



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:02 PM UTC

PDB ID : 1NCD / pdb_00001ncd
Title : REFINED CRYSTAL STRUCTURE OF THE INFLUENZA VIRUS N9
NEURAMINIDASE-NC41 FAB COMPLEX
Authors : Tulip, W.R.; Varghese, J.N.; Colman, P.M.
Deposited on : 1992-01-21
Resolution : 2.90 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

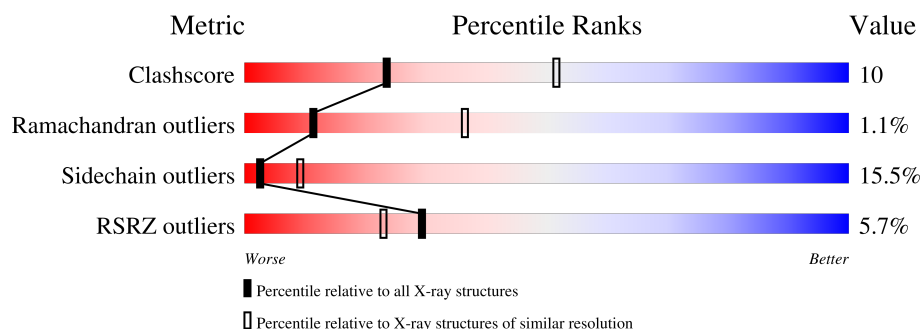
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	N	389	2% 52% 35% 11% .
2	L	214	7% 50% 36% 11% .
3	H	221	10% 56% 36% 7% .
4	A	6	100%
5	B	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6585 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 INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	389	Total	C	N	O	S	0	0	0
			3069	1912	539	595	23			

- Molecule 2 is a protein called IGG2A-KAPPA NC41 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1667	1043	280	336	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	THR	SER	conflict	EMBL Y11589
L	21	ILE	VAL	conflict	EMBL Y11589
L	28	ASP	ILE	conflict	EMBL Y11589
L	30	SER	GLY	conflict	EMBL Y11589
L	32	ALA	ASN	conflict	EMBL Y11589
L	34	VAL	ALA	conflict	EMBL Y11589
L	46	LEU	ALA	conflict	EMBL Y11589
L	50	TRP	SER	conflict	EMBL Y11589
L	53	THR	TYR	conflict	EMBL Y11589
L	55	HIS	TYR	conflict	EMBL Y11589
L	56	ILE	SER	conflict	EMBL Y11589
L	63	ALA	THR	conflict	EMBL Y11589
L	71	TYR	PHE	conflict	EMBL Y11589
L	77	SER	ASN	conflict	EMBL Y11589
L	80	ALA	SER	conflict	EMBL Y11589
L	85	LEU	GLU	conflict	EMBL Y11589
L	87	TYR	PHE	conflict	EMBL Y11589
L	91	HIS	TYR	conflict	EMBL Y11589
L	92	TYR	ASN	conflict	EMBL Y11589
L	93	SER	ARG	conflict	EMBL Y11589

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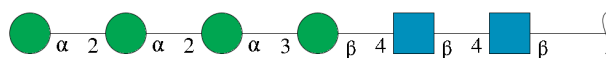
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Chain	Residue	Modelled	Actual	Comment	Reference
L	94	PRO	TYR	conflict	EMBL Y11589

- Molecule 3 is a protein called IGG2A-KAPPA NC41 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1665	1050	273	335	7			

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



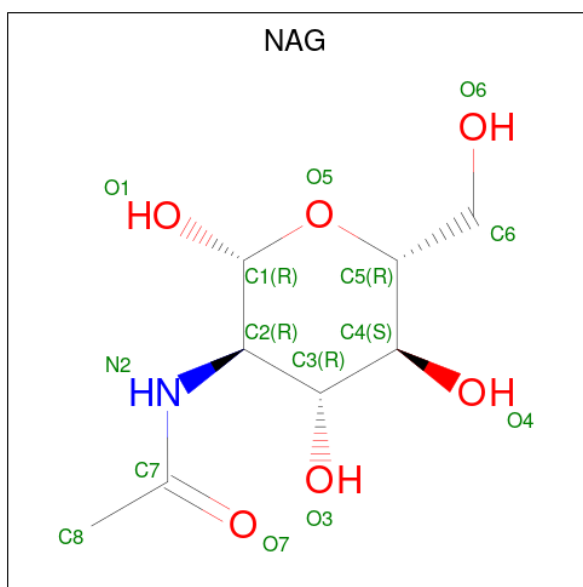
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 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
5	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	N	1	Total	Ca	0	0
			1	1		

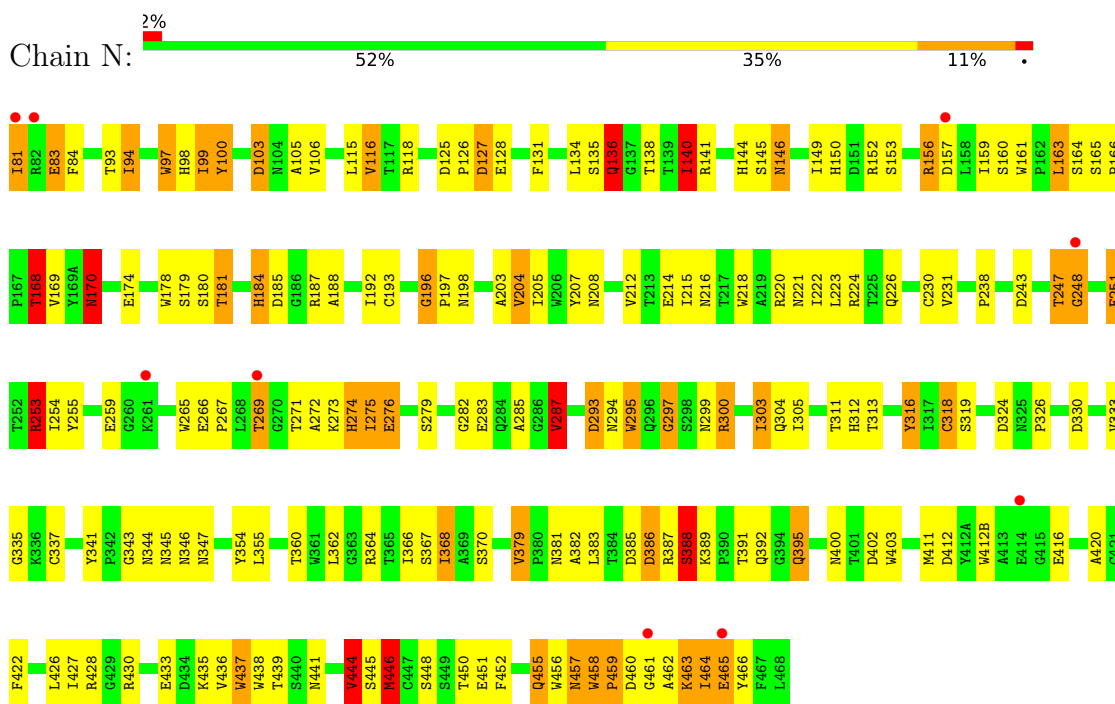
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	63	Total	O	0	0
			63	63		
8	L	2	Total	O	0	0
			2	2		
8	H	4	Total	O	0	0
			4	4		

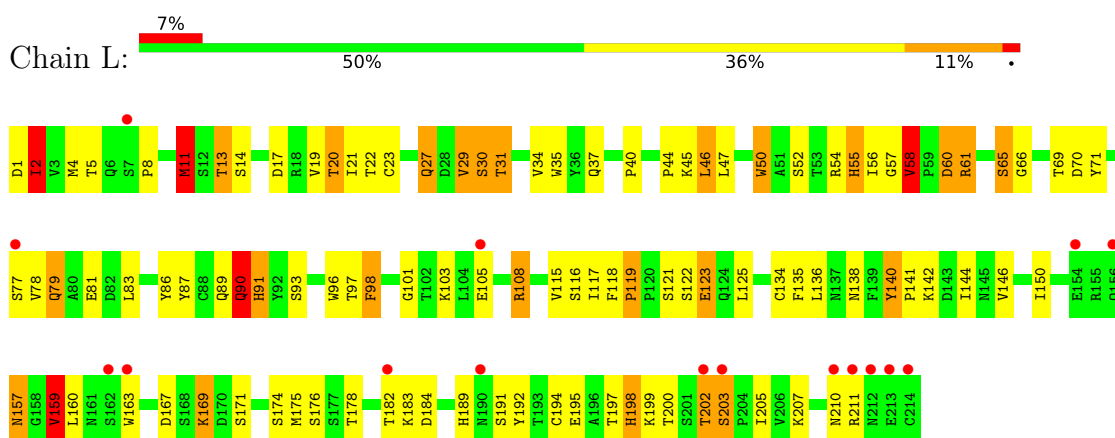
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

