



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 AM UTC

PDB ID : 8ZER / pdb_00008zer
Title : Crystal structure of the complex of Wuhan SARS-CoV-2 RBD (319-541) with P2C5 nanobody
Authors : Sluchanko, N.N.; Varfolomeeva, L.A.; Shcheblyakov, D.V.; Logunov, D.Y.; Gintsburg, A.L.; Popov, V.O.; Boyko, K.M.
Deposited on : 2024-05-06
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:

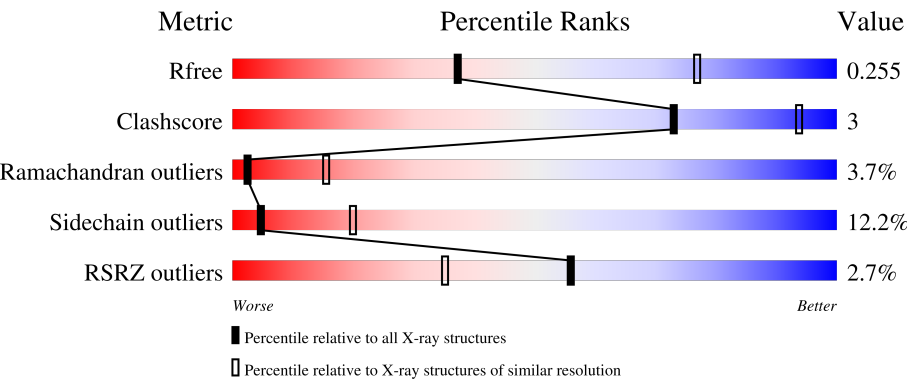
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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	B	235	3% 54%23%17%
1	C	235	3% 55%18%7%18%
1	E	235	3% 50%24%7%17%
1	G	235	3% 50%23%6%18%
1	I	235	3% 56%20%6%18%

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Mol	Chain	Length	Quality of chain
2	A	146	59%18%18%
2	D	146	3% 61%18%18%
2	F	146	% 63%16%18%
2	H	146	% 60%21%16%
2	J	146	3% 63%15%18%
3	K	3	100%
3	N	3	100%
4	L	2	100%
4	M	2	100%
5	O	7	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12475 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	B	195	Total	C	N	O	S	0	1	0
			1542	988	259	287	8			
1	C	192	Total	C	N	O	S	0	0	0
			1514	972	252	282	8			
1	E	194	Total	C	N	O	S	0	0	0
			1525	977	254	286	8			
1	G	192	Total	C	N	O	S	0	0	0
			1520	976	253	283	8			
1	I	193	Total	C	N	O	S	0	0	0
			1521	975	253	285	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	542	GLY	-	expression tag	UNP P0DTC2
B	543	SER	-	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
B	550	HIS	-	expression tag	UNP P0DTC2
B	551	HIS	-	expression tag	UNP P0DTC2
B	552	HIS	-	expression tag	UNP P0DTC2
B	553	HIS	-	expression tag	UNP P0DTC2
C	542	GLY	-	expression tag	UNP P0DTC2
C	543	SER	-	expression tag	UNP P0DTC2
C	544	HIS	-	expression tag	UNP P0DTC2
C	545	HIS	-	expression tag	UNP P0DTC2
C	546	HIS	-	expression tag	UNP P0DTC2
C	547	HIS	-	expression tag	UNP P0DTC2
C	548	HIS	-	expression tag	UNP P0DTC2

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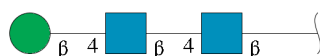
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Chain	Residue	Modelled	Actual	Comment	Reference
C	549	HIS	-	expression tag	UNP P0DTC2
C	550	HIS	-	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
C	552	HIS	-	expression tag	UNP P0DTC2
C	553	HIS	-	expression tag	UNP P0DTC2
E	542	GLY	-	expression tag	UNP P0DTC2
E	543	SER	-	expression tag	UNP P0DTC2
E	544	HIS	-	expression tag	UNP P0DTC2
E	545	HIS	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	HIS	-	expression tag	UNP P0DTC2
E	548	HIS	-	expression tag	UNP P0DTC2
E	549	HIS	-	expression tag	UNP P0DTC2
E	550	HIS	-	expression tag	UNP P0DTC2
E	551	HIS	-	expression tag	UNP P0DTC2
E	552	HIS	-	expression tag	UNP P0DTC2
E	553	HIS	-	expression tag	UNP P0DTC2
G	542	GLY	-	expression tag	UNP P0DTC2
G	543	SER	-	expression tag	UNP P0DTC2
G	544	HIS	-	expression tag	UNP P0DTC2
G	545	HIS	-	expression tag	UNP P0DTC2
G	546	HIS	-	expression tag	UNP P0DTC2
G	547	HIS	-	expression tag	UNP P0DTC2
G	548	HIS	-	expression tag	UNP P0DTC2
G	549	HIS	-	expression tag	UNP P0DTC2
G	550	HIS	-	expression tag	UNP P0DTC2
G	551	HIS	-	expression tag	UNP P0DTC2
G	552	HIS	-	expression tag	UNP P0DTC2
G	553	HIS	-	expression tag	UNP P0DTC2
I	542	GLY	-	expression tag	UNP P0DTC2
I	543	SER	-	expression tag	UNP P0DTC2
I	544	HIS	-	expression tag	UNP P0DTC2
I	545	HIS	-	expression tag	UNP P0DTC2
I	546	HIS	-	expression tag	UNP P0DTC2
I	547	HIS	-	expression tag	UNP P0DTC2
I	548	HIS	-	expression tag	UNP P0DTC2
I	549	HIS	-	expression tag	UNP P0DTC2
I	550	HIS	-	expression tag	UNP P0DTC2
I	551	HIS	-	expression tag	UNP P0DTC2
I	552	HIS	-	expression tag	UNP P0DTC2
I	553	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody P2C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	120	Total	C	N	O	S	0	0	0
			922	572	157	186	7			
2	D	120	Total	C	N	O	S	0	1	0
			929	575	160	187	7			
2	F	120	Total	C	N	O	S	0	0	0
			914	567	155	185	7			
2	H	123	Total	C	N	O	S	0	0	0
			945	585	161	192	7			
2	J	120	Total	C	N	O	S	0	1	0
			923	572	157	187	7			

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



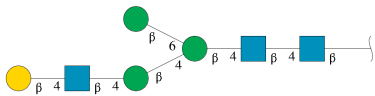
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

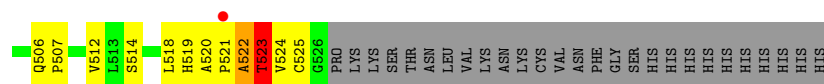


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

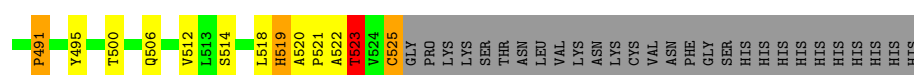
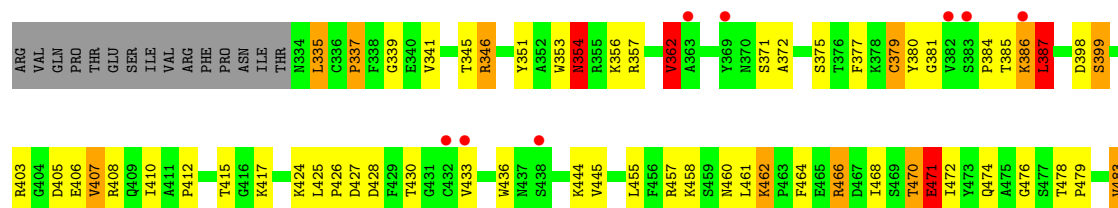
- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



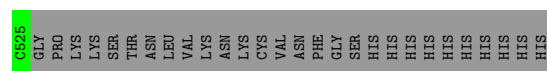
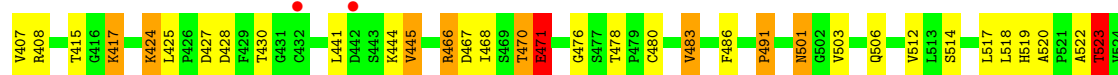
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	O	7	86	48	3	35	0	0	0



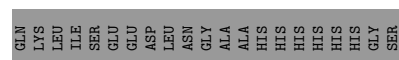
• Molecule 1: Spike protein S1



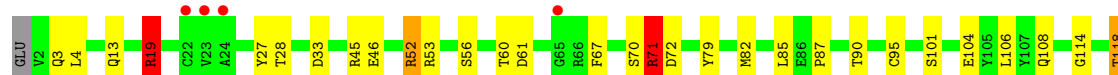
• Molecule 1: Spike protein S1

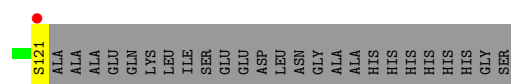


• Molecule 2: Nanobody P2C5

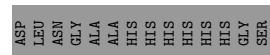


• Molecule 2: Nanobody P2C5

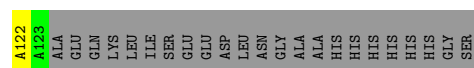
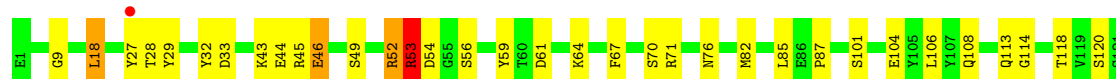




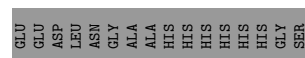
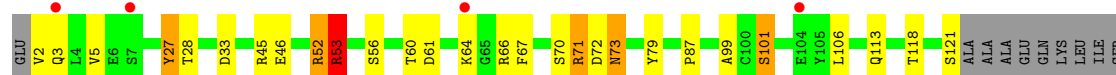
• Molecule 2: Nanobody P2C5



• Molecule 2: Nanobody P2C5



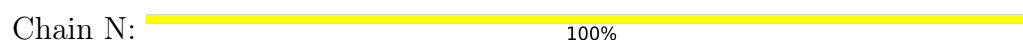
• Molecule 2: Nanobody P2C5



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



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



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

Chain L:  100%

NAG1
NAG2

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

Chain M:  100%

NAG1
NAG2

- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

NAG1
NAG2
BMA3
BMA4
NAG5
GAL6
BMA7

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.48Å 177.46Å 209.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 3.10 45.17 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.17-3.10) 98.7 (45.17-3.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.222 , 0.283 (Not available) , 0.255	Depositor DCC
R_{free} test set	2386 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12475	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, GAL, BMA

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	B	1.06	1/1591 (0.1%)	1.82	36/2167 (1.7%)
1	C	1.09	0/1557	1.89	35/2120 (1.7%)
1	E	1.09	2/1568 (0.1%)	1.88	44/2137 (2.1%)
1	G	1.08	4/1563 (0.3%)	1.92	43/2128 (2.0%)
1	I	1.01	0/1564	1.81	31/2132 (1.5%)
2	A	0.98	0/941	1.76	17/1272 (1.3%)
2	D	0.99	0/952	1.88	28/1287 (2.2%)
2	F	0.99	0/933	1.77	21/1263 (1.7%)
2	H	0.95	0/964	1.77	17/1303 (1.3%)
2	J	1.03	0/946	1.79	23/1280 (1.8%)
All	All	1.04	7/12579 (0.1%)	1.84	295/17089 (1.7%)

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	B	0	8
1	C	0	6
1	E	0	7
1	G	0	10
1	I	0	6
2	A	0	5
2	D	0	5
2	F	0	3
2	H	0	4
2	J	0	4
All	All	0	58

