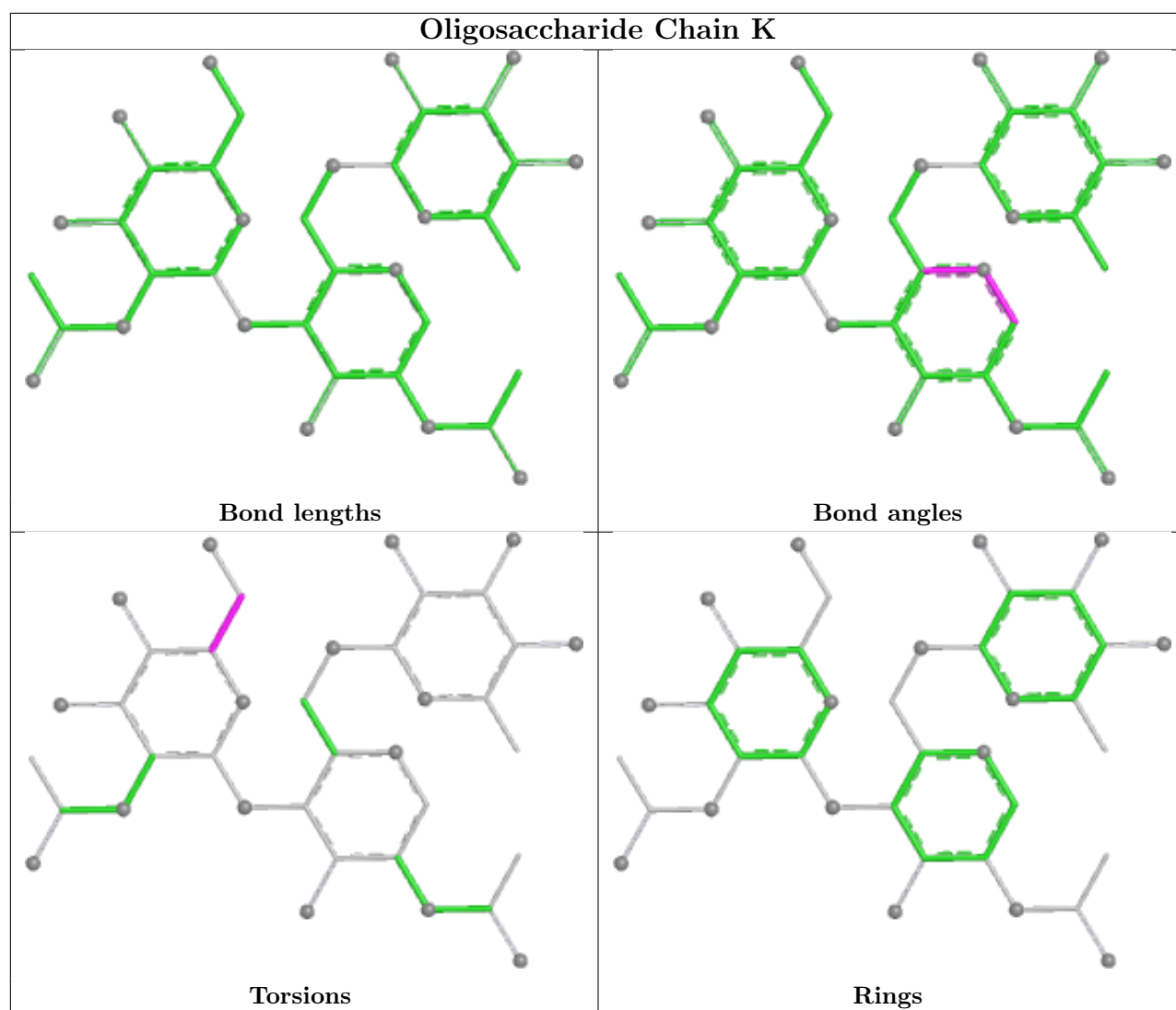
Mol	Chain	Res	Type	Atoms
6	K	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6

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](#)

There are no ligands in this entry.