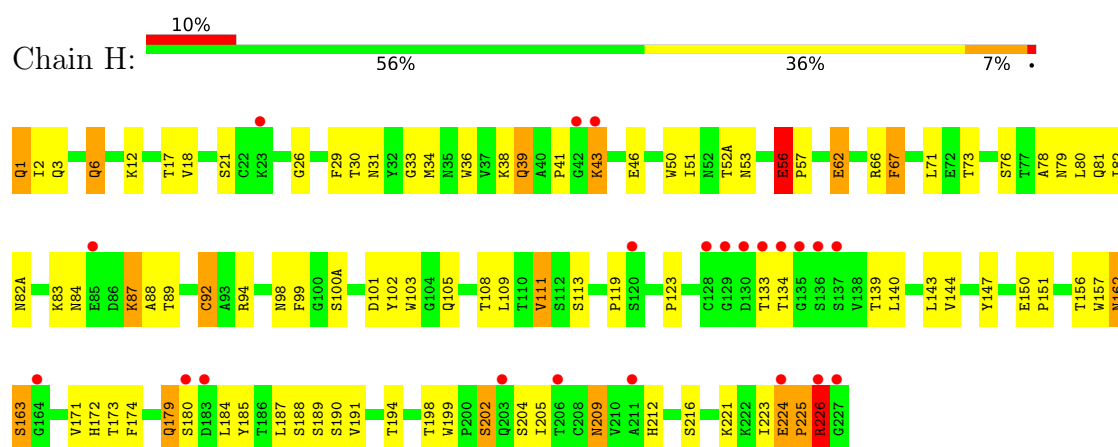
• Molecule 1: INFLUENZA A SUBTYPE N9 NEURAMINIDASE



• Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)



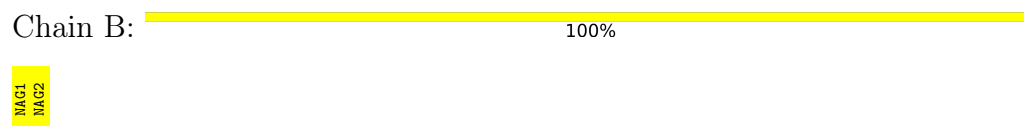
• Molecule 3: IGG2A-KAPPA NC41 FAB (HEAVY CHAIN)



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.00Å 167.00Å 124.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 124.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 69.3 (124.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.157 , (Not available) 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6585	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, CA, 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	N	1.24	15/3151 (0.5%)	2.20	158/4292 (3.7%)
2	L	1.10	9/1708 (0.5%)	2.00	52/2323 (2.2%)
3	H	1.00	2/1707 (0.1%)	1.95	40/2326 (1.7%)
All	All	1.15	26/6566 (0.4%)	2.09	250/8941 (2.8%)

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	N	0	2
2	L	0	1
All	All	0	3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	91	HIS	CD2-NE2	-8.02	1.29	1.37
1	N	287	VAL	CA-CB	7.60	1.63	1.54
2	L	58	VAL	CA-CB	7.43	1.61	1.53
1	N	204	VAL	CA-CB	7.37	1.63	1.54
1	N	184	HIS	CD2-NE2	-7.19	1.29	1.37
1	N	144	HIS	CD2-NE2	-7.04	1.30	1.37
2	L	56	ILE	CA-CB	6.97	1.64	1.54
2	L	198	HIS	CD2-NE2	-6.72	1.30	1.37
1	N	312	HIS	CG-ND1	-6.62	1.30	1.38
1	N	312	HIS	CD2-NE2	-6.60	1.30	1.37
2	L	97	THR	CA-CB	6.58	1.63	1.53
1	N	150	HIS	CD2-NE2	-6.55	1.30	1.37
1	N	274	HIS	CD2-NE2	-6.25	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	172	HIS	CD2-NE2	-6.19	1.31	1.37
2	L	189	HIS	CD2-NE2	-6.08	1.31	1.37
2	L	202	THR	CA-CB	5.98	1.63	1.53
1	N	466	TYR	C-N	-5.89	1.25	1.33
1	N	184	HIS	CG-ND1	-5.85	1.31	1.38
1	N	98	HIS	CD2-NE2	-5.59	1.31	1.37
1	N	144	HIS	CG-ND1	-5.54	1.32	1.38
3	H	212	HIS	CD2-NE2	-5.54	1.31	1.37
1	N	457	ASN	CG-ND2	-5.54	1.21	1.33
1	N	297	GLY	C-O	5.43	1.31	1.23
2	L	198	HIS	CG-ND1	-5.28	1.32	1.38
1	N	205	ILE	CA-CB	5.23	1.59	1.53
2	L	55	HIS	CG-ND1	-5.16	1.32	1.38