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	468	ILE	CB-CG1	-8.01	1.37	1.53
1	G	346	ARG	NE-CZ	7.45	1.41	1.33
1	E	417	LYS	CB-CG	7.14	1.73	1.52
1	G	468	ILE	CB-CG1	-6.68	1.40	1.53
1	E	525	CYS	N-CA	6.06	1.50	1.46
1	G	427	ASP	CG-OD1	5.51	1.35	1.25
1	G	525	CYS	C-O	5.24	1.34	1.23

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	417	LYS	CB-CG-CD	12.69	140.49	111.30
2	D	46	GLU	CB-CG-CD	12.47	133.80	112.60
2	F	104	GLU	CB-CG-CD	11.66	132.42	112.60
1	G	362	VAL	N-CA-CB	10.91	124.08	110.99
1	C	405	ASP	CA-CB-CG	10.56	123.17	112.60
2	A	27	TYR	CB-CA-C	10.12	127.95	110.45
1	G	346	ARG	CD-NE-CZ	10.00	138.40	124.40
1	C	506	GLN	CB-CA-C	9.90	124.06	108.91
1	G	471	GLU	N-CA-CB	9.86	127.15	110.49
1	I	337	PRO	N-CA-CB	-9.66	95.04	102.28
1	B	506	GLN	CB-CA-C	9.59	123.58	108.91
1	B	415	THR	CA-CB-OG1	-9.58	95.23	109.60
2	F	104	GLU	CB-CA-C	9.55	129.00	110.67
2	H	67	PHE	CA-CB-CG	9.40	123.20	113.80
1	E	506	GLN	CB-CA-C	9.35	123.21	108.91
1	B	471	GLU	N-CA-CB	9.21	126.06	110.49
1	G	506	GLN	CB-CA-C	9.18	122.96	108.91
1	E	471	GLU	N-CA-CB	9.17	125.99	110.49
2	D	27	TYR	CB-CA-C	9.11	126.21	110.45
1	C	337	PRO	N-CA-CB	-9.07	96.74	102.81
1	I	506	GLN	CB-CA-C	8.93	122.56	108.91
2	F	27	TYR	CB-CA-C	8.88	125.81	110.45
2	J	67	PHE	CA-CB-CG	8.71	122.51	113.80
1	C	351	TYR	N-CA-CB	8.70	122.90	110.12
2	D	13	GLN	CB-CA-C	8.68	124.12	109.72
2	D	28	THR	OG1-CB-CG2	8.66	126.63	109.30
2	A	67	PHE	CA-CB-CG	8.64	122.44	113.80
2	J	60	THR	CA-CB-OG1	-8.59	96.72	109.60
1	G	337	PRO	N-CA-CB	-8.49	95.91	102.28
2	H	27	TYR	CB-CA-C	8.46	125.08	110.45
2	J	61	ASP	CA-CB-CG	8.41	121.01	112.60
1	G	458	LYS	CA-CB-CG	8.39	130.88	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	351	TYR	N-CA-CB	8.36	122.40	110.12
2	D	61	ASP	CA-CB-CG	8.34	120.94	112.60
2	D	60	THR	CA-CB-OG1	-8.31	97.14	109.60
1	B	420	ASP	CB-CA-C	8.25	125.71	110.11
2	D	46	GLU	CG-CD-OE2	8.22	137.30	118.40
2	D	67	PHE	CA-CB-CG	8.20	122.00	113.80
2	F	92	MET	CG-SD-CE	8.19	118.92	100.90
2	H	104	GLU	CB-CA-C	8.10	124.23	110.79
2	F	27	TYR	CA-CB-CG	8.09	128.46	113.90
2	F	67	PHE	CA-CB-CG	8.04	121.84	113.80
1	I	483	VAL	N-CA-CB	7.99	122.11	111.25
2	D	28	THR	CA-CB-OG1	-7.95	97.68	109.60
2	J	99	ALA	CA-C-O	-7.93	112.30	120.71
1	G	470	THR	CA-CB-OG1	-7.92	97.73	109.60
1	G	379	CYS	CB-CA-C	7.82	122.71	109.80
1	E	483	VAL	N-CA-CB	7.78	121.83	111.25
2	A	71	ARG	CB-CA-C	7.68	123.20	109.38
1	B	467	ASP	CA-CB-CG	7.60	120.20	112.60
1	I	354	ASN	CA-CB-CG	-7.57	105.03	112.60
2	D	104	GLU	CB-CA-C	7.57	125.20	110.67
2	D	13	GLN	N-CA-CB	-7.49	98.51	109.83
1	I	470	THR	CA-CB-OG1	-7.42	98.47	109.60
1	G	354	ASN	CB-CA-C	-7.41	95.83	109.46
1	C	415	THR	CA-CB-CG2	7.38	123.05	110.50
2	D	53	ARG	N-CA-CB	7.32	120.88	110.12
1	C	417	LYS	CA-CB-CG	7.25	128.60	114.10
2	D	19	ARG	CG-CD-NE	7.20	127.83	112.00
1	E	387	LEU	N-CA-CB	7.14	122.03	110.40
2	A	2	VAL	N-CA-CB	7.11	123.58	111.50
2	A	53	ARG	N-CA-CB	7.09	120.54	110.12
2	J	27	TYR	CB-CA-C	7.07	125.73	111.60
1	E	523	THR	N-CA-CB	7.06	122.42	110.49
2	A	60	THR	CA-CB-OG1	-7.05	99.03	109.60
1	B	415	THR	OG1-CB-CG2	7.03	123.37	109.30
1	G	346	ARG	CA-CB-CG	7.01	128.12	114.10
1	I	470	THR	OG1-CB-CG2	7.01	123.32	109.30
1	E	427	ASP	CB-CA-C	6.99	124.10	110.67
1	E	354	ASN	CA-CB-CG	-6.95	105.65	112.60
2	H	46	GLU	CB-CA-C	6.90	120.92	109.53
1	B	387	LEU	N-CA-CB	6.88	121.61	110.40
1	G	345	THR	CA-CB-OG1	-6.84	99.34	109.60
1	C	471	GLU	N-CA-CB	6.83	122.04	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	71	ARG	CB-CA-C	6.81	121.63	109.38
2	F	46	GLU	CB-CA-C	6.79	120.72	109.53
1	G	427	ASP	CB-CA-C	6.74	121.98	110.79
1	I	471	GLU	N-CA-CB	6.74	121.88	110.49
1	G	462	LYS	CB-CG-CD	6.72	126.75	111.30
1	C	470	THR	CA-CB-OG1	-6.67	99.59	109.60
2	A	61	ASP	CA-CB-CG	6.66	119.26	112.60
1	E	405	ASP	CB-CA-C	6.65	124.21	110.31
2	H	45	ARG	N-CA-CB	6.65	120.58	109.94
1	C	374	PHE	N-CA-CB	6.64	121.67	110.46
1	G	415	THR	CA-CB-OG1	-6.62	99.67	109.60
1	G	399	SER	CA-CB-OG	6.60	124.31	111.10
1	E	486	PHE	CA-CB-CG	6.58	120.38	113.80
2	H	108	GLN	CB-CA-C	6.55	123.28	111.03
1	I	491	PRO	N-CA-CB	-6.55	95.29	102.17
1	C	483	VAL	N-CA-CB	6.53	123.28	111.21
2	J	28	THR	CA-CB-OG1	-6.49	99.87	109.60
1	E	416	GLY	N-CA-C	6.47	118.64	112.04
2	F	53	ARG	N-CA-CB	6.43	119.57	110.12
1	G	335	LEU	N-CA-CB	6.42	121.34	110.49
1	B	456	PHE	CA-CB-CG	6.42	120.22	113.80
1	G	523	THR	N-CA-CB	6.42	121.33	110.49
1	I	523	THR	N-CA-CB	6.40	121.31	110.49
1	G	491	PRO	N-CA-CB	-6.40	95.45	102.17
1	E	525	CYS	N-CA-C	6.39	117.74	108.34
1	B	468	ILE	CA-C-O	-6.39	113.23	120.26
2	D	114	GLY	CA-C-O	-6.39	117.82	122.23
1	G	460	ASN	CA-CB-CG	6.38	118.98	112.60
1	E	403	ARG	CB-CA-C	-6.38	97.81	109.54
1	G	471	GLU	CB-CA-C	-6.37	97.75	110.42
1	B	501	ASN	CA-CB-CG	6.36	118.96	112.60
1	G	346	ARG	NE-CZ-NH1	6.35	127.85	121.50
2	H	29	TYR	N-CA-CB	-6.34	101.38	110.57
1	B	483	VAL	N-CA-CB	6.33	122.93	111.21
1	C	354	ASN	CA-CB-CG	-6.30	106.30	112.60
1	G	346	ARG	CG-CD-NE	6.29	125.83	112.00
1	G	428	ASP	CA-CB-CG	6.27	118.87	112.60
1	E	362	VAL	CA-C-O	-6.26	112.95	120.78
1	G	483	VAL	N-CA-CB	6.25	119.18	110.56
1	G	500	THR	OG1-CB-CG2	6.25	121.79	109.30
1	I	424	LYS	N-CA-CB	6.24	120.82	110.52
2	F	45	ARG	N-CA-CB	6.23	119.91	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	45	ARG	CB-CA-C	-6.21	100.41	110.77
1	B	470	THR	CA-CB-OG1	-6.18	100.33	109.60
2	A	13	GLN	CB-CA-C	6.18	120.21	109.65
1	E	490	PHE	O-C-N	-6.17	115.94	121.31
1	G	405	ASP	CB-CA-C	6.16	123.18	110.31
1	B	427	ASP	CB-CA-C	6.14	120.99	110.79
2	D	71[A]	ARG	CG-CD-NE	6.13	125.50	112.00
2	D	71[B]	ARG	CG-CD-NE	6.13	125.50	112.00
2	J	2	VAL	N-CA-CB	6.13	121.92	111.50
2	J	46	GLU	CB-CA-C	6.13	119.78	109.48
1	B	523	THR	N-CA-CB	6.12	120.83	110.49
2	D	19	ARG	CB-CA-C	6.12	120.32	110.16
1	G	387	LEU	N-CA-CB	6.12	120.69	110.41
1	G	462	LYS	CG-CD-CE	6.12	125.37	111.30
2	H	108	GLN	N-CA-CB	-6.12	100.60	110.14
1	I	428	ASP	CA-CB-CG	6.10	118.70	112.60
1	I	387	LEU	N-CA-CB	6.08	119.27	110.88
1	E	424	LYS	N-CA-CB	6.05	120.51	110.52
1	C	523	THR	N-CA-CB	6.04	120.71	110.49
2	J	72	ASP	CA-CB-CG	6.04	118.64	112.60
1	I	417	LYS	CB-CG-CD	6.03	125.17	111.30
2	F	57	THR	CA-CB-OG1	6.03	118.64	109.60
1	C	403	ARG	CG-CD-NE	6.01	125.23	112.00
1	B	466	ARG	CD-NE-CZ	6.01	132.81	124.40
1	G	386	LYS	CA-CB-CG	6.00	126.11	114.10
2	F	114	GLY	CA-C-O	-5.98	118.11	122.23
1	B	468	ILE	O-C-N	5.96	129.86	122.11
2	J	52	ARG	N-CA-CB	-5.95	101.83	110.70
2	J	71	ARG	CA-C-O	-5.92	113.97	120.36
2	D	104	GLU	CB-CG-CD	5.91	122.65	112.60
2	F	61	ASP	CA-CB-CG	5.91	118.51	112.60
1	C	417	LYS	CD-CE-NZ	5.90	130.79	111.90
1	B	405	ASP	CB-CA-C	5.90	122.63	110.31
2	A	46	GLU	CB-CA-C	5.88	119.35	109.48
1	B	525	CYS	CB-CA-C	5.87	122.11	110.42
1	B	337	PRO	N-CA-CB	-5.86	97.88	102.28
1	G	351	TYR	N-CA-CB	5.84	118.71	110.12
1	E	407	VAL	N-CA-CB	5.84	120.63	110.65
1	B	355	ARG	CD-NE-CZ	5.82	132.55	124.40
2	J	28	THR	OG1-CB-CG2	5.82	120.94	109.30
1	I	385	THR	CA-CB-OG1	-5.82	100.87	109.60
1	E	355	ARG	CD-NE-CZ	5.82	132.54	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	71	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	E	415	THR	CA-CB-OG1	-5.79	100.91	109.60
2	A	27	TYR	CA-CB-CG	5.79	124.33	113.90
2	H	45	ARG	CB-CA-C	-5.78	101.11	110.77
2	D	33	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	467	ASP	CA-CB-CG	5.78	118.38	112.60
2	D	79	TYR	CB-CA-C	5.77	120.14	109.70
2	D	46	GLU	CB-CA-C	5.76	119.16	109.48
1	E	524	VAL	CA-C-O	-5.76	114.38	120.48
2	J	27	TYR	N-CA-CB	-5.75	101.24	110.51
1	I	467	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	484	GLU	CB-CG-CD	5.74	122.36	112.60
1	I	470	THR	CB-CA-C	5.73	121.82	110.42
2	H	53	ARG	N-CA-CB	5.73	118.65	110.06
1	I	353	TRP	N-CA-C	5.72	118.75	110.28
1	E	383	SER	CB-CA-C	5.71	119.10	109.67
1	E	360	ASN	CA-CB-CG	5.71	118.31	112.60
2	A	114	GLY	CA-C-O	-5.71	118.29	122.23
1	I	405	ASP	CB-CA-C	5.69	122.20	110.31
2	H	33	ASP	CA-CB-CG	5.68	118.28	112.60
2	H	52	ARG	N-CA-CB	-5.68	102.24	110.70
2	J	27	TYR	CA-CB-CG	5.67	124.11	113.90
1	E	345	THR	CA-CB-OG1	-5.66	101.11	109.60
2	J	53	ARG	N-CA-CB	5.64	118.42	110.12
1	B	341	VAL	N-CA-CB	5.64	117.41	110.64
1	I	389	ASP	CB-CA-C	5.63	119.79	111.17
2	A	45	ARG	CB-CA-C	-5.63	101.37	110.77
1	I	417	LYS	N-CA-CB	5.60	118.47	110.06
1	I	334	ASN	CA-C-N	5.59	132.22	121.54
1	I	334	ASN	C-N-CA	5.59	132.22	121.54
1	C	507	PRO	N-CA-CB	-5.58	97.89	103.19
1	C	501	ASN	CA-CB-CG	5.57	118.17	112.60
2	D	45	ARG	CB-CA-C	-5.57	101.47	110.77
1	E	501	ASN	N-CA-CB	5.56	118.31	110.36
1	G	470	THR	CB-CA-C	5.56	121.48	110.42
1	G	407	VAL	N-CA-CB	5.56	120.15	110.65
1	E	379	CYS	CB-CA-C	5.55	121.01	110.51
1	C	430	THR	OG1-CB-CG2	5.55	120.40	109.30
1	B	428	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	351	TYR	O-C-N	5.54	127.99	122.12
1	E	501	ASN	CA-CB-CG	5.54	118.14	112.60
1	G	471	GLU	CB-CG-CD	5.54	122.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	427	ASP	CB-CA-C	5.53	119.98	110.79
2	J	64	LYS	CG-CD-CE	5.52	124.00	111.30
2	J	52	ARG	CB-CA-C	5.52	120.19	110.36
1	E	346	ARG	CD-NE-CZ	5.51	132.12	124.40
1	C	389	ASP	CB-CA-C	5.51	119.60	111.17
1	E	353	TRP	N-CA-C	5.50	118.42	110.28
1	E	428	ASP	CA-CB-CG	5.50	118.10	112.60
2	A	26	GLY	CA-C-O	-5.50	118.65	122.22
1	E	470	THR	CA-CB-OG1	-5.49	101.36	109.60
1	I	486	PHE	CA-CB-CG	5.49	119.29	113.80
2	F	54	ASP	CA-CB-CG	5.49	118.09	112.60
1	E	463	PRO	N-CA-CB	5.47	109.00	103.25
2	J	71	ARG	CB-CG-CD	5.47	123.88	111.30
2	H	114	GLY	CA-C-O	-5.47	118.20	122.52
1	E	362	VAL	CB-CA-C	5.46	120.25	111.29
2	J	5	VAL	N-CA-CB	5.46	120.23	111.23
1	G	458	LYS	CB-CG-CD	5.45	123.83	111.30
2	D	87	PRO	CA-C-N	5.44	128.33	120.38
2	D	87	PRO	C-N-CA	5.44	128.33	120.38
1	I	501	ASN	N-CA-CB	5.44	118.72	110.45
1	C	468	ILE	O-C-N	5.44	129.18	122.11
2	F	2	VAL	CA-C-O	-5.44	111.55	120.80
1	G	470	THR	OG1-CB-CG2	5.43	120.16	109.30
1	I	468	ILE	O-C-N	5.42	129.16	122.11
1	B	490	PHE	CA-CB-CG	-5.42	108.38	113.80
2	D	52	ARG	N-CA-CB	-5.42	102.37	110.60
2	J	45	ARG	N-CA-CB	5.42	118.70	109.87
2	A	46	GLU	CB-CG-CD	5.41	121.80	112.60
1	C	347	PHE	CA-CB-CG	5.41	119.21	113.80
1	E	507	PRO	N-CA-CB	-5.40	98.06	103.19
1	B	398	ASP	CA-C-O	-5.39	115.12	121.16
1	E	363	ALA	N-CA-CB	5.39	119.60	110.49
1	B	351	TYR	N-CA-CB	5.38	118.03	110.12
2	H	87	PRO	CA-C-N	5.38	128.23	120.38
2	H	87	PRO	C-N-CA	5.38	128.23	120.38
2	A	105	TYR	CA-CB-CG	5.38	123.58	113.90
1	C	525	CYS	CB-CA-C	5.36	121.09	110.42
1	G	455	LEU	N-CA-CB	-5.36	102.65	110.47
1	C	385	THR	OG1-CB-CG2	-5.35	98.59	109.30
1	E	484	GLU	CB-CG-CD	5.35	121.69	112.60
2	J	33	ASP	CA-CB-CG	5.33	117.93	112.60
2	F	72	ASP	CA-CB-CG	5.33	117.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	385	THR	CA-CB-CG2	5.33	119.56	110.50
1	C	385	THR	CA-CB-CG2	5.32	119.55	110.50
1	C	407	VAL	N-CA-CB	5.32	119.75	110.65
1	B	466	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	E	523	THR	CA-CB-OG1	5.31	117.56	109.60
2	J	87	PRO	CA-C-N	5.29	128.10	120.38
2	J	87	PRO	C-N-CA	5.29	128.10	120.38
1	I	350	VAL	CA-C-O	-5.28	114.76	120.47
2	H	61	ASP	CA-CB-CG	5.28	117.88	112.60
1	I	503	VAL	N-CA-CB	5.27	117.71	110.54
2	A	19	ARG	CB-CA-C	5.25	118.88	110.16
2	F	33	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	376	THR	OG1-CB-CG2	5.24	119.78	109.30
1	C	428	ASP	CA-CB-CG	5.23	117.83	112.60
1	G	483	VAL	CA-CB-CG2	5.23	119.29	110.40
1	C	460	ASN	CA-C-O	-5.21	115.47	121.47
1	E	369	TYR	CA-CB-CG	5.21	123.28	113.90
1	C	424	LYS	CG-CD-CE	5.20	123.26	111.30
1	C	509	ARG	CA-CB-CG	-5.20	103.71	114.10
1	G	353	TRP	N-CA-C	5.19	117.96	110.28
1	G	424	LYS	N-CA-CB	5.18	119.06	110.52
1	G	405	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	355	ARG	CD-NE-CZ	5.17	131.63	124.40
1	C	470	THR	CB-CA-C	5.16	120.69	110.42
1	B	385	THR	CA-CB-CG2	5.16	119.27	110.50
1	B	415	THR	N-CA-CB	-5.14	103.58	111.56
1	G	362	VAL	N-CA-C	-5.13	101.02	108.36
2	H	54	ASP	CA-CB-CG	5.13	117.73	112.60
1	I	346	ARG	CB-CA-C	5.13	119.88	110.24
1	E	418	ILE	N-CA-C	5.11	115.34	110.53
2	F	108	GLN	CB-CA-C	5.09	120.55	111.03
1	B	394	ASN	CB-CA-C	-5.08	101.17	110.62
1	E	445	VAL	CB-CA-C	5.08	116.72	111.23
1	B	351	TYR	O-C-N	5.08	127.50	122.12
1	B	424	LYS	N-CA-CB	5.08	118.90	110.52
1	C	491	PRO	N-CA-CB	-5.08	96.84	102.17
1	E	522	ALA	CA-C-N	5.07	131.22	121.54
1	E	522	ALA	C-N-CA	5.07	131.22	121.54
1	G	385	THR	CA-CB-CG2	5.07	119.12	110.50
2	D	104	GLU	CA-C-O	-5.06	114.15	119.97
1	B	466	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	C	501	ASN	N-CA-CB	5.04	117.57	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	53	ARG	CG-CD-NE	5.04	123.09	112.00
1	I	445	VAL	CB-CA-C	5.04	116.67	111.23
1	C	495	TYR	N-CA-CB	5.03	117.75	110.26
1	E	471	GLU	CB-CG-CD	5.03	121.15	112.60
2	D	72	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	422	ASN	CA-C-O	-5.02	112.75	119.47
1	B	470	THR	OG1-CB-CG2	5.01	119.33	109.30
2	D	108	GLN	CB-CA-C	5.01	118.61	110.24
1	G	445	VAL	CB-CA-C	5.01	116.81	111.35
2	F	29	TYR	N-CA-CB	-5.00	103.31	110.57
1	E	491	PRO	N-CA-CB	-5.00	96.92	102.17

