



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:41 PM UTC

PDB ID : 1NCB / pdb_00001ncb
Title : CRYSTAL STRUCTURES OF TWO MUTANT NEURAMINIDASE-AN
TIBODY COMPLEXES WITH AMINO ACID SUBSTITUTIONS IN THE
INTERFACE
Authors : Tulip, W.R.; Varghese, J.N.; Colman, P.M.
Deposited on : 1992-01-21
Resolution : 2.50 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

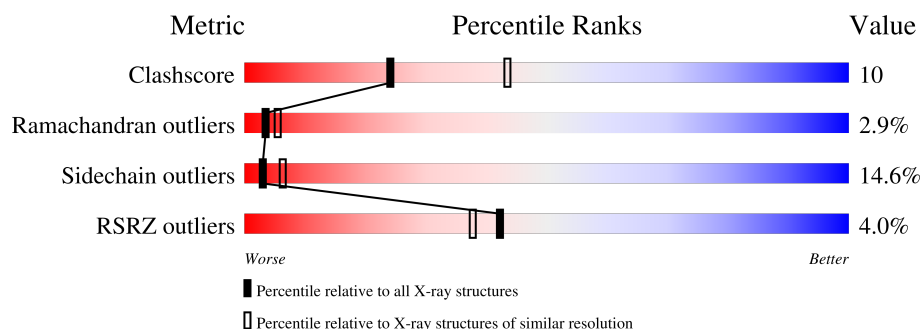
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	54% 35% 10% .
2	L	214	50% 33% 14% .
3	H	221	51% 39% 9% .
4	A	6	100%
5	B	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6594 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
			3075	1920	538	594	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	329	ASP	ASN	conflict	UNP P03472

- 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

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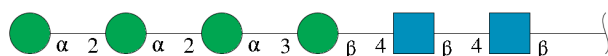
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Chain	Residue	Modelled	Actual	Comment	Reference
L	85	LEU	GLU	conflict	EMBL Y11589
L	87	TYR	PHE	conflict	EMBL Y11589
L	91	HIS	TYR	conflict	EMBL Y11589
L	92	TYR	ASN	conflict	EMBL Y11589
L	93	SER	ARG	conflict	EMBL Y11589
L	94	PRO	TYR	conflict	EMBL Y11589

- 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.



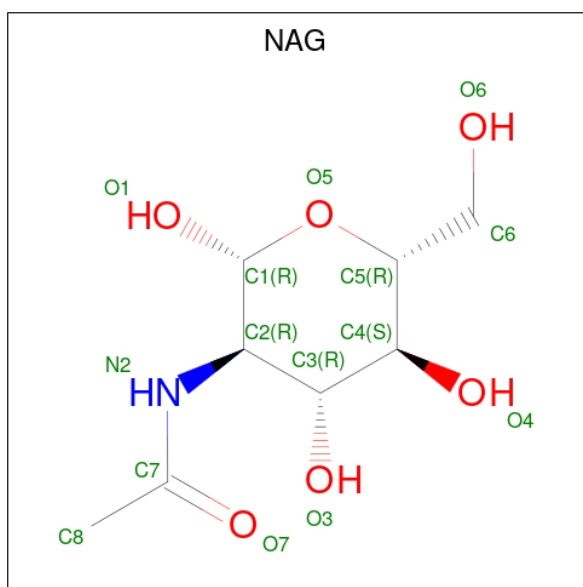
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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
			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		