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	157	ASP	CA-CB-CG	14.35	126.95	112.60
1	N	347	ASN	CA-CB-CG	12.52	125.12	112.60
1	N	386	ASP	CA-CB-CG	12.03	124.63	112.60
2	L	210	ASN	CA-CB-CG	-11.87	100.73	112.60
1	N	185	ASP	CA-CB-CG	11.28	123.88	112.60
3	H	162	ASN	CA-CB-CG	-11.12	101.48	112.60
1	N	136	GLN	CG-CD-NE2	11.02	132.93	116.40
2	L	91	HIS	CA-CB-CG	10.06	123.86	113.80
1	N	170	ASN	OD1-CG-ND2	-9.58	113.02	122.60
1	N	198	ASN	OD1-CG-ND2	-9.49	113.11	122.60
1	N	198	ASN	CB-CG-ND2	9.36	130.45	116.40
2	L	29	VAL	N-CA-CB	-8.98	101.88	112.39
1	N	136	GLN	OE1-CD-NE2	-8.89	113.71	122.60
1	N	99	ILE	N-CA-CB	8.83	121.18	110.31
1	N	457	ASN	CA-C-N	8.76	135.92	123.30
1	N	457	ASN	C-N-CA	8.76	135.92	123.30
1	N	455	GLN	OE1-CD-NE2	-8.60	114.00	122.60
1	N	438	TRP	CG-CD2-CE3	8.55	142.45	133.90
1	N	226	GLN	N-CA-C	8.44	128.78	110.80
1	N	416	GLU	N-CA-C	-8.42	103.14	113.50
2	L	57	GLY	CA-C-N	-8.28	116.63	122.59
2	L	57	GLY	C-N-CA	-8.28	116.63	122.59
3	H	105	GLN	N-CA-C	8.20	123.00	112.34
1	N	381	ASN	CA-CB-CG	-8.00	104.60	112.60
1	N	456	TRP	CG-CD2-CE3	8.00	141.90	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	99	ILE	CB-CA-C	-7.92	99.53	111.33
1	N	385	ASP	CA-CB-CG	7.89	120.49	112.60
3	H	162	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	N	247	THR	N-CA-CB	-7.74	100.21	110.88
1	N	127	ASP	N-CA-CB	-7.68	100.69	110.90
2	L	90	GLN	CG-CD-NE2	7.51	127.67	116.40
1	N	221	ASN	OD1-CG-ND2	-7.50	115.10	122.60
2	L	31	THR	N-CA-CB	-7.41	102.76	113.65
2	L	91	HIS	CB-CG-CD2	-7.39	121.60	131.20
1	N	438	TRP	CB-CG-CD1	-7.30	115.95	126.90
1	N	458	TRP	CA-C-N	7.28	127.04	119.76
1	N	458	TRP	C-N-CA	7.28	127.04	119.76
2	L	169	LYS	N-CA-C	-7.26	95.34	110.80
3	H	185	TYR	N-CA-C	7.24	121.63	109.76
3	H	6	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	N	266	GLU	CA-C-N	7.08	127.07	119.78
1	N	266	GLU	C-N-CA	7.08	127.07	119.78
1	N	385	ASP	CA-C-O	-7.06	112.74	120.30
1	N	293	ASP	CA-CB-CG	7.04	119.64	112.60
3	H	79	ASN	OD1-CG-ND2	-7.00	115.59	122.60
1	N	247	THR	N-CA-C	-6.96	104.45	114.12
1	N	319	SER	N-CA-C	6.94	117.58	109.60
2	L	205	ILE	N-CA-C	-6.92	99.76	108.89
3	H	209	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	N	184	HIS	CB-CG-CD2	-6.87	122.27	131.20
2	L	11	MET	CA-CB-CG	-6.84	100.41	114.10
1	N	293	ASP	N-CA-C	-6.84	97.59	108.73
3	H	162	ASN	CB-CG-ND2	6.83	126.64	116.40
2	L	184	ASP	CA-CB-CG	6.79	119.39	112.60
3	H	101	ASP	CA-CB-CG	6.75	119.35	112.60
3	H	39	GLN	N-CA-C	-6.75	96.22	108.02
1	N	105	ALA	N-CA-C	6.72	118.26	111.07
1	N	97	TRP	CG-CD2-CE3	6.71	140.61	133.90
1	N	403	TRP	CG-CD2-CE3	6.71	140.61	133.90
1	N	125	ASP	CA-CB-CG	6.71	119.31	112.60
1	N	455	GLN	CG-CD-NE2	6.69	126.44	116.40
1	N	318	CYS	N-CA-C	6.58	119.28	111.71
1	N	220	ARG	N-CA-C	6.57	120.57	111.90
2	L	54	ARG	NE-CZ-NH2	-6.56	113.29	119.20
1	N	267	PRO	N-CA-C	6.55	121.62	111.21
3	H	179	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	N	303	ILE	O-C-N	-6.53	115.46	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	203	SER	CA-C-N	6.50	126.53	119.90
2	L	203	SER	C-N-CA	6.50	126.53	119.90
1	N	170	ASN	CA-CB-CG	6.46	119.06	112.60
1	N	299	ASN	CA-CB-CG	6.42	119.02	112.60
3	H	226	ARG	N-CA-C	6.41	124.45	110.80
3	H	21	SER	CA-C-O	-6.40	113.70	120.80
1	N	170	ASN	CB-CG-ND2	6.37	125.96	116.40
1	N	412	ASP	CA-CB-CG	6.36	118.96	112.60
1	N	208	ASN	CA-CB-CG	-6.36	106.24	112.60
1	N	446	MET	CG-SD-CE	-6.36	86.92	100.90
2	L	2	ILE	N-CA-C	-6.35	99.08	109.12
3	H	150	GLU	N-CA-C	-6.34	101.77	109.83
1	N	297	GLY	O-C-N	6.30	130.89	122.70
3	H	225	PRO	N-CA-C	6.28	121.74	114.20
2	L	91	HIS	CB-CG-ND1	6.28	132.12	122.70
1	N	403	TRP	CB-CG-CD1	-6.27	117.49	126.90
1	N	451	GLU	N-CA-C	-6.27	102.26	110.53
1	N	196	GLY	CA-C-N	6.23	126.25	119.89
1	N	196	GLY	C-N-CA	6.23	126.25	119.89
1	N	458	TRP	O-C-N	6.23	127.14	121.04
1	N	161	TRP	CG-CD2-CE3	6.23	140.13	133.90
1	N	444	VAL	CB-CA-C	-6.21	100.75	110.69
2	L	30	SER	N-CA-C	6.21	119.75	111.30
1	N	300	ARG	N-CA-C	6.21	117.63	109.93
3	H	29	PHE	N-CA-C	6.20	118.55	111.11
1	N	437	TRP	CG-CD2-CE3	6.18	140.08	133.90
2	L	138	ASN	N-CA-C	6.17	120.16	111.52
1	N	161	TRP	N-CA-C	-6.17	102.58	108.07
1	N	103	ASP	N-CA-C	6.17	120.54	112.89
2	L	58	VAL	N-CA-C	-6.14	101.56	107.76
3	H	172	HIS	CB-CG-CD2	-6.12	123.25	131.20
2	L	189	HIS	CA-CB-CG	-6.10	107.70	113.80
1	N	103	ASP	CA-CB-CG	6.10	118.70	112.60
2	L	159	VAL	N-CA-CB	-6.10	102.96	111.25
1	N	366	ILE	N-CA-C	-6.09	105.13	111.58
1	N	461	GLY	O-C-N	-6.05	115.52	122.42
1	N	294	ASN	O-C-N	6.03	129.25	122.32
2	L	87	TYR	CA-C-O	-6.03	113.73	120.66
1	N	197	PRO	N-CA-CB	6.02	108.38	103.32
1	N	269	THR	CA-CB-OG1	-6.01	100.58	109.60
2	L	157	ASN	CA-CB-CG	6.00	118.61	112.60
1	N	335	GLY	CA-C-O	-6.00	115.17	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	221	ASN	CA-CB-CG	-5.99	106.61	112.60
1	N	279	SER	CA-C-O	-5.97	114.33	120.54
1	N	164	SER	N-CA-C	5.95	120.49	113.23
2	L	29	VAL	CA-C-O	5.95	126.09	120.14
3	H	223	ILE	N-CA-C	-5.95	96.75	106.32
1	N	247	THR	CB-CA-C	5.94	119.36	109.38
3	H	92	CYS	N-CA-C	-5.94	100.03	109.76
2	L	65	SER	N-CA-C	5.93	117.25	108.60
1	N	203	ALA	CA-C-O	-5.92	114.12	120.92
1	N	389	LYS	CA-C-N	5.90	125.87	120.03
1	N	389	LYS	C-N-CA	5.90	125.87	120.03
1	N	157	ASP	O-C-N	-5.88	116.21	123.44
2	L	211	ARG	N-CA-C	5.88	118.72	109.96
3	H	94	ARG	CB-CG-CD	-5.88	97.79	111.30
1	N	168	THR	CA-CB-OG1	-5.86	100.81	109.60
2	L	89	GLN	N-CA-C	-5.86	101.34	110.42
1	N	140	ILE	CA-C-O	-5.83	115.00	121.17