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	101	SER	Peptide
2	A	2	VAL	Mainchain
2	A	45	ARG	Sidechain
2	A	52	ARG	Sidechain
2	A	9	GLY	Peptide
1	B	333	THR	Peptide
1	B	357	ARG	Sidechain
1	B	371	SER	Peptide
1	B	381	GLY	Peptide
1	B	408	ARG	Sidechain
1	B	466	ARG	Sidechain
1	B	476	GLY	Peptide
1	B	526	GLY	Peptide
1	C	346	ARG	Sidechain
1	C	357	ARG	Sidechain
1	C	371	SER	Peptide
1	C	381	GLY	Peptide
1	C	476	GLY	Peptide
1	C	519	HIS	Peptide
2	D	101	SER	Peptide
2	D	19	ARG	Sidechain
2	D	52	ARG	Sidechain
2	D	71[A]	ARG	Sidechain
2	D	71[B]	ARG	Sidechain
1	E	357	ARG	Sidechain
1	E	371	SER	Peptide

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Mol	Chain	Res	Type	Group
1	E	379	CYS	Mainchain
1	E	381	GLY	Peptide
1	E	408	ARG	Sidechain
1	E	466	ARG	Sidechain
1	E	476	GLY	Peptide
2	F	101	SER	Peptide
2	F	52	ARG	Sidechain
2	F	71	ARG	Sidechain
1	G	346	ARG	Sidechain
1	G	357	ARG	Sidechain
1	G	371	SER	Peptide
1	G	379	CYS	Mainchain
1	G	381	GLY	Peptide
1	G	408	ARG	Sidechain
1	G	466	ARG	Sidechain
1	G	476	GLY	Peptide
1	G	483	VAL	Peptide
1	G	519	HIS	Peptide
2	H	101	SER	Peptide
2	H	122	ALA	Peptide
2	H	52	ARG	Sidechain
2	H	53	ARG	Sidechain
1	I	357	ARG	Sidechain
1	I	371	SER	Peptide
1	I	381	GLY	Peptide
1	I	408	ARG	Sidechain
1	I	466	ARG	Sidechain
1	I	476	GLY	Peptide
2	J	101	SER	Peptide
2	J	52	ARG	Sidechain
2	J	53	ARG	Sidechain
2	J	66	ARG	Sidechain