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	A	216/226 (95%)	0.16	3 (1%) 73 53	61, 86, 118, 147	0
1	F	216/226 (95%)	0.51	6 (2%) 55 34	77, 118, 157, 225	0
2	B	213/214 (99%)	0.22	5 (2%) 61 39	63, 94, 136, 162	0
2	G	213/214 (99%)	0.57	5 (2%) 61 39	72, 139, 175, 228	0
3	C	220/228 (96%)	0.56	8 (3%) 46 26	75, 103, 140, 188	0
3	H	218/228 (95%)	0.09	1 (0%) 87 73	52, 78, 120, 146	0
4	D	215/215 (100%)	0.53	10 (4%) 36 19	86, 122, 167, 213	0
4	L	215/215 (100%)	0.18	4 (1%) 66 45	70, 99, 144, 207	0
5	E	193/210 (91%)	0.54	9 (4%) 36 19	71, 102, 152, 206	0
5	I	193/210 (91%)	0.47	6 (3%) 51 30	63, 93, 158, 227	0
All	All	2112/2186 (96%)	0.38	57 (2%) 56 35	52, 103, 158, 228	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	373	SER	5.0
4	D	29	VAL	4.8
4	L	29	VAL	4.3
1	F	101	SER	3.6
5	E	373	SER	3.4
1	F	100	GLY	3.4
4	D	44	PRO	3.3
2	B	93	ASN	3.2
3	C	11	LEU	3.2
2	G	51	ALA	3.1
2	B	148	TRP	3.1
4	L	30	THR	3.1
3	C	15	SER	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	363	ALA	3.0
1	F	63	SER	2.9
5	I	416	GLY	2.9
3	C	106	THR	2.8
5	I	503	VAL	2.8
5	E	487	ASN	2.8
2	G	159	SER	2.8
3	C	57	GLU	2.7
5	E	440	ASN	2.7
1	F	45	LEU	2.6
2	G	194	CYS	2.6
4	D	128	SER	2.6
1	F	26	GLY	2.6
4	D	4	MET	2.4
2	G	177	SER	2.4
1	F	91	THR	2.4
4	D	30	THR	2.4
2	B	163	VAL	2.4
4	D	89	GLN	2.4
5	I	362	VAL	2.4
5	E	526	GLY	2.3
5	I	385	THR	2.3
5	E	386	LYS	2.3
4	D	2	ILE	2.3
3	C	13	LYS	2.3
1	A	93	VAL	2.3
4	L	2	ILE	2.2
1	A	141	GLY	2.2
3	C	120	THR	2.2
1	A	45	LEU	2.2
3	C	9	PRO	2.2
4	D	25	THR	2.2
5	E	445	VAL	2.2
3	H	2	VAL	2.1
4	L	31	SER	2.1
5	E	387	LEU	2.1
4	D	90	LEU	2.0
2	G	58	VAL	2.0
2	B	162	SER	2.0
2	B	152	ASN	2.0
3	C	108	CYS	2.0
5	E	374	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	101	GLN	2.0
5	I	390	LEU	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](#)

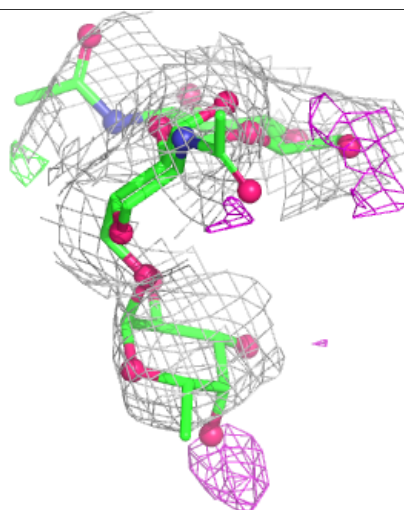
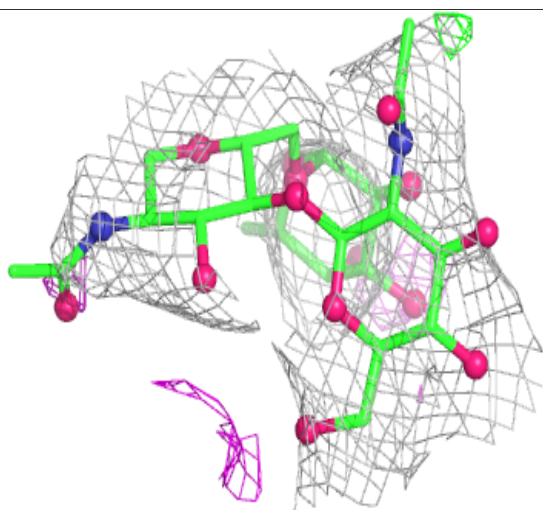
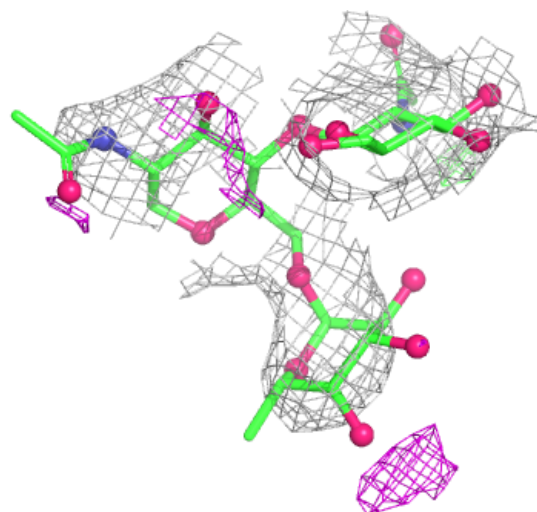
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