1	N	274	HIS	CB-CG-CD2	-5.80	123.66	131.20
3	H	67	PHE	CA-CB-CG	-5.79	108.01	113.80
1	N	153	SER	CA-CB-OG	5.78	122.66	111.10
3	H	87	LYS	CA-CB-CG	-5.76	102.57	114.10
1	N	294	ASN	CA-CB-CG	-5.76	106.84	112.60
1	N	116	VAL	N-CA-C	-5.72	101.33	108.89
3	H	190	SER	CA-CB-OG	5.72	122.54	111.10
1	N	412(B)	TRP	CE2-CD2-CG	-5.72	100.34	107.20
1	N	402	ASP	CA-C-O	-5.70	114.95	121.68
1	N	251	GLU	CB-CG-CD	-5.70	102.91	112.60
1	N	316	TYR	N-CA-C	-5.70	101.77	110.14
2	L	20	THR	CA-CB-OG1	-5.68	101.08	109.60
1	N	295	TRP	CG-CD2-CE3	5.68	139.58	133.90
1	N	152	ARG	CA-CB-CG	5.67	125.44	114.10
1	N	165	SER	CA-C-N	5.66	123.74	119.66
1	N	165	SER	C-N-CA	5.66	123.74	119.66
1	N	184	HIS	CB-CG-ND1	5.66	131.19	122.70
1	N	439	THR	N-CA-C	-5.64	101.39	110.14
1	N	456	TRP	CE2-CD2-CG	-5.62	100.45	107.20
1	N	166	PRO	O-C-N	-5.61	118.51	121.15
1	N	438	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	N	433	GLU	N-CA-C	-5.59	100.66	108.54
1	N	346	ASN	OD1-CG-ND2	-5.58	117.02	122.60
2	L	13	THR	CA-CB-OG1	-5.58	101.23	109.60
1	N	388	SER	N-CA-C	5.58	117.82	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	128	GLU	O-C-N	-5.58	117.94	123.46
2	L	163	TRP	CG-CD2-CE3	5.56	139.46	133.90
1	N	174	GLU	N-CA-C	5.56	120.18	112.90
1	N	294	ASN	CA-C-O	-5.56	113.83	120.56
3	H	67	PHE	O-C-N	5.56	129.69	123.19
2	L	140	TYR	O-C-N	-5.55	114.93	121.32
1	N	179	SER	O-C-N	-5.55	117.06	123.33
3	H	202	SER	N-CA-CB	-5.51	101.98	109.98
3	H	82(A)	ASN	OD1-CG-ND2	-5.51	117.09	122.60
3	H	83	LYS	CA-CB-CG	-5.51	103.09	114.10
1	N	368	ILE	CB-CG1-CD1	5.50	125.36	113.80
1	N	144	HIS	CB-CG-CD2	-5.48	124.07	131.20
3	H	1	GLN	CA-C-O	-5.48	111.49	120.80
1	N	385	ASP	O-C-N	-5.47	116.92	123.27
2	L	194	CYS	N-CA-C	-5.47	98.44	108.02
1	N	412(B)	TRP	CG-CD2-CE3	5.46	139.36	133.90
1	N	243	ASP	CA-CB-CG	5.46	118.06	112.60
1	N	435	LYS	CA-CB-CG	-5.45	103.20	114.10
1	N	368	ILE	CA-CB-CG2	-5.45	101.24	110.50
1	N	275	ILE	N-CA-C	5.44	115.78	108.17
1	N	253	ARG	CB-CG-CD	-5.42	98.84	111.30
1	N	299	ASN	N-CA-C	-5.41	100.58	109.40
3	H	163	SER	N-CA-CB	-5.41	104.08	112.30
3	H	157	TRP	CA-C-O	5.41	126.27	120.38
3	H	78	ALA	N-CA-C	-5.40	100.90	109.59
1	N	140	ILE	N-CA-CB	5.39	116.86	110.55
2	L	1	ASP	CA-CB-CG	5.39	117.99	112.60
1	N	341	TYR	N-CA-C	-5.38	101.76	109.24
1	N	216	ASN	CB-CG-ND2	5.36	124.43	116.40
1	N	354	TYR	N-CA-C	-5.35	99.80	108.52
3	H	36	TRP	O-C-N	-5.35	116.96	123.27
2	L	189	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	N	146	ASN	O-C-N	5.33	129.74	122.82
1	N	178	TRP	CE2-CD2-CG	-5.32	100.82	107.20
2	L	98	PHE	CA-CB-CG	5.32	119.12	113.80
2	L	210	ASN	OD1-CG-ND2	-5.30	117.30	122.60
2	L	60	ASP	N-CA-C	5.30	122.08	110.80
1	N	83	GLU	N-CA-CB	-5.29	101.68	111.53
1	N	97	TRP	CB-CG-CD1	-5.29	118.96	126.90
1	N	161	TRP	CB-CG-CD1	-5.28	118.97	126.90
3	H	62	GLU	CB-CG-CD	5.28	121.57	112.60
2	L	29	VAL	CB-CA-C	5.27	118.25	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	459	PRO	CB-CA-C	-5.26	104.22	111.21
1	N	436	VAL	N-CA-C	-5.25	100.79	108.99
1	N	216	ASN	N-CA-CB	-5.25	102.87	110.70
2	L	119	PRO	N-CA-C	5.25	117.11	110.70
2	L	79	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	N	247	THR	CA-CB-OG1	-5.25	101.72	109.60
2	L	202	THR	N-CA-C	-5.24	99.64	110.80
1	N	161	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	N	326	PRO	N-CD-CG	-5.22	97.53	103.80
2	L	45	LYS	N-CA-C	-5.22	100.38	108.90
1	N	379	VAL	CA-C-N	5.22	125.13	119.76
1	N	379	VAL	C-N-CA	5.22	125.13	119.76
1	N	344	ASN	CA-CB-CG	-5.21	107.39	112.60
1	N	97	TRP	CE2-CD2-CG	-5.20	100.96	107.20
3	H	157	TRP	O-C-N	5.19	129.42	123.29
2	L	52	SER	CA-CB-OG	-5.19	100.71	111.10
1	N	223	LEU	N-CA-C	-5.18	100.86	109.46
2	L	91	HIS	N-CA-C	5.17	117.08	110.61
3	H	29	PHE	CA-C-N	5.17	128.86	120.60
3	H	29	PHE	C-N-CA	5.17	128.86	120.60
1	N	450	THR	CA-C-O	5.16	125.31	119.27
1	N	168	THR	N-CA-CB	-5.15	102.02	110.52
1	N	253	ARG	N-CA-C	5.15	116.77	108.32
1	N	178	TRP	CG-CD2-CE3	5.14	139.04	133.90
3	H	3	GLN	CA-CB-CG	5.13	124.36	114.10
1	N	99	ILE	O-C-N	5.13	128.26	122.67
1	N	444	VAL	N-CA-C	-5.12	100.51	108.86
1	N	178	TRP	CB-CG-CD1	-5.11	119.23	126.90
1	N	193	CYS	N-CA-C	5.11	116.85	108.52
1	N	465	GLU	CA-C-N	-5.10	114.48	122.65
1	N	465	GLU	C-N-CA	-5.10	114.48	122.65
2	L	90	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	N	265	TRP	CG-CD1-NE1	-5.09	103.58	110.20
2	L	90	GLN	CA-CB-CG	5.09	124.28	114.10
1	N	100	TYR	N-CA-C	-5.09	105.91	112.68
1	N	212	VAL	N-CA-CB	-5.08	105.82	111.41
2	L	205	ILE	O-C-N	-5.08	117.17	122.81
1	N	422	PHE	CA-CB-CG	5.08	118.88	113.80
2	L	117	ILE	N-CA-C	-5.08	101.15	108.71
2	L	189	HIS	N-CA-C	5.07	117.00	109.69
1	N	218	TRP	CE2-CD2-CG	-5.07	101.12	107.20
2	L	40	PRO	O-C-N	5.06	128.40	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	50	TRP	CG-CD2-CE3	5.06	138.96	133.90
1	N	276	GLU	N-CA-CB	-5.06	102.13	111.53
1	N	215	ILE	N-CA-C	-5.05	100.93	108.46
1	N	343	GLY	CA-C-N	-5.05	115.69	123.07
1	N	343	GLY	C-N-CA	-5.05	115.69	123.07
1	N	274	HIS	CA-CB-CG	5.05	118.85	113.80
1	N	150	HIS	O-C-N	5.04	129.31	122.96
1	N	94	ILE	CA-CB-CG2	-5.04	101.94	110.50
3	H	66	ARG	N-CA-C	-5.03	107.82	114.31
1	N	285	ALA	N-CA-C	5.02	118.53	111.90
3	H	56	GLU	N-CA-C	5.02	117.24	110.31
1	N	127	ASP	CA-CB-CG	5.02	117.62	112.60
1	N	160	SER	O-C-N	-5.01	117.11	123.17
1	N	403	TRP	CE2-CD2-CG	-5.00	101.19	107.20
3	H	103	TRP	CG-CD2-CE3	5.00	138.90	133.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	140	TYR	Sidechain
1	N	196	GLY	Peptide
1	N	248	GLY	Peptide