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	B	1542	0	1455	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1514	0	1426	10	0
1	E	1525	0	1428	10	0
1	G	1520	0	1435	14	0
1	I	1521	0	1425	7	0
2	A	922	0	860	9	0
2	D	929	0	864	8	0
2	F	914	0	843	4	0
2	H	945	0	885	7	0
2	J	923	0	853	3	0
3	K	39	0	34	0	0
3	N	39	0	34	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
5	O	86	0	73	0	0
All	All	12475	0	11665	75	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 (75) 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:I:466:ARG:HH21	2:J:106:LEU:HD22	1.59	0.68
2:A:53:ARG:HH11	2:A:53:ARG:HB3	1.59	0.67
1:I:425:LEU:HD21	1:I:512:VAL:HG11	1.85	0.58
2:D:19:ARG:HH11	2:D:19:ARG:HG3	1.68	0.58
1:B:406:GLU:OE2	1:B:495:TYR:OH	2.22	0.56
2:A:53:ARG:HH11	2:A:53:ARG:CB	2.19	0.56
1:B:470:THR:HG21	2:A:50:ILE:HD11	1.88	0.54
1:C:406:GLU:OE2	1:C:495:TYR:OH	2.22	0.53
1:G:425:LEU:HD21	1:G:512:VAL:HG11	1.91	0.53
2:H:53:ARG:HB3	2:H:53:ARG:HH11	1.74	0.52
1:B:425:LEU:HD21	1:B:512:VAL:HG11	1.91	0.52
1:I:480:CYS:O	1:I:483:VAL:HG22	2.10	0.52
1:C:466:ARG:HH21	2:D:106:LEU:HD13	1.75	0.51
1:C:425:LEU:HD21	1:C:512:VAL:HG11	1.91	0.51
2:H:49:SER:HB3	2:H:59:TYR:HD1	1.75	0.51
1:G:362:VAL:HG12	1:G:525:CYS:C	2.36	0.50
2:F:82:MET:HB3	2:F:85:LEU:HD21	1.94	0.50
1:G:466:ARG:HH21	2:H:106:LEU:HD22	1.77	0.50
2:H:28:THR:HG21	2:H:32:TYR:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:70:SER:OG	2:J:79:TYR:HB2	2.13	0.49
1:I:522:ALA:O	1:I:523:THR:HG23	2.12	0.49
1:G:406:GLU:OE2	1:G:495:TYR:OH	2.23	0.49
1:B:341:VAL:HG11	1:B:397:ALA:HB1	1.95	0.47
1:G:375:SER:HB3	1:G:436:TRP:HA	1.96	0.47
1:E:522:ALA:O	1:E:523:THR:HG23	2.15	0.47
2:H:53:ARG:HH11	2:H:53:ARG:CB	2.28	0.47
1:G:380:TYR:CE2	1:G:412:PRO:HD2	2.50	0.46
1:G:384:PRO:HA	1:G:387:LEU:HG	1.96	0.46
1:G:410:ILE:O	1:G:433:VAL:HG21	2.16	0.46
2:A:82:MET:HB3	2:A:85:LEU:HD21	1.97	0.46
2:D:82:MET:HB3	2:D:85:LEU:HD21	1.98	0.46
1:C:522:ALA:O	1:C:523:THR:HG23	2.16	0.46
1:B:468:ILE:HD12	2:A:99:ALA:HB3	1.98	0.46
2:F:53:ARG:HH11	2:F:53:ARG:HB3	1.81	0.46
1:G:474:GLN:HE22	1:G:479:PRO:HA	1.81	0.46
1:E:410:ILE:HD11	1:E:418:ILE:HG21	1.97	0.45
2:F:53:ARG:HH11	2:F:53:ARG:CB	2.29	0.45
1:C:470:THR:O	1:C:471:GLU:HB2	2.16	0.45
1:B:522:ALA:O	1:B:523:THR:HG23	2.16	0.45
1:I:341:VAL:HG11	1:I:397:ALA:HB1	1.99	0.45
1:G:426:PRO:HD3	1:G:464:PHE:CE2	2.51	0.45
1:B:468:ILE:HD12	2:A:99:ALA:CB	2.47	0.44
1:C:466:ARG:NH2	2:D:106:LEU:HD22	2.32	0.44
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.98	0.44
1:E:380:TYR:CE2	1:E:412:PRO:HD2	2.53	0.44
1:I:470:THR:O	1:I:471:GLU:CB	2.65	0.44
1:B:380:TYR:CE2	1:B:412:PRO:HD2	2.53	0.43
1:B:468:ILE:HD11	2:A:100:CYS:HA	1.99	0.43
1:E:470:THR:O	1:E:471:GLU:HB2	2.17	0.43
1:B:492:LEU:HD13	2:A:98:TRP:CZ3	2.53	0.43
1:E:382:VAL:HG12	1:E:386:LYS:NZ	2.33	0.43
2:H:9:GLY:H	2:H:18:LEU:HD11	1.84	0.43
1:G:522:ALA:O	1:G:523:THR:HG23	2.19	0.43
1:I:354:ASN:O	1:I:398:ASP:HA	2.20	0.42
2:D:4:LEU:HB3	2:D:95:CYS:SG	2.59	0.42
1:E:425:LEU:HD21	1:E:512:VAL:HG11	2.01	0.42
1:E:457:ARG:CZ	1:E:461:LEU:HD23	2.50	0.42
1:G:470:THR:O	1:G:471:GLU:CB	2.67	0.42
1:C:354:ASN:O	1:C:398:ASP:HA	2.19	0.42
1:C:453:TYR:CZ	1:C:493:GLN:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:THR:O	1:C:471:GLU:CB	2.67	0.42
2:D:71[A]:ARG:HH11	2:D:71[A]:ARG:HD2	1.67	0.41
2:D:71[B]:ARG:HH11	2:D:71[B]:ARG:HG2	1.85	0.41
2:F:29:TYR:CD1	2:F:29:TYR:N	2.87	0.41
1:G:457:ARG:CZ	1:G:461:LEU:HD23	2.50	0.41
1:B:384:PRO:HA	1:B:387:LEU:HG	2.02	0.41
1:E:354:ASN:O	1:E:398:ASP:HA	2.20	0.41
2:A:34:MET:HB3	2:A:78:LEU:HD22	2.02	0.41
1:E:358:ILE:HB	1:E:395:VAL:HB	2.02	0.41
1:C:380:TYR:HE1	1:C:433:VAL:HG23	1.85	0.41
1:E:364:ASP:OD2	1:E:367:VAL:HG23	2.21	0.41
1:G:354:ASN:O	1:G:398:ASP:HA	2.21	0.41
1:B:470:THR:O	1:B:471:GLU:HB2	2.21	0.40
2:D:90:THR:HG23	2:D:118:THR:HA	2.04	0.40
2:J:73:ASN:OD1	2:J:73:ASN:N	2.52	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	B	194/235 (83%)	161 (83%)	21 (11%)	12 (6%)	1	7
1	C	190/235 (81%)	157 (83%)	22 (12%)	11 (6%)	1	8
1	E	192/235 (82%)	158 (82%)	21 (11%)	13 (7%)	1	5
1	G	190/235 (81%)	158 (83%)	21 (11%)	11 (6%)	1	8
1	I	191/235 (81%)	162 (85%)	19 (10%)	10 (5%)	1	10
2	A	118/146 (81%)	111 (94%)	7 (6%)	0	100	100
2	D	119/146 (82%)	113 (95%)	6 (5%)	0	100	100
2	F	118/146 (81%)	110 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	121/146 (83%)	112 (93%)	8 (7%)	1 (1%)	16	47
2	J	119/146 (82%)	110 (92%)	9 (8%)	0	100	100
All	All	1552/1905 (82%)	1352 (87%)	142 (9%)	58 (4%)	2	15

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	363	ALA
1	B	372	ALA
1	C	363	ALA
1	C	372	ALA
1	C	417	LYS
1	C	519	HIS
1	E	363	ALA
1	E	372	ALA
1	E	519	HIS
1	G	372	ALA
1	G	471	GLU
1	G	519	HIS
1	I	335	LEU
1	I	363	ALA
1	I	372	ALA
1	B	471	GLU
1	B	519	HIS
1	B	523	THR
1	C	471	GLU
1	C	523	THR
1	E	471	GLU
1	E	523	THR
1	G	335	LEU
1	G	472	ILE
1	G	523	THR
1	I	471	GLU
1	I	519	HIS
1	I	523	THR
1	B	339	GLY
1	B	362	VAL
1	E	417	LYS
1	B	478	THR
1	C	339	GLY
1	C	478	THR

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Mol	Chain	Res	Type
1	E	339	GLY
1	E	478	THR
1	G	339	GLY
1	G	377	PHE
1	G	478	THR
1	I	339	GLY
1	I	478	THR
1	E	470	THR
1	G	521	PRO
2	H	64	LYS
1	B	335	LEU
1	B	417	LYS
1	B	470	THR
1	C	362	VAL
1	C	520	ALA
1	E	360	ASN
1	E	521	PRO
1	I	362	VAL
1	I	520	ALA
1	B	520	ALA
1	E	520	ALA
1	C	521	PRO
1	G	520	ALA
1	E	362	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	B	167/207 (81%)	146 (87%)	21 (13%)	4	19
1	C	163/207 (79%)	139 (85%)	24 (15%)	3	14
1	E	164/207 (79%)	142 (87%)	22 (13%)	4	17
1	G	164/207 (79%)	146 (89%)	18 (11%)	6	24
1	I	164/207 (79%)	142 (87%)	22 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	97/117 (83%)	83 (86%)	14 (14%)	3	14
2	D	98/117 (84%)	90 (92%)	8 (8%)	10	36
2	F	95/117 (81%)	86 (90%)	9 (10%)	8	30
2	H	99/117 (85%)	87 (88%)	12 (12%)	5	20
2	J	97/117 (83%)	86 (89%)	11 (11%)	5	23
All	All	1308/1620 (81%)	1147 (88%)	161 (12%)	5	20

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	334	ASN
1	B	335	LEU
1	B	337	PRO
1	B	341	VAL
1	B	347	PHE
1	B	356	LYS
1	B	368	LEU
1	B	383	SER
1	B	385	THR
1	B	386	LYS
1	B	387	LEU
1	B	407	VAL
1	B	417	LYS
1	B	424	LYS
1	B	430	THR
1	B	441	LEU
1	B	445	VAL
1	B	491	PRO
1	B	501	ASN
1	B	514	SER
1	B	518	LEU
2	A	3	GLN
2	A	13	GLN
2	A	18	LEU
2	A	19	ARG
2	A	27	TYR
2	A	43	LYS
2	A	44	GLU
2	A	53	ARG
2	A	56	SER

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Mol	Chain	Res	Type
2	A	70	SER
2	A	75	LYS
2	A	101	SER
2	A	118	THR
2	A	121	SER
1	C	337	PRO
1	C	341	VAL
1	C	356	LYS
1	C	373	SER
1	C	383	SER
1	C	385	THR
1	C	399	SER
1	C	403	ARG
1	C	407	VAL
1	C	415	THR
1	C	417	LYS
1	C	424	LYS
1	C	430	THR
1	C	441	LEU
1	C	444	LYS
1	C	466	ARG
1	C	468	ILE
1	C	483	VAL
1	C	484	GLU
1	C	491	PRO
1	C	493	GLN
1	C	501	ASN
1	C	514	SER
1	C	518	LEU
2	D	3	GLN
2	D	19	ARG
2	D	56	SER
2	D	70	SER
2	D	71[A]	ARG
2	D	71[B]	ARG
2	D	118	THR
2	D	121	SER
1	E	333	THR
1	E	334	ASN
1	E	337	PRO
1	E	341	VAL
1	E	347	PHE