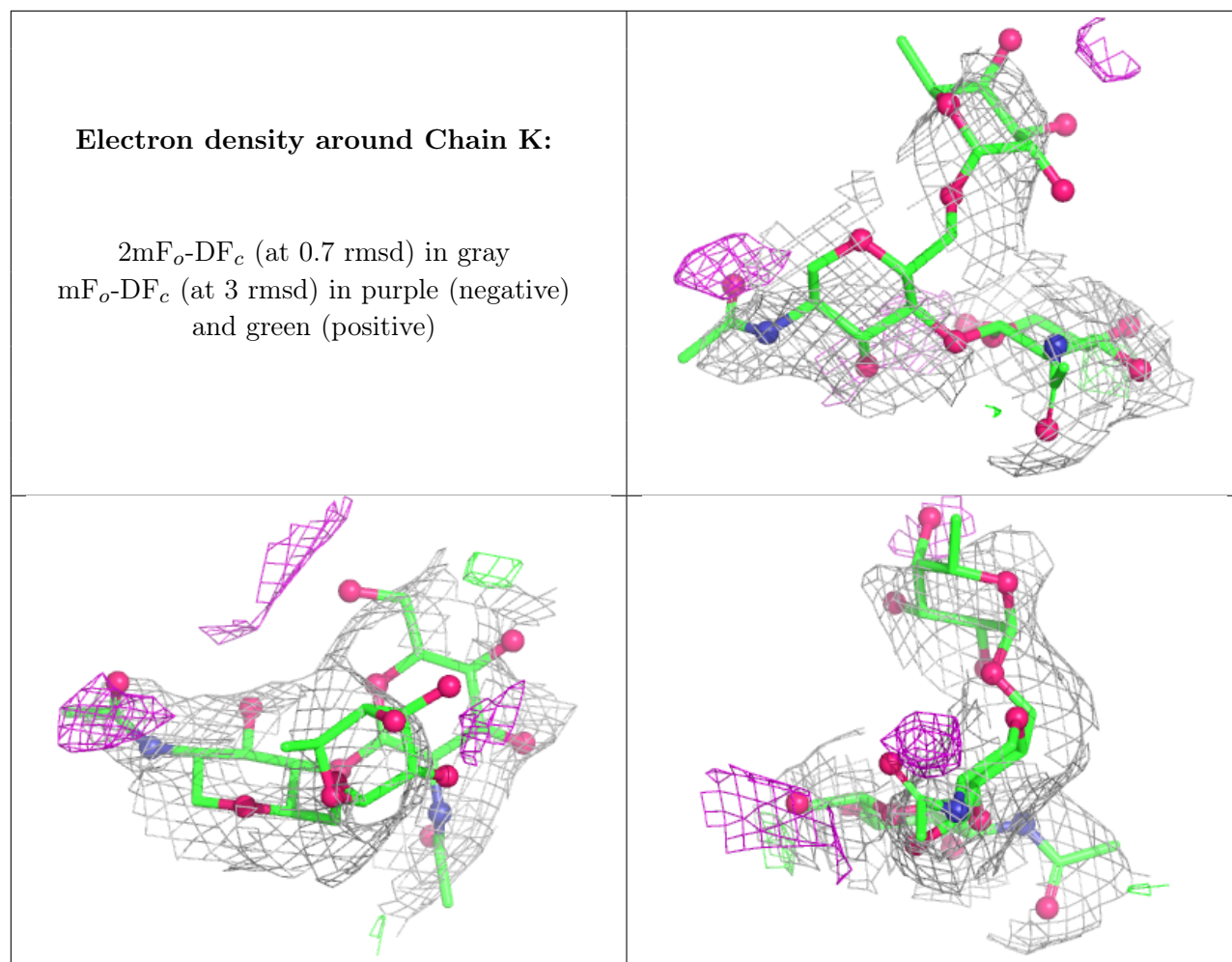
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	J	1	14/15	-	-	103,126,146,155	0
6	NAG	J	2	14/15	-	-	119,146,157,158	0
6	FUC	J	3	10/11	-	-	146,155,170,174	0
6	FUC	K	3	10/11	0.20	0.28	159,171,174,177	0
6	NAG	K	2	14/15	0.34	0.15	130,145,158,171	0
6	NAG	K	1	14/15	0.83	0.15	91,115,138,151	0

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.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.