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	N	3069	0	2886	62	0
2	L	1667	0	1598	39	0
3	H	1665	0	1612	33	0
4	A	72	0	61	0	0
5	B	28	0	25	0	0
6	N	14	0	13	0	0
7	N	1	0	0	0	0
8	H	4	0	0	0	0
8	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	63	0	0	0	0
All	All	6585	0	6195	129	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 10.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:91:HIS:HB2	3:H:100(A):SER:HB2	1.65	0.77
1:N:426:LEU:HD11	1:N:444:VAL:HG22	1.67	0.75
1:N:97:TRP:H	1:N:395:GLN:HE22	1.40	0.69
2:L:108:ARG:HG3	2:L:171:SER:HB2	1.75	0.67
1:N:81:ILE:HG13	1:N:83:GLU:H	1.59	0.66
1:N:272:ALA:HA	1:N:316:TYR:CE1	2.32	0.65
1:N:168:THR:HB	1:N:170:ASN:ND2	2.11	0.64
2:L:46:LEU:HD22	2:L:55:HIS:HB2	1.79	0.64
1:N:287:VAL:HG22	1:N:305:ILE:HB	1.78	0.64
2:L:2:ILE:H	2:L:2:ILE:HD12	1.63	0.63
1:N:97:TRP:HB3	1:N:446:MET:HG2	1.81	0.63
3:H:123:PRO:HD3	3:H:221:LYS:NZ	2.15	0.62
3:H:84:ASN:HA	3:H:111:VAL:HB	1.82	0.62
2:L:2:ILE:HD13	2:L:90:GLN:NE2	2.14	0.61
3:H:173:THR:HA	3:H:189:SER:HB3	1.84	0.60
1:N:135:SER:O	1:N:156:ARG:HA	2.03	0.59
2:L:96:TRP:HZ2	3:H:99:PHE:HB3	1.66	0.59
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.38	0.59
3:H:199:TRP:HD1	3:H:205:ILE:HG12	1.69	0.58
3:H:12:LYS:O	3:H:111:VAL:HA	2.04	0.58
2:L:47:LEU:HA	2:L:58:VAL:HG11	1.85	0.58
1:N:300:ARG:NH1	1:N:324:ASP:HA	2.19	0.57
1:N:97:TRP:H	1:N:395:GLN:NE2	2.01	0.57
3:H:123:PRO:HD3	3:H:221:LYS:HZ3	1.70	0.57
1:N:135:SER:HB2	1:N:159:ILE:HD13	1.87	0.56
1:N:94:ILE:HG23	1:N:448:SER:HB2	1.88	0.55
1:N:457:ASN:ND2	1:N:457:ASN:N	2.54	0.55
3:H:143:LEU:HD12	3:H:188:SER:HB3	1.89	0.55
3:H:67:PHE:CE2	3:H:82:ILE:HG12	2.42	0.54
1:N:392:GLN:NE2	1:N:452:PHE:HE2	2.06	0.54
1:N:238:PRO:HB2	1:N:305:ILE:HD13	1.91	0.53
1:N:457:ASN:N	1:N:457:ASN:HD22	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:146:ASN:OD1	1:N:437:TRP:HB3	2.09	0.52
3:H:18:VAL:O	3:H:81:GLN:HA	2.10	0.52
2:L:23:CYS:HB2	2:L:35:TRP:HH2	1.75	0.52
2:L:115:VAL:HG22	2:L:136:LEU:HD23	1.92	0.52
1:N:275:ILE:HG12	1:N:303:ILE:HD11	1.91	0.52
1:N:103:ASP:HB3	1:N:131:PHE:HE2	1.75	0.51
2:L:86:TYR:O	2:L:101:GLY:HA2	2.10	0.51
3:H:162:ASN:OD1	3:H:205:ILE:HA	2.10	0.51
2:L:160:LEU:HD11	3:H:179:GLN:NE2	2.25	0.51
3:H:224:GLU:HG2	3:H:225:PRO:HD2	1.92	0.51
1:N:181:THR:HG22	1:N:192:ILE:HB	1.93	0.51
2:L:8:PRO:HD2	2:L:11:MET:HE1	1.93	0.51
3:H:34:MET:O	3:H:50:TRP:HA	2.10	0.51
3:H:144:VAL:HB	3:H:187:LEU:HB3	1.93	0.50
1:N:395:GLN:HA	1:N:455:GLN:NE2	2.25	0.50
1:N:463:LYS:C	1:N:465:GLU:H	2.19	0.50
1:N:272:ALA:HA	1:N:316:TYR:HE1	1.76	0.50
3:H:39:GLN:O	3:H:88:ALA:HB1	2.11	0.49
1:N:293:ASP:HB3	1:N:297:GLY:HA3	1.94	0.49
3:H:199:TRP:CD1	3:H:205:ILE:HG12	2.46	0.49
2:L:125:LEU:O	2:L:183:LYS:HE2	2.11	0.49
1:N:457:ASN:ND2	1:N:457:ASN:H	2.10	0.49
1:N:106:VAL:HG12	1:N:462:ALA:CB	2.43	0.49
1:N:333:VAL:HA	1:N:386:ASP:O	2.12	0.49
2:L:61:ARG:HG2	2:L:61:ARG:HH11	1.78	0.48
1:N:100:TYR:CE2	1:N:163:LEU:HD11	2.50	0.47
2:L:34:VAL:HG23	2:L:91:HIS:HD2	1.79	0.47
1:N:463:LYS:C	1:N:465:GLU:N	2.72	0.47
2:L:121:SER:OG	2:L:123:GLU:HG2	2.13	0.47
2:L:141:PRO:HG2	2:L:199:LYS:HD3	1.97	0.47
1:N:428:ARG:NH1	1:N:460:ASP:OD2	2.47	0.47
1:N:180:SER:HA	1:N:192:ILE:O	2.15	0.47
2:L:174:SER:C	3:H:174:PHE:HE1	2.22	0.46
3:H:1:GLN:HA	3:H:1:GLN:OE1	2.15	0.46
1:N:430:ARG:HE	1:N:437:TRP:HA	1.81	0.46
2:L:30:SER:O	2:L:31:THR:HB	2.14	0.46
2:L:159:VAL:HA	2:L:178:THR:O	2.15	0.46
2:L:17:ASP:O	2:L:78:VAL:HG23	2.15	0.45
1:N:136:GLN:NE2	1:N:156:ARG:HD3	2.31	0.45
2:L:31:THR:HG22	2:L:50:TRP:HE3	1.82	0.45
1:N:231:VAL:HG11	1:N:282:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:MET:HB2	2:L:98:PHE:O	2.17	0.45
2:L:2:ILE:HD13	2:L:90:GLN:HE22	1.79	0.45
2:L:116:SER:O	2:L:134:CYS:HA	2.17	0.45
2:L:118:PHE:HE2	2:L:135:PHE:CD2	2.36	0.45
3:H:6:GLN:NE2	3:H:92:CYS:H	2.15	0.45
1:N:395:GLN:HG2	1:N:455:GLN:HE21	1.82	0.44
2:L:136:LEU:HD13	2:L:146:VAL:HG11	1.99	0.44
1:N:360:THR:HG21	1:N:382:ALA:HB3	1.99	0.44
1:N:395:GLN:HA	1:N:455:GLN:HE21	1.82	0.44
1:N:138:THR:HG21	1:N:145:SER:HA	1.98	0.44
3:H:2:ILE:HA	3:H:26:GLY:HA3	1.99	0.44
3:H:98:ASN:O	3:H:99:PHE:HB2	2.16	0.44
2:L:144:ILE:HG13	2:L:198:HIS:HB2	2.00	0.44
2:L:150:ILE:HG23	2:L:192:TYR:CE1	2.52	0.44
3:H:38:LYS:HB3	3:H:46:GLU:HB3	1.99	0.44
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.99	0.44
2:L:19:VAL:HG22	2:L:20:THR:N	2.33	0.43
2:L:27:GLN:HE21	2:L:27:GLN:HB3	1.65	0.43
1:N:367:SER:HB3	1:N:370:SER:O	2.19	0.43
2:L:37:GLN:O	2:L:44:PRO:HA	2.19	0.43
1:N:464:ILE:O	1:N:464:ILE:CG2	2.66	0.43
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.99	0.43
3:H:30:THR:HG22	3:H:53:ASN:HD22	1.83	0.43
2:L:2:ILE:HD12	2:L:2:ILE:N	2.32	0.43
1:N:400:ASN:HB3	3:H:31:ASN:O	2.19	0.42
3:H:17:THR:HA	3:H:82:ILE:O	2.18	0.42
1:N:106:VAL:HG12	1:N:462:ALA:HB2	2.00	0.42
1:N:116:VAL:HG22	1:N:140:ILE:HA	2.01	0.42
1:N:355:LEU:HD13	1:N:383:LEU:HD13	2.01	0.42
1:N:248:GLY:O	1:N:274:HIS:HD2	2.01	0.42
2:L:2:ILE:HD11	2:L:93:SER:HB2	2.02	0.42
3:H:56:GLU:HA	3:H:57:PRO:HD3	1.70	0.42
1:N:379:VAL:CG1	1:N:388:SER:HB2	2.49	0.42
1:N:430:ARG:NE	1:N:437:TRP:HA	2.34	0.42
1:N:188:ALA:HB3	1:N:207:TYR:CZ	2.55	0.42
1:N:458:TRP:HA	1:N:459:PRO:HD2	1.80	0.42
1:N:115:LEU:HD21	1:N:169:VAL:HG22	2.01	0.41
1:N:271:THR:O	1:N:273:LYS:HD2	2.19	0.41
1:N:126:PRO:HD2	1:N:184:HIS:CD2	2.55	0.41
3:H:33:GLY:HA2	3:H:52(A):THR:HG23	2.03	0.41
3:H:139:THR:HA	3:H:191:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:94:ILE:HD12	1:N:420:ALA:HB3	2.03	0.41
1:N:168:THR:HB	1:N:170:ASN:HD21	1.82	0.41
1:N:253:ARG:HG3	1:N:255:TYR:HE1	1.86	0.41
1:N:318:CYS:SG	1:N:383:LEU:O	2.79	0.41
1:N:140:ILE:HG21	1:N:140:ILE:HD13	1.80	0.40
1:N:94:ILE:HG21	1:N:97:TRP:CZ2	2.55	0.40
2:L:118:PHE:HA	2:L:119:PRO:HD2	1.79	0.40
2:L:167:ASP:O	2:L:171:SER:HA	2.21	0.40
1:N:84:PHE:CE1	1:N:187:ARG:HD3	2.56	0.40
1:N:207:TYR:CE2	1:N:259:GLU:HG2	2.57	0.40
3:H:34:MET:HB2	3:H:51:ILE:HG22	2.02	0.40
3:H:109:LEU:HA	3:H:109:LEU:HD12	1.83	0.40
1:N:81:ILE:HG13	1:N:83:GLU:N	2.30	0.40
1:N:427:ILE:O	1:N:428:ARG:HD2	2.21	0.40
2:L:175:MET:HG2	2:L:176:SER:N	2.37	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	N	387/389 (100%)	352 (91%)	33 (8%)	2 (0%)	24	54
2	L	212/214 (99%)	197 (93%)	14 (7%)	1 (0%)	24	54
3	H	219/221 (99%)	192 (88%)	21 (10%)	6 (3%)	4	16
All	All	818/824 (99%)	741 (91%)	68 (8%)	9 (1%)	11	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	295	TRP
2	L	60	ASP