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Mol	Chain	Res	Type
1	E	356	LYS
1	E	373	SER
1	E	383	SER
1	E	385	THR
1	E	386	LYS
1	E	387	LEU
1	E	390	LEU
1	E	403	ARG
1	E	407	VAL
1	E	415	THR
1	E	417	LYS
1	E	430	THR
1	E	441	LEU
1	E	491	PRO
1	E	501	ASN
1	E	514	SER
1	E	518	LEU
2	F	3	GLN
2	F	19	ARG
2	F	21	SER
2	F	53	ARG
2	F	56	SER
2	F	70	SER
2	F	101	SER
2	F	118	THR
2	F	121	SER
1	G	337	PRO
1	G	341	VAL
1	G	354	ASN
1	G	356	LYS
1	G	362	VAL
1	G	386	LYS
1	G	387	LEU
1	G	399	SER
1	G	403	ARG
1	G	407	VAL
1	G	417	LYS
1	G	430	THR
1	G	444	LYS
1	G	462	LYS
1	G	471	GLU
1	G	491	PRO

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Mol	Chain	Res	Type
1	G	514	SER
1	G	518	LEU
2	H	18	LEU
2	H	43	LYS
2	H	44	GLU
2	H	46	GLU
2	H	53	ARG
2	H	56	SER
2	H	70	SER
2	H	71	ARG
2	H	76	ASN
2	H	113	GLN
2	H	118	THR
2	H	120	SER
1	I	334	ASN
1	I	337	PRO
1	I	341	VAL
1	I	356	LYS
1	I	373	SER
1	I	383	SER
1	I	387	LEU
1	I	388	ASN
1	I	390	LEU
1	I	407	VAL
1	I	415	THR
1	I	417	LYS
1	I	424	LYS
1	I	430	THR
1	I	441	LEU
1	I	444	LYS
1	I	445	VAL
1	I	491	PRO
1	I	501	ASN
1	I	514	SER
1	I	517	LEU
1	I	518	LEU
2	J	3[A]	GLN
2	J	3[B]	GLN
2	J	27	TYR
2	J	53	ARG
2	J	56	SER
2	J	71	ARG

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Mol	Chain	Res	Type
2	J	73	ASN
2	J	101	SER
2	J	113	GLN
2	J	118	THR
2	J	121	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	ASN
1	B	388	ASN
2	A	73	ASN
2	A	81	GLN
2	A	83	ASN
1	C	409	GLN
1	C	501	ASN
2	D	73	ASN
2	D	81	GLN
2	D	83	ASN
2	D	108	GLN
2	D	116	GLN
1	E	360	ASN
1	E	388	ASN
1	E	501	ASN
1	G	388	ASN
2	H	39	GLN
2	H	73	ASN
2	J	83	ASN
2	J	108	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 ⓘ

17 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
3	NAG	K	1	3,1	14,14,15	1.40	3 (21%)	17,19,21	2.85	8 (47%)
3	NAG	K	2	3	14,14,15	0.85	0	17,19,21	1.49	3 (17%)
3	BMA	K	3	3	11,11,12	0.74	0	15,15,17	2.49	2 (13%)
4	NAG	L	1	4,1	14,14,15	0.67	0	17,19,21	2.83	9 (52%)
4	NAG	L	2	4	14,14,15	1.31	2 (14%)	17,19,21	3.57	10 (58%)
4	NAG	M	1	4,1	14,14,15	1.04	0	17,19,21	2.67	5 (29%)
4	NAG	M	2	4	14,14,15	0.73	0	17,19,21	2.62	7 (41%)
3	NAG	N	1	3,1	14,14,15	0.56	0	17,19,21	2.16	5 (29%)
3	NAG	N	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.98	4 (23%)
3	BMA	N	3	3	11,11,12	1.87	3 (27%)	15,15,17	2.51	5 (33%)
5	NAG	O	1	5,1	14,14,15	0.87	0	17,19,21	3.71	4 (23%)
5	NAG	O	2	5	14,14,15	0.77	0	17,19,21	3.33	7 (41%)
5	BMA	O	3	5	11,11,12	1.87	2 (18%)	15,15,17	2.39	6 (40%)
5	BMA	O	4	5	11,11,12	1.93	2 (18%)	15,15,17	2.54	5 (33%)
5	NAG	O	5	5	14,14,15	0.99	1 (7%)	17,19,21	1.61	3 (17%)
5	GAL	O	6	5	11,11,12	0.94	0	15,15,17	1.49	1 (6%)
5	BMA	O	7	5	11,11,12	1.18	2 (18%)	15,15,17	1.46	3 (20%)

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
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	M	2	4	-	3/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	BMA	N	3	3	-	1/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	3/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	BMA	O	4	5	-	2/2/19/22	0/1/1/1
5	NAG	O	5	5	-	2/6/23/26	0/1/1/1
5	GAL	O	6	5	-	2/2/19/22	0/1/1/1
5	BMA	O	7	5	-	2/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	3	BMA	C2-C3	4.71	1.59	1.52
5	O	4	BMA	C2-C3	4.25	1.59	1.52
5	O	3	BMA	O5-C5	4.13	1.51	1.43
5	O	4	BMA	O5-C5	3.59	1.50	1.43
5	O	3	BMA	C2-C3	3.32	1.57	1.52
3	K	1	NAG	O6-C6	3.00	1.55	1.42
5	O	5	NAG	C1-C2	2.87	1.56	1.52
5	O	7	BMA	C2-C3	2.81	1.56	1.52
3	K	1	NAG	C6-C5	2.60	1.60	1.51
4	L	2	NAG	C2-N2	2.59	1.50	1.46
3	K	1	NAG	O4-C4	2.50	1.49	1.43
4	L	2	NAG	C3-C2	2.48	1.57	1.52
3	N	3	BMA	C1-C2	2.28	1.57	1.52
3	N	3	BMA	O5-C5	2.26	1.47	1.43
5	O	7	BMA	O5-C5	2.20	1.47	1.43
3	N	2	NAG	O4-C4	2.09	1.48	1.43

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C1-O5-C5	10.60	126.39	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C2-N2-C7	10.27	136.67	122.90
5	O	2	NAG	C2-N2-C7	9.63	135.80	122.90
5	O	1	NAG	C1-C2-N2	8.11	123.22	110.43
3	K	3	BMA	C1-O5-C5	7.38	122.08	112.19
4	M	1	NAG	C1-O5-C5	6.95	121.50	112.19
5	O	3	BMA	C1-O5-C5	6.68	121.14	112.19
5	O	4	BMA	C1-O5-C5	6.45	120.84	112.19
3	N	3	BMA	C1-O5-C5	6.42	120.79	112.19
5	O	2	NAG	C1-C2-N2	6.17	120.15	110.43
4	M	1	NAG	C2-N2-C7	6.14	131.13	122.90
5	O	1	NAG	C2-N2-C7	6.09	131.06	122.90
3	K	1	NAG	C1-O5-C5	5.76	119.90	112.19
3	N	1	NAG	C2-N2-C7	5.64	130.46	122.90
4	L	1	NAG	C2-N2-C7	5.45	130.21	122.90
3	K	1	NAG	C2-N2-C7	5.30	130.01	122.90
4	M	2	NAG	C1-O5-C5	5.25	119.22	112.19
4	L	1	NAG	O5-C1-C2	5.11	119.20	111.29
3	N	3	BMA	C1-C2-C3	5.02	116.95	109.64
3	K	3	BMA	C1-C2-C3	4.95	116.85	109.64
4	L	2	NAG	O5-C1-C2	4.93	118.92	111.29
5	O	6	GAL	C1-O5-C5	4.93	118.79	112.19
4	M	2	NAG	C2-N2-C7	4.92	129.50	122.90
3	N	2	NAG	C1-C2-N2	4.79	117.97	110.43
4	L	2	NAG	C4-C3-C2	4.69	117.89	111.02
4	M	2	NAG	C1-C2-N2	4.65	117.77	110.43
4	L	1	NAG	C1-O5-C5	4.63	118.39	112.19
3	K	1	NAG	O6-C6-C5	4.46	126.51	111.33
4	M	2	NAG	O3-C3-C2	4.45	118.65	109.40
5	O	5	NAG	C2-N2-C7	4.32	128.69	122.90
4	L	1	NAG	O5-C5-C4	-3.89	101.36	110.83
5	O	2	NAG	C1-O5-C5	3.88	117.38	112.19
3	K	1	NAG	O3-C3-C2	-3.85	101.40	109.40
5	O	4	BMA	C1-C2-C3	3.73	115.07	109.64
3	K	2	NAG	C2-N2-C7	3.65	127.79	122.90
3	N	2	NAG	C4-C3-C2	3.64	116.35	111.02
4	L	2	NAG	O5-C5-C4	-3.63	102.00	110.83
5	O	5	NAG	C1-C2-N2	3.55	116.03	110.43
4	L	2	NAG	O4-C4-C3	3.47	118.55	110.38
3	N	1	NAG	C1-C2-N2	3.46	115.88	110.43
5	O	2	NAG	O5-C5-C6	3.38	114.24	107.66
4	L	2	NAG	C1-C2-N2	3.35	115.71	110.43
4	L	1	NAG	C4-C3-C2	-3.30	106.19	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C1-C2-N2	-3.13	105.50	110.43
3	K	1	NAG	C4-C3-C2	3.07	115.52	111.02
5	O	4	BMA	O4-C4-C3	3.04	117.54	110.38
3	N	1	NAG	C4-C3-C2	3.00	115.41	111.02
5	O	4	BMA	C3-C4-C5	-2.97	104.84	110.23
3	K	1	NAG	C6-C5-C4	2.95	120.27	113.02
5	O	3	BMA	C1-C2-C3	2.94	113.93	109.64
5	O	4	BMA	O4-C4-C5	2.91	116.48	109.32
5	O	7	BMA	C1-O5-C5	2.90	116.07	112.19
4	M	1	NAG	C6-C5-C4	2.87	120.06	113.02
5	O	2	NAG	O3-C3-C2	2.79	115.20	109.40
5	O	7	BMA	C2-C3-C4	2.77	115.73	110.86
5	O	2	NAG	O4-C4-C3	-2.72	103.95	110.38
5	O	3	BMA	O4-C4-C5	2.65	115.86	109.32
4	L	1	NAG	O3-C3-C2	2.64	114.88	109.40
4	M	1	NAG	C3-C4-C5	-2.63	105.46	110.23
5	O	3	BMA	C3-C4-C5	-2.61	105.49	110.23
4	L	2	NAG	O3-C3-C2	-2.58	104.04	109.40
3	N	3	BMA	C3-C4-C5	-2.48	105.74	110.23
3	N	3	BMA	O2-C2-C1	2.44	114.81	109.22
4	M	1	NAG	O6-C6-C5	2.42	119.58	111.33
3	K	2	NAG	O7-C7-N2	-2.41	117.73	121.98
4	L	2	NAG	C1-O5-C5	2.41	115.41	112.19
5	O	3	BMA	O2-C2-C3	2.39	115.09	110.15
3	N	2	NAG	C1-O5-C5	2.38	115.38	112.19
5	O	1	NAG	O6-C6-C5	2.38	119.44	111.33
4	L	2	NAG	O4-C4-C5	-2.36	103.51	109.32
4	L	1	NAG	C8-C7-N2	2.35	120.02	116.12
4	L	1	NAG	O6-C6-C5	2.32	119.25	111.33
5	O	2	NAG	O4-C4-C5	2.32	115.03	109.32
3	N	1	NAG	O4-C4-C5	2.28	114.94	109.32
4	L	1	NAG	C6-C5-C4	2.26	118.56	113.02
4	M	2	NAG	O5-C1-C2	-2.20	107.88	111.29
4	M	2	NAG	O7-C7-N2	-2.20	118.09	121.98
3	K	2	NAG	C4-C3-C2	2.20	114.24	111.02
5	O	7	BMA	O2-C2-C3	2.17	114.64	110.15
3	N	3	BMA	O4-C4-C5	2.12	114.55	109.32
4	M	2	NAG	C4-C3-C2	-2.12	107.91	111.02
5	O	5	NAG	O4-C4-C5	2.12	114.54	109.32
5	O	3	BMA	O6-C6-C5	2.11	118.53	111.33
3	K	1	NAG	O3-C3-C4	2.09	115.30	110.38
4	L	2	NAG	C6-C5-C4	2.06	118.08	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	2	NAG	O3-C3-C2	-2.05	105.15	109.40
3	N	1	NAG	O5-C5-C4	-2.04	105.87	110.83