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Mol	Chain	Res	Type
3	H	216	SER
3	H	226	ARG
1	N	222	ILE
3	H	43	LYS
3	H	102	TYR
3	H	180	SER
3	H	41	PRO

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	N	341/341 (100%)	294 (86%)	47 (14%)	3	12
2	L	190/190 (100%)	153 (80%)	37 (20%)	1	5
3	H	187/187 (100%)	160 (86%)	27 (14%)	3	11
All	All	718/718 (100%)	607 (84%)	111 (16%)	2	9

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	81	ILE
1	N	93	THR
1	N	99	ILE
1	N	118	ARG
1	N	127	ASP
1	N	134	LEU
1	N	136	GLN
1	N	140	ILE
1	N	141	ARG
1	N	149	ILE
1	N	156	ARG
1	N	163	LEU
1	N	168	THR
1	N	170	ASN
1	N	181	THR

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Mol	Chain	Res	Type
1	N	204	VAL
1	N	214	GLU
1	N	224	ARG
1	N	230	CYS
1	N	247	THR
1	N	251	GLU
1	N	253	ARG
1	N	254	ILE
1	N	269	THR
1	N	276	GLU
1	N	283	GLU
1	N	287	VAL
1	N	304	GLN
1	N	311	THR
1	N	313	THR
1	N	330	ASP
1	N	337	CYS
1	N	345	ASN
1	N	362	LEU
1	N	364	ARG
1	N	368	ILE
1	N	387	ARG
1	N	388	SER
1	N	391	THR
1	N	395	GLN
1	N	411	MET
1	N	441	ASN
1	N	444	VAL
1	N	445	SER
1	N	446	MET
1	N	463	LYS
1	N	464	ILE
2	L	2	ILE
2	L	5	THR
2	L	11	MET
2	L	13	THR
2	L	14	SER
2	L	21	ILE
2	L	22	THR
2	L	27	GLN
2	L	29	VAL
2	L	46	LEU

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Mol	Chain	Res	Type
2	L	58	VAL
2	L	61	ARG
2	L	65	SER
2	L	69	THR
2	L	70	ASP
2	L	77	SER
2	L	79	GLN
2	L	81	GLU
2	L	83	LEU
2	L	90	GLN
2	L	103	LYS
2	L	105	GLU
2	L	108	ARG
2	L	122	SER
2	L	123	GLU
2	L	142	LYS
2	L	157	ASN
2	L	159	VAL
2	L	169	LYS
2	L	182	THR
2	L	191	SER
2	L	195	GLU
2	L	197	THR
2	L	200	THR
2	L	202	THR
2	L	203	SER
2	L	207	LYS
3	H	43	LYS
3	H	56	GLU
3	H	62	GLU
3	H	71	LEU
3	H	73	THR
3	H	76	SER
3	H	80	LEU
3	H	87	LYS
3	H	89	THR
3	H	108	THR
3	H	111	VAL
3	H	113	SER
3	H	133	THR
3	H	134	THR
3	H	140	LEU

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Mol	Chain	Res	Type
3	H	151	PRO
3	H	156	THR
3	H	163	SER
3	H	171	VAL
3	H	184	LEU
3	H	194	THR
3	H	198	THR
3	H	202	SER
3	H	204	SER
3	H	209	ASN
3	H	224	GLU
3	H	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	95	ASN
1	N	136	GLN
1	N	144	HIS
1	N	170	ASN
1	N	216	ASN
1	N	226	GLN
1	N	234	ASN
1	N	346	ASN
1	N	381	ASN
1	N	395	GLN
1	N	455	GLN
1	N	457	ASN
2	L	27	GLN
2	L	37	GLN
2	L	38	GLN
2	L	137	ASN
3	H	6	GLN
3	H	39	GLN
3	H	53	ASN
3	H	81	GLN
3	H	82(A)	ASN
3	H	82(B)	ASN
3	H	179	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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	A	1	4,1	14,14,15	1.06	0	17,19,21	1.41	1 (5%)
4	NAG	A	2	4	14,14,15	0.81	0	17,19,21	1.39	2 (11%)
4	BMA	A	3	4	11,11,12	1.18	1 (9%)	15,15,17	1.53	4 (26%)
4	MAN	A	4	4	11,11,12	0.98	0	15,15,17	1.56	3 (20%)
4	MAN	A	5	4	11,11,12	1.58	1 (9%)	15,15,17	0.99	0
4	MAN	A	6	4	11,11,12	1.41	2 (18%)	15,15,17	2.01	1 (6%)
5	NAG	B	1	5,1	14,14,15	0.81	0	17,19,21	1.82	4 (23%)
5	NAG	B	2	5	14,14,15	1.26	1 (7%)	17,19,21	2.48	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
4	MAN	A	4	4	-	1/2/19/22	0/1/1/1
4	MAN	A	5	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	6	4	-	2/2/19/22	0/1/1/1
5	NAG	B	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	B	2	5	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	NAG	C1-C2	4.26	1.58	1.52
4	A	5	MAN	C2-C3	4.25	1.59	1.52
4	A	3	BMA	C2-C3	2.69	1.56	1.52
4	A	6	MAN	C2-C3	-2.65	1.48	1.52
4	A	6	MAN	O3-C3	-2.06	1.37	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6	MAN	C1-O5-C5	6.97	121.53	112.19
5	B	2	NAG	C1-C2-N2	5.88	119.71	110.43
5	B	2	NAG	C1-O5-C5	4.69	118.47	112.19
5	B	2	NAG	C2-N2-C7	4.65	129.13	122.90
5	B	1	NAG	C4-C3-C2	-4.19	104.88	111.02
4	A	1	NAG	C1-C2-N2	-3.86	104.36	110.43
5	B	1	NAG	C1-C2-N2	3.52	115.98	110.43
4	A	2	NAG	C8-C7-N2	3.32	121.62	116.12
4	A	4	MAN	C1-O5-C5	3.24	116.53	112.19
4	A	4	MAN	O2-C2-C1	-3.15	102.00	109.22
5	B	1	NAG	C6-C5-C4	2.78	119.85	113.02
4	A	3	BMA	O5-C5-C4	-2.70	104.27	110.83
4	A	3	BMA	O4-C4-C3	-2.54	104.38	110.38
5	B	1	NAG	O5-C1-C2	-2.42	107.55	111.29
4	A	2	NAG	C1-O5-C5	2.34	115.32	112.19
5	B	2	NAG	C3-C4-C5	-2.15	106.34	110.23
4	A	4	MAN	O3-C3-C4	-2.14	105.33	110.38
4	A	3	BMA	C6-C5-C4	2.04	118.04	113.02
4	A	3	BMA	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	NAG	C1-C2-N2-C7