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C1-C2-N2-C7
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C1-C2-N2-C7
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
5	O	1	NAG	C1-C2-N2-C7
5	O	2	NAG	C1-C2-N2-C7
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
3	K	2	NAG	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
5	O	4	BMA	O5-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6
5	O	6	GAL	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
5	O	7	BMA	C4-C5-C6-O6
5	O	4	BMA	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
5	O	7	BMA	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
5	O	5	NAG	O5-C5-C6-O6
4	L	1	NAG	C3-C2-N2-C7

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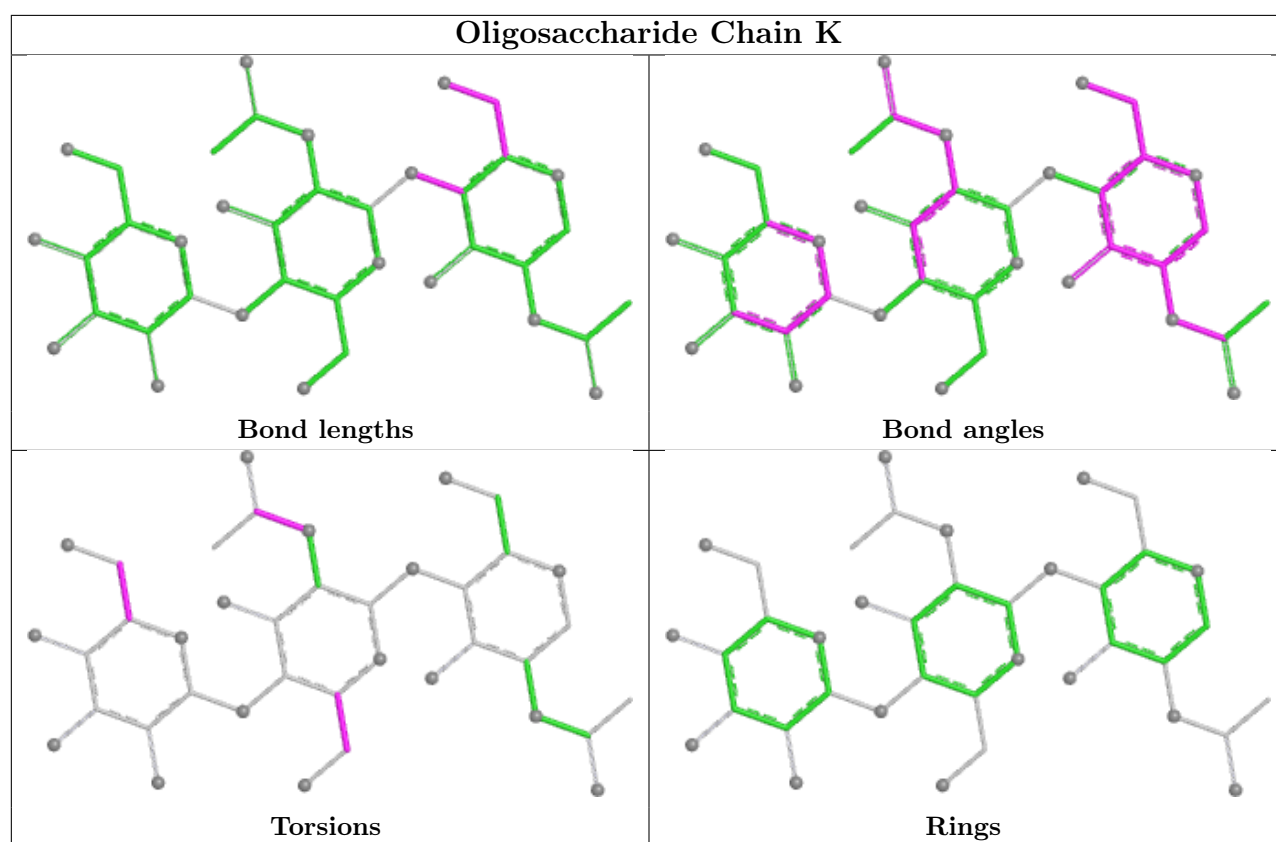
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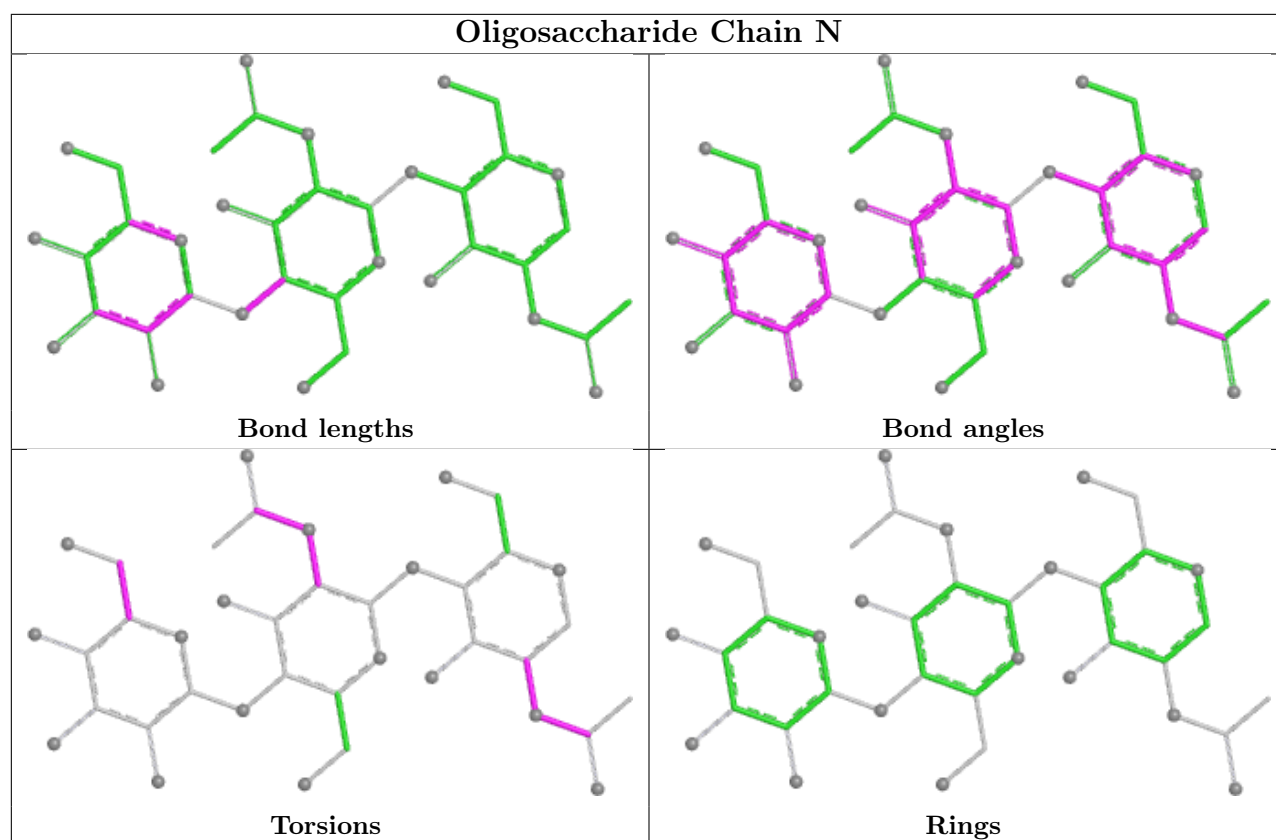
Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C3-C2-N2-C7
4	M	2	NAG	C1-C2-N2-C7
3	N	2	NAG	C1-C2-N2-C7
5	O	5	NAG	O7-C7-N2-C2
5	O	6	GAL	C4-C5-C6-O6

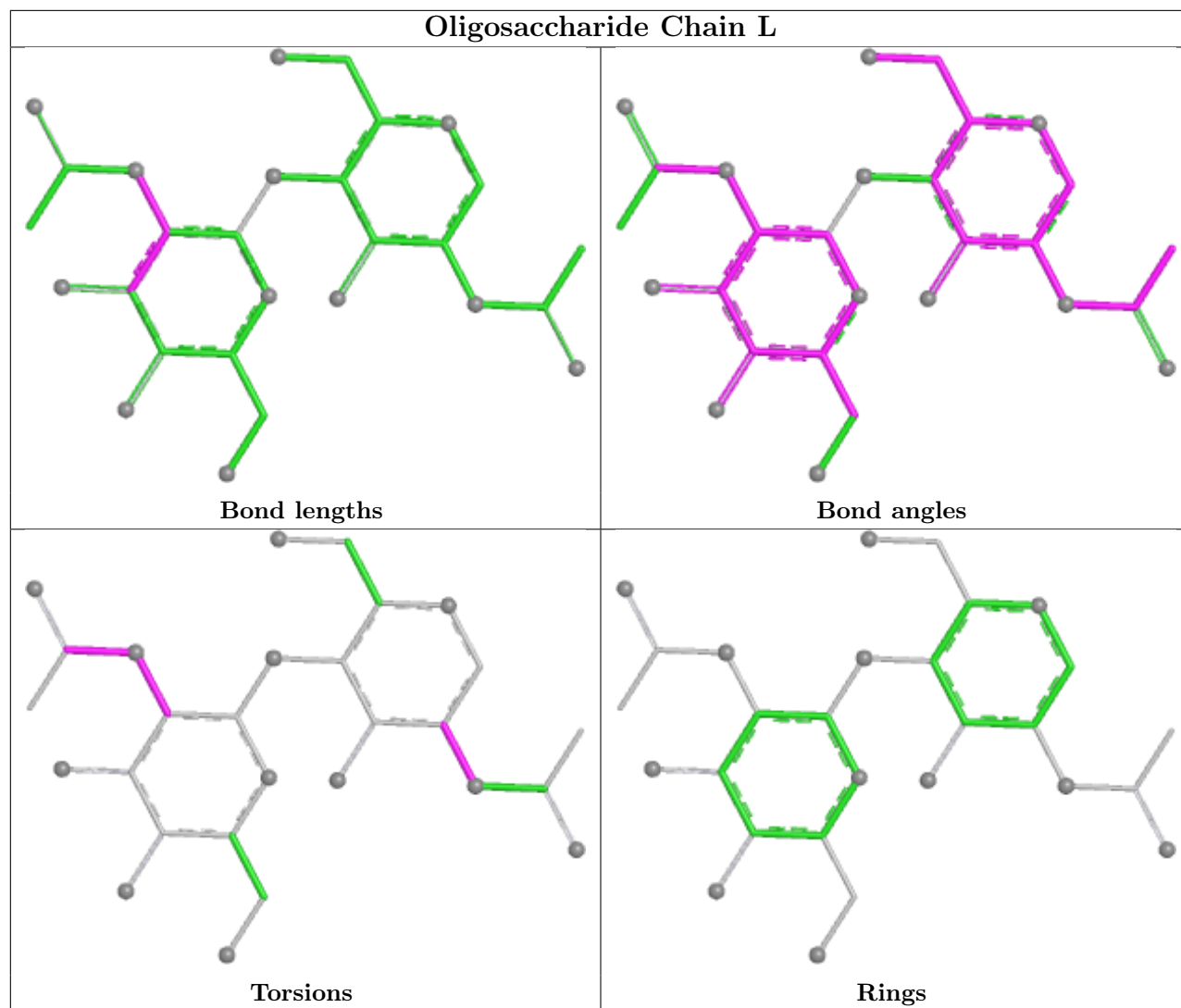
There are no ring outliers.