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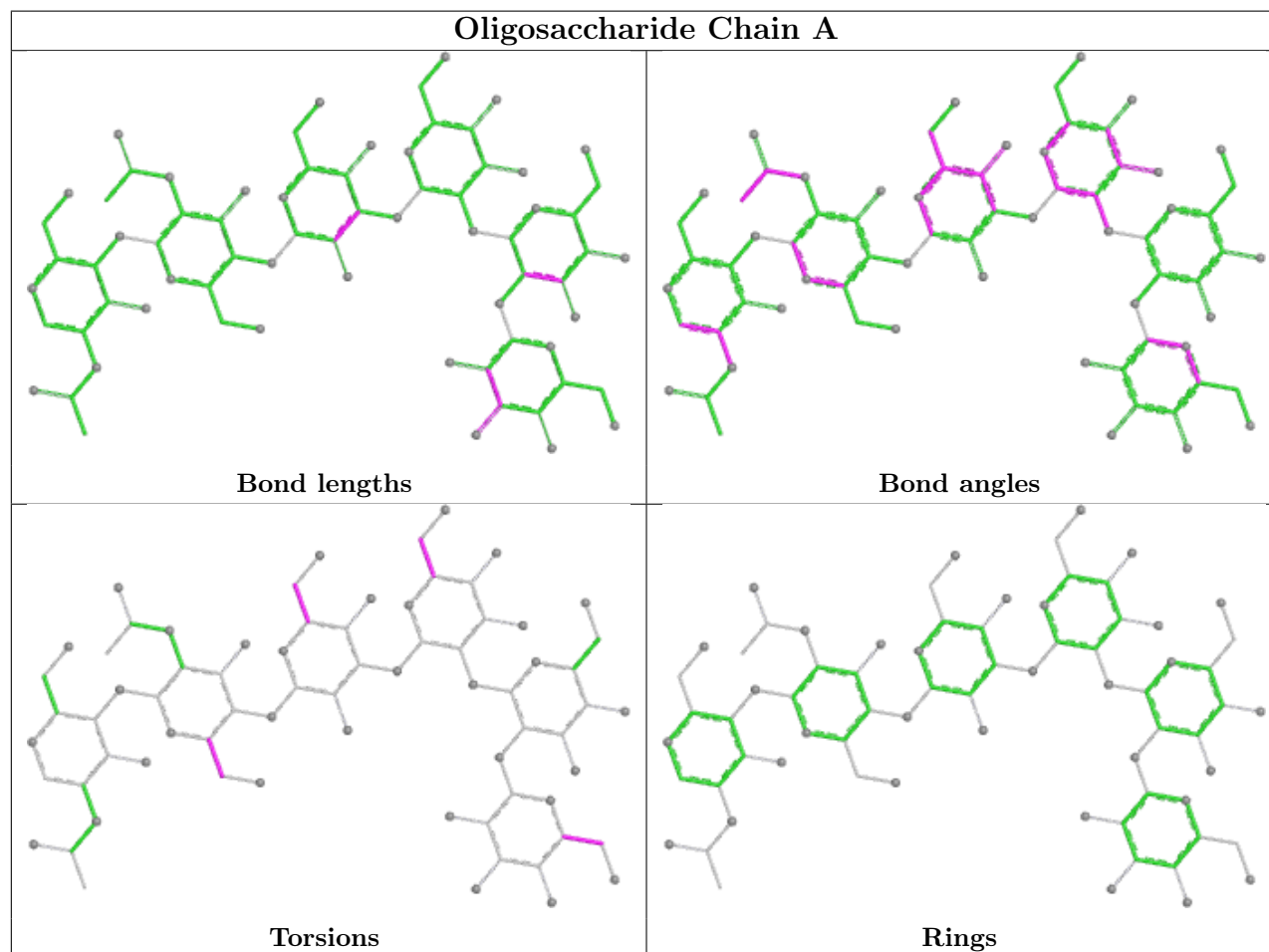
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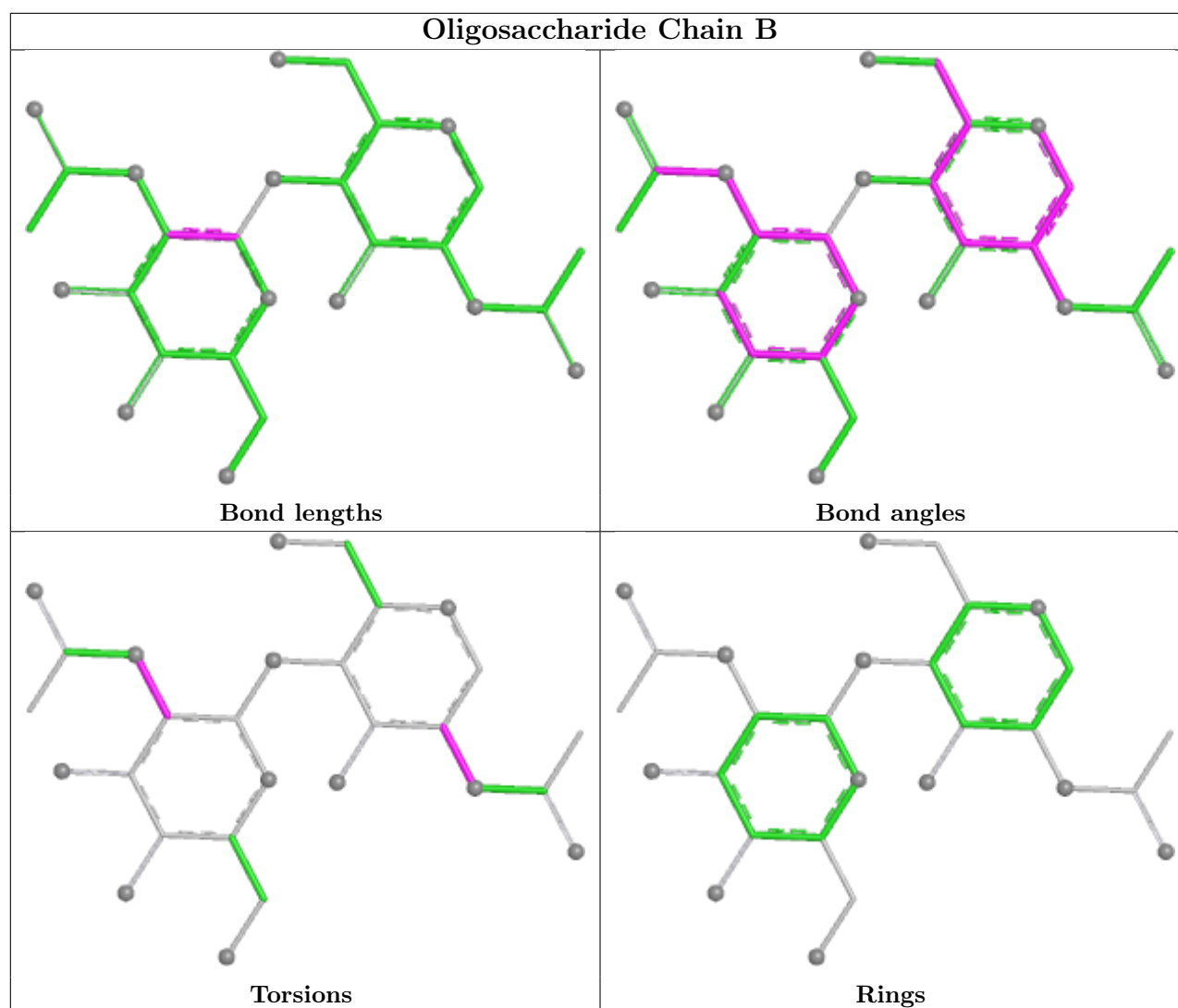
Mol	Chain	Res	Type	Atoms
5	B	2	NAG	C1-C2-N2-C7
4	A	3	BMA	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	6	MAN	C4-C5-C6-O6
4	A	4	MAN	O5-C5-C6-O6
4	A	6	MAN	O5-C5-C6-O6

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	N	475(A)	1	14,14,15	0.80	0	17,19,21	1.78	4 (23%)

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	N	475(A)	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	475(A)	NAG	C1-O5-C5	3.82	117.31	112.19
6	N	475(A)	NAG	C8-C7-N2	3.77	122.37	116.12
6	N	475(A)	NAG	C1-C2-N2	2.08	113.71	110.43
6	N	475(A)	NAG	O7-C7-N2	-2.00	118.44	121.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	N	389/389 (100%)	-0.13	9 (2%) 61 52	2, 8, 24, 47	0
2	L	214/214 (100%)	0.56	16 (7%) 20 16	4, 25, 42, 47	0
3	H	221/221 (100%)	0.70	22 (9%) 12 10	4, 26, 40, 45	0
All	All	824/824 (100%)	0.27	47 (5%) 29 23	2, 17, 38, 47	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	128	CYS	10.1
2	L	214	CYS	9.3
3	H	134	THR	8.9
3	H	180	SER	8.1
2	L	213	GLU	7.8
3	H	129	GLY	7.7
3	H	133	THR	6.9
3	H	135	GLY	6.8
3	H	130	ASP	6.7
3	H	227	GLY	6.0
2	L	211	ARG	5.6
3	H	137	SER	5.1
3	H	183	ASP	4.6
2	L	7	SER	4.5
3	H	136	SER	4.2
2	L	154	GLU	4.0
2	L	105	GLU	3.7
3	H	226	ARG	3.6
2	L	212	ASN	3.5
3	H	224	GLU	3.4
1	N	465	GLU	3.4
1	N	81	ILE	3.3
2	L	156	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	N	461	GLY	3.3
2	L	77	SER	3.2
2	L	210	ASN	3.2
1	N	261	LYS	3.0
1	N	82	ARG	2.9
1	N	269	THR	2.9
2	L	202	THR	2.9
3	H	85	GLU	2.9
3	H	164	GLY	2.8
3	H	42	GLY	2.8
2	L	182	THR	2.7
2	L	203	SER	2.6
3	H	43	LYS	2.6
3	H	23	LYS	2.6
1	N	157	ASP	2.3
2	L	163	TRP	2.3
2	L	190	ASN	2.2
3	H	120	SER	2.2
1	N	414	GLU	2.2
1	N	248	GLY	2.2
3	H	206	THR	2.1
3	H	211	ALA	2.1
2	L	162	SER	2.1
3	H	203	GLN	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.

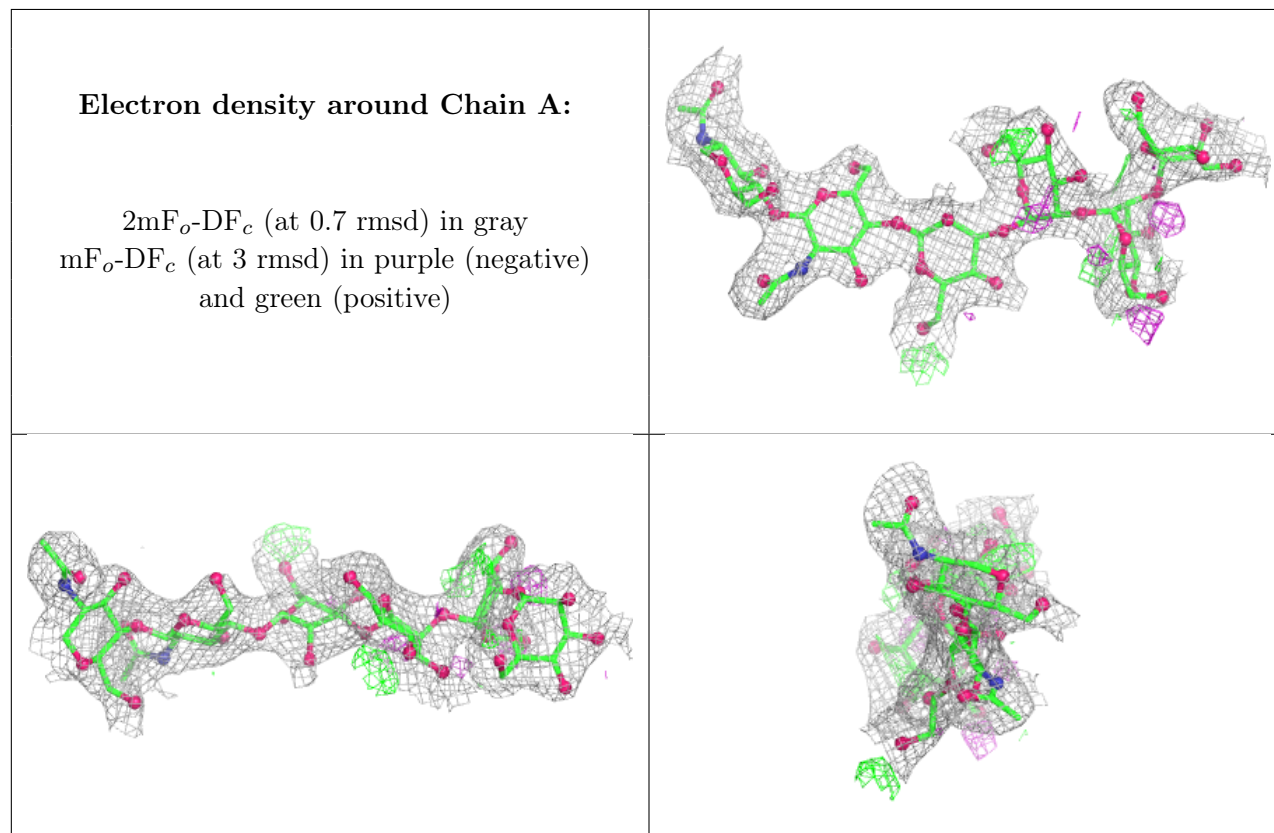
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1	14/15	-	-	5,11,23,24	0
4	NAG	A	2	14/15	-	-	12,14,16,20	0
4	BMA	A	3	11/12	-	-	8,11,13,13	0
4	MAN	A	4	11/12	-	-	9,11,14,19	0

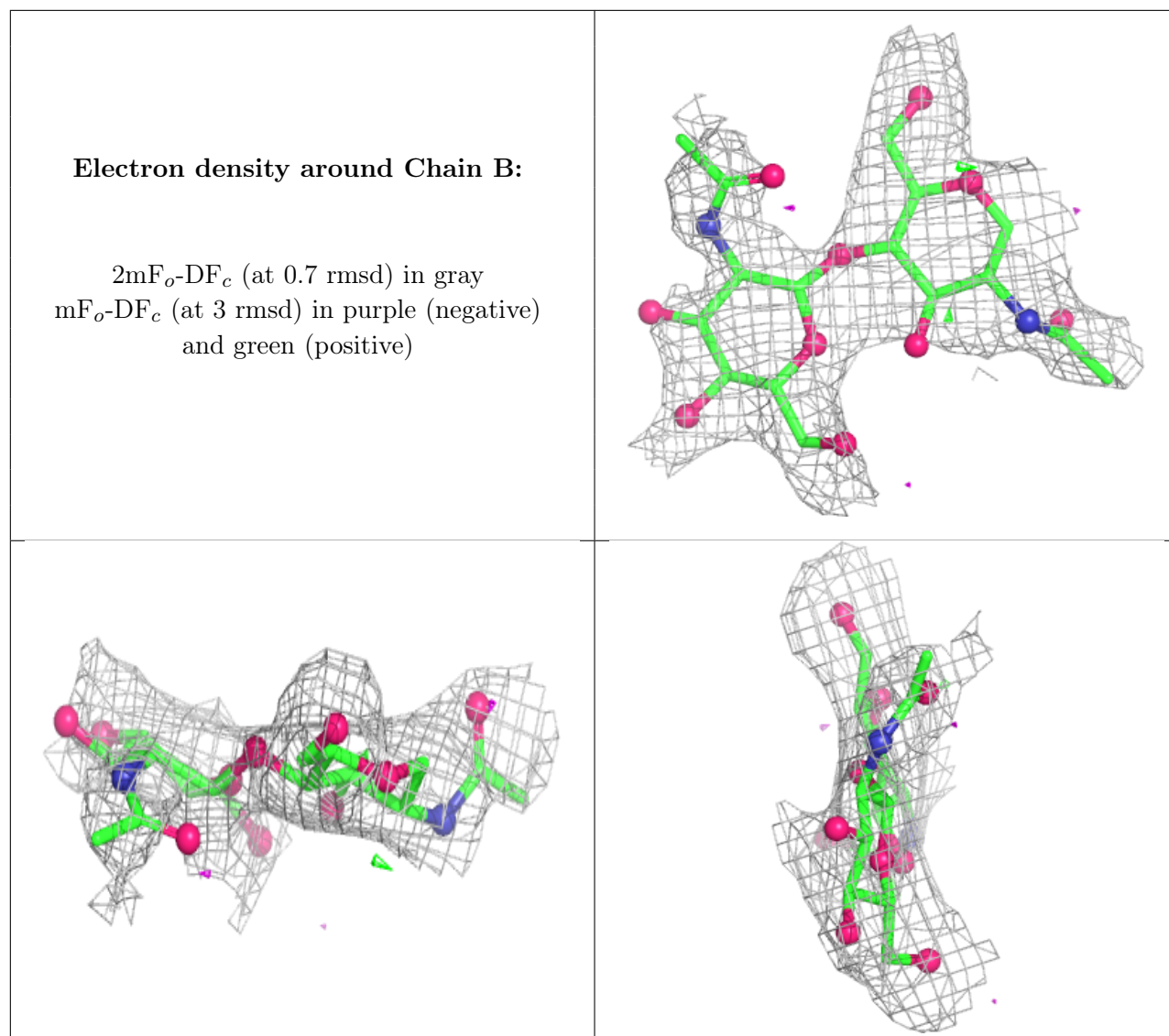
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	A	5	11/12	-	-	14,17,19,19	0
4	MAN	A	6	11/12	-	-	11,13,15,16	0
5	NAG	B	1	14/15	-	-	41,46,53,57	0
5	NAG	B	2	14/15	-	-	54,57,59,61	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	N	475(A)	14/15	0.68	0.15	37,40,44,46	0
7	CA	N	0	1/1	0.90	0.08	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.