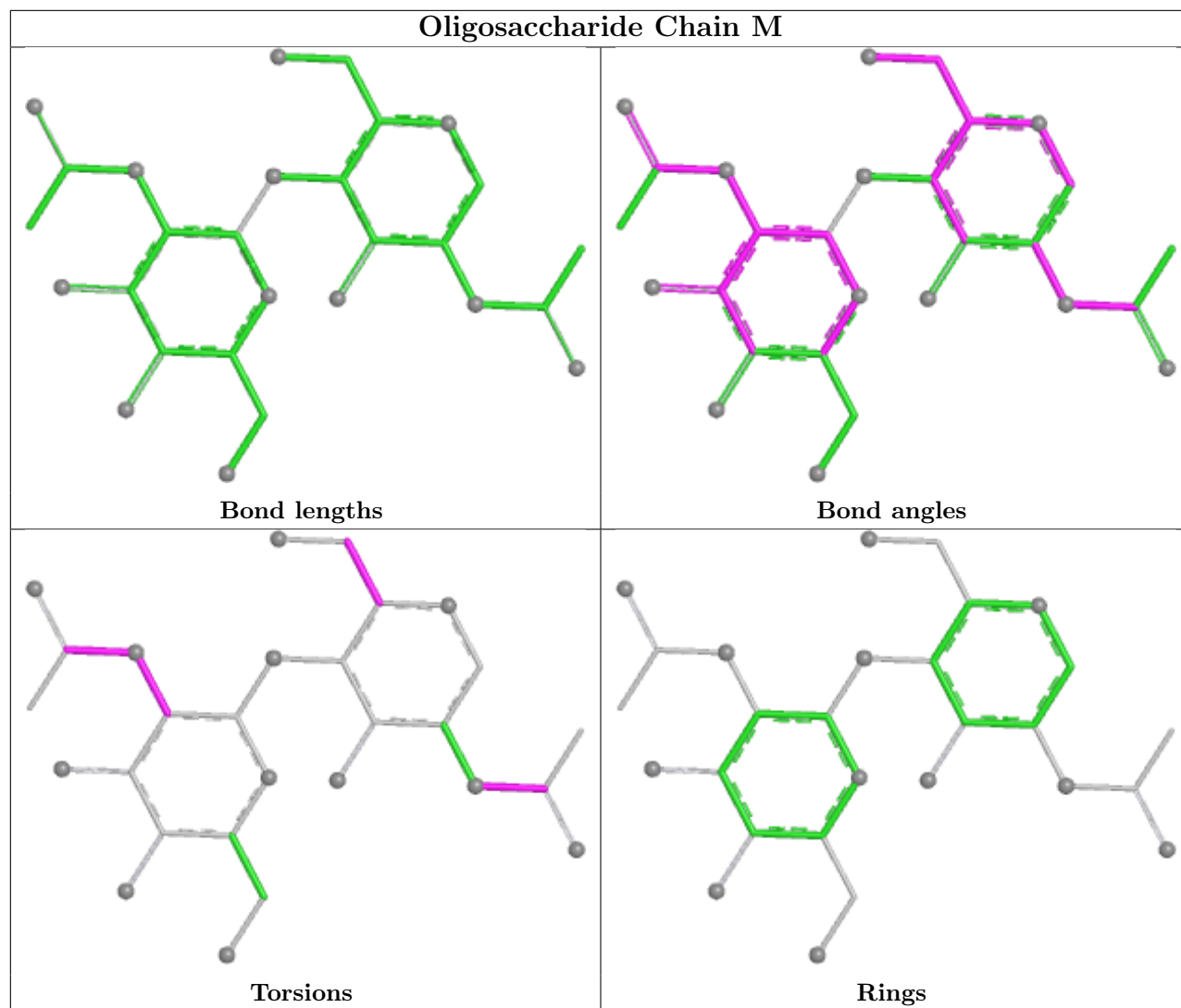
No monomer is involved in short contacts.

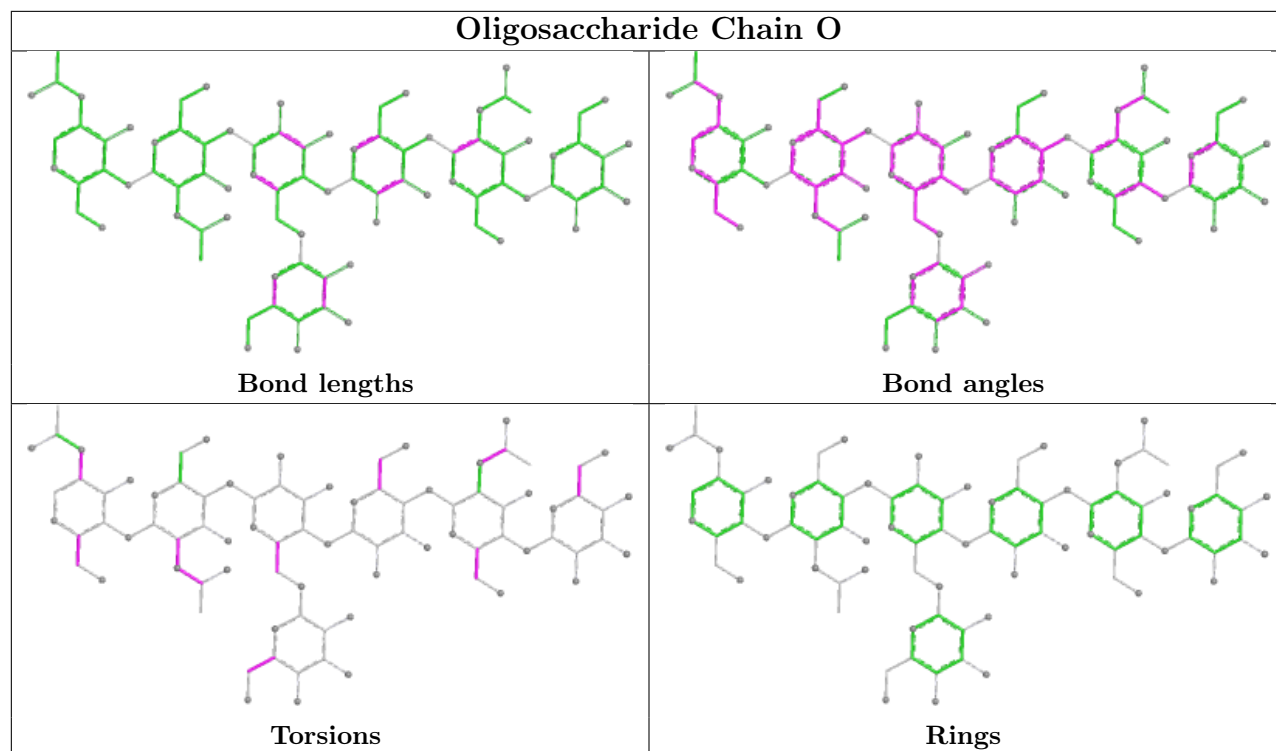
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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	B	195/235 (82%)	0.17	3 (1%)	72	52	47, 83, 143, 190	1 (0%)
1	C	192/235 (81%)	0.28	6 (3%)	51	30	46, 76, 136, 203	0
1	E	194/235 (82%)	0.21	6 (3%)	51	30	50, 80, 128, 189	0
1	G	192/235 (81%)	0.41	8 (4%)	40	22	50, 85, 134, 161	0
1	I	193/235 (82%)	0.41	8 (4%)	41	23	54, 91, 144, 172	0
2	A	120/146 (82%)	0.02	0	100	100	45, 74, 113, 145	0
2	D	120/146 (82%)	0.34	5 (4%)	40	22	43, 86, 112, 127	1 (0%)
2	F	120/146 (82%)	0.09	1 (0%)	82	65	52, 86, 117, 130	0
2	H	123/146 (84%)	0.10	1 (0%)	82	65	56, 78, 104, 133	0
2	J	120/146 (82%)	0.25	4 (3%)	49	29	53, 86, 111, 122	1 (0%)
All	All	1569/1905 (82%)	0.24	42 (2%)	56	35	43, 83, 132, 203	3 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	24	ALA	5.2
1	G	432	CYS	4.9
1	I	363	ALA	4.3
1	I	383	SER	4.0
2	D	23	VAL	3.6
1	G	382	VAL	3.5
1	I	442	ASP	3.3
2	D	22	CYS	3.3
1	E	417	LYS	3.2
1	G	386	LYS	3.1
2	H	27	TYR	2.9
2	J	3[A]	GLN	2.9
1	B	346[A]	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	383	SER	2.8
1	E	424	LYS	2.8
2	D	121	SER	2.7
2	J	104	GLU	2.7
1	I	341	VAL	2.7
1	C	383	SER	2.6
1	C	448	ASN	2.6
1	E	480	CYS	2.6
1	G	433	VAL	2.5
1	I	432	CYS	2.4
1	G	369	TYR	2.3
1	E	521	PRO	2.3
2	D	65	GLY	2.3
1	C	526	GLY	2.3
1	E	420	ASP	2.3
1	C	521	PRO	2.3
2	J	7	SER	2.3
1	C	480	CYS	2.2
2	J	64	LYS	2.2
1	B	436	TRP	2.1
1	C	443	SER	2.1
1	I	334	ASN	2.1
1	G	438	SER	2.1
1	G	363	ALA	2.1
1	I	367	VAL	2.1
1	B	424	LYS	2.0
1	E	483	VAL	2.0
2	F	121	SER	2.0
1	I	385	THR	2.0

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

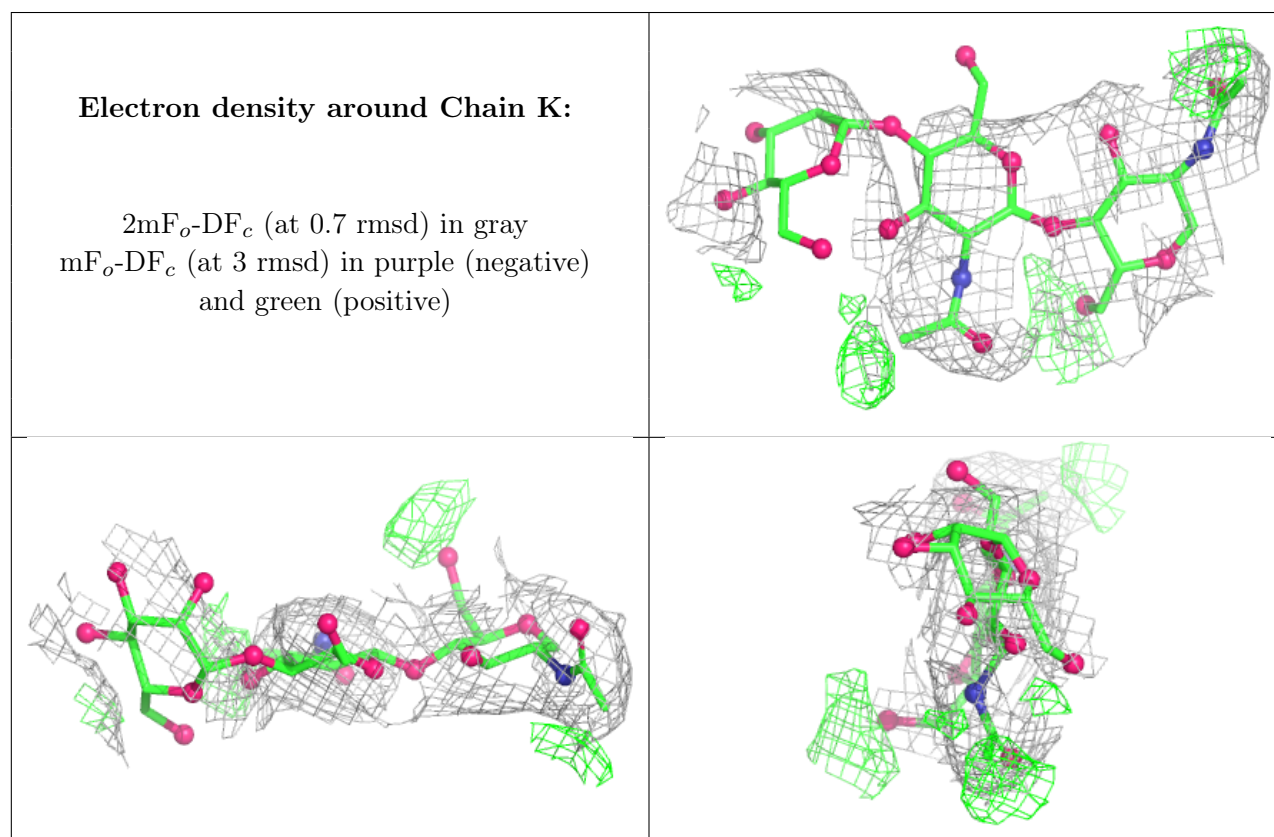
There are no non-standard protein/DNA/RNA residues in this entry.

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.

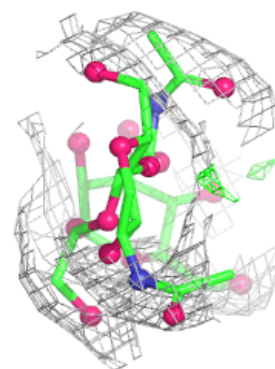
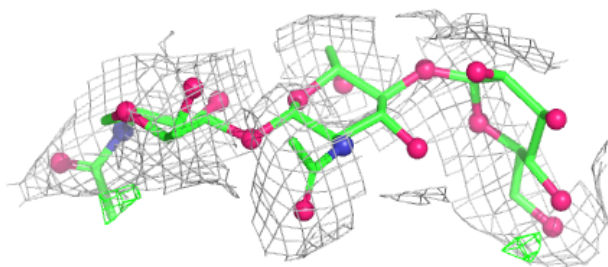
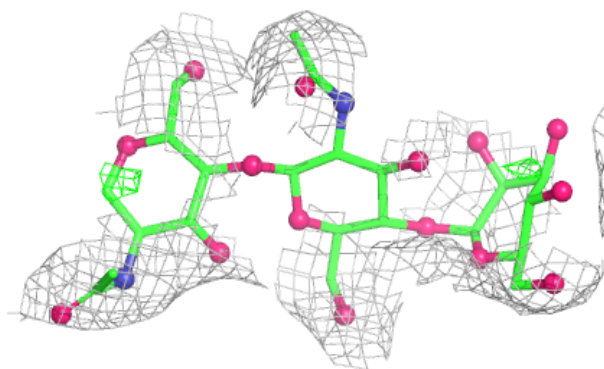
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	K	2	14/15	0.35	0.17	131,161,185,186	0
3	BMA	K	3	11/12	0.41	0.12	143,161,167,179	0
5	BMA	O	7	11/12	0.50	0.10	138,152,190,227	0
4	NAG	L	2	14/15	0.58	0.12	102,128,155,155	0
5	GAL	O	6	11/12	0.64	0.08	163,175,189,199	0
5	NAG	O	5	14/15	0.64	0.10	156,203,221,233	0
5	NAG	O	2	14/15	0.65	0.13	115,158,190,205	0
4	NAG	M	2	14/15	0.67	0.13	97,146,175,191	0
5	BMA	O	3	11/12	0.71	0.09	177,189,208,248	0
3	BMA	N	3	11/12	0.73	0.09	104,137,168,173	0
5	BMA	O	4	11/12	0.75	0.10	144,206,244,258	0
3	NAG	N	2	14/15	0.80	0.08	82,130,160,164	0
3	NAG	K	1	14/15	0.84	0.10	77,91,110,126	0
5	NAG	O	1	14/15	0.89	0.11	82,111,127,146	0
4	NAG	M	1	14/15	0.90	0.09	96,106,112,131	0
3	NAG	N	1	14/15	0.91	0.12	90,116,137,140	0
4	NAG	L	1	14/15	0.91	0.08	77,100,111,125	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.



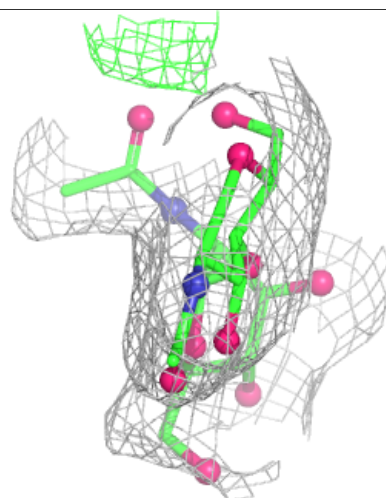
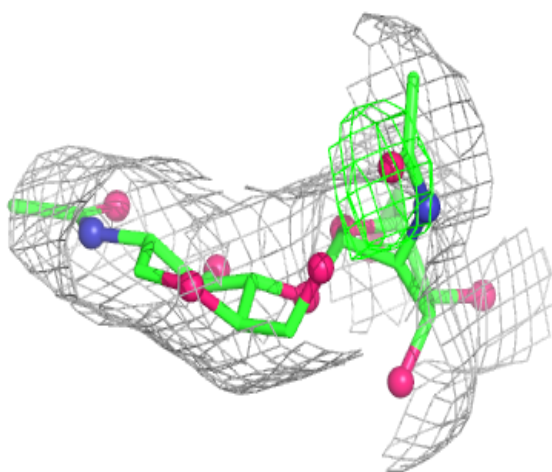
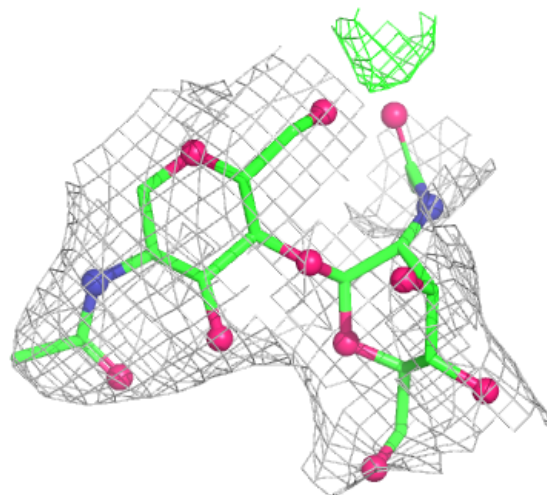
Electron density around Chain N:

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



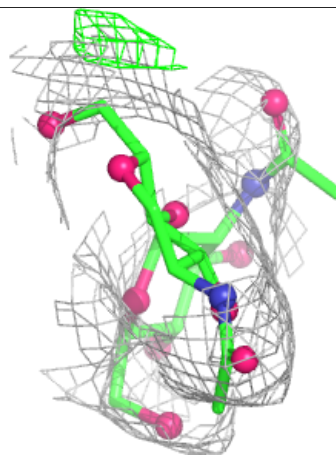
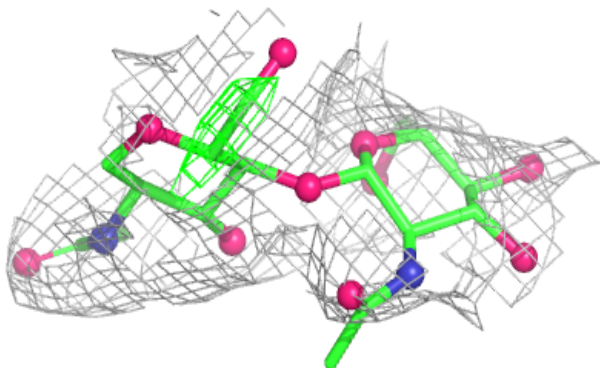
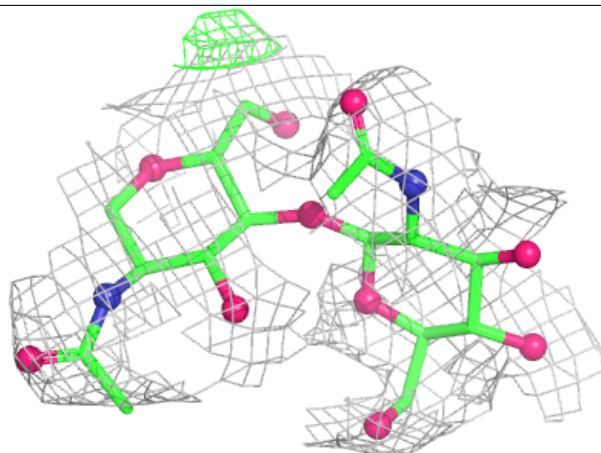
Electron density around Chain L:

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

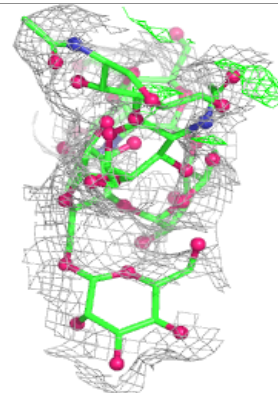
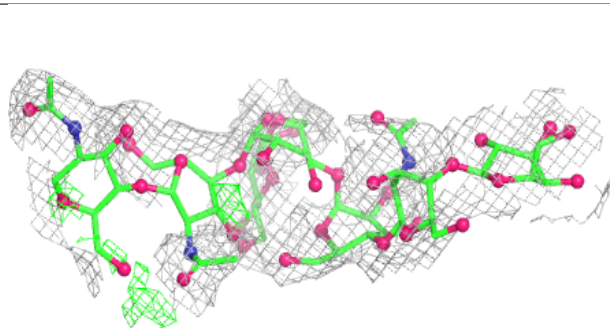
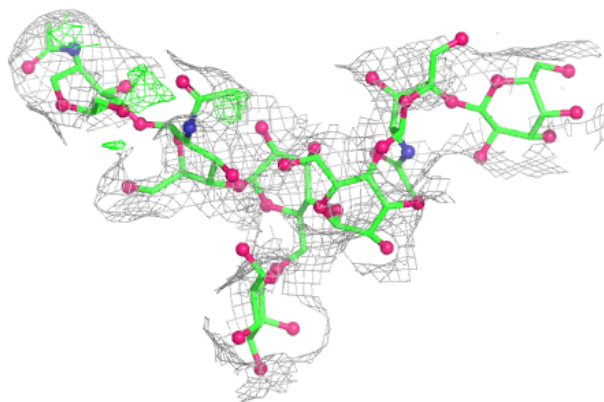


Electron density around Chain M:

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

**Electron density around Chain O:**

$2mF_o - DF_c$ (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.