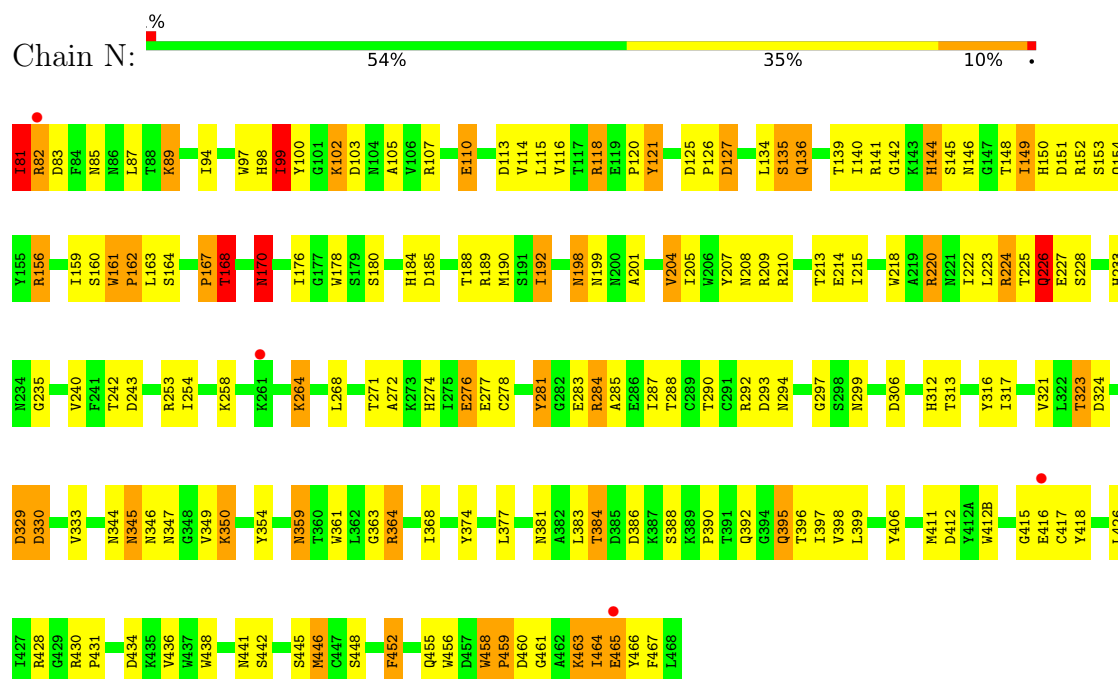
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	66	Total	O	0	0
			66	66		
8	L	2	Total	O	0	0
			2	2		
8	H	4	Total	O	0	0
			4	4		

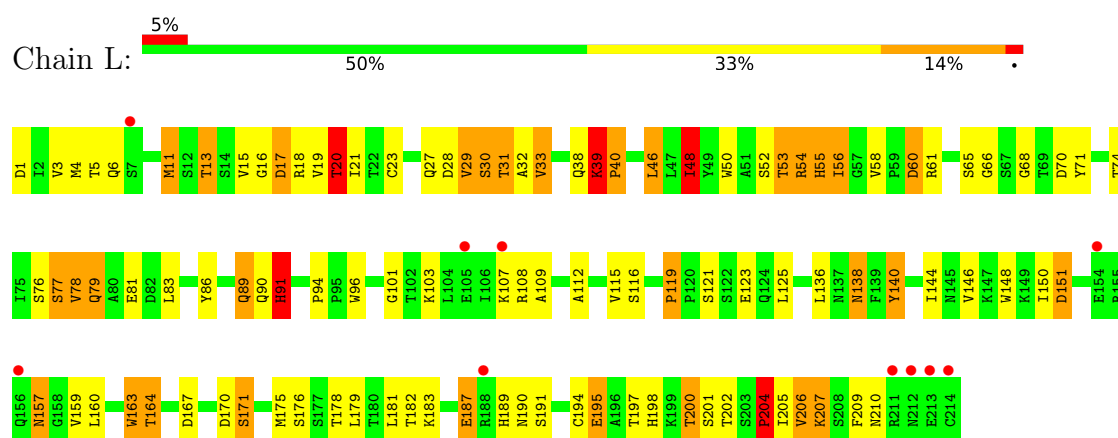
3 Residue-property plots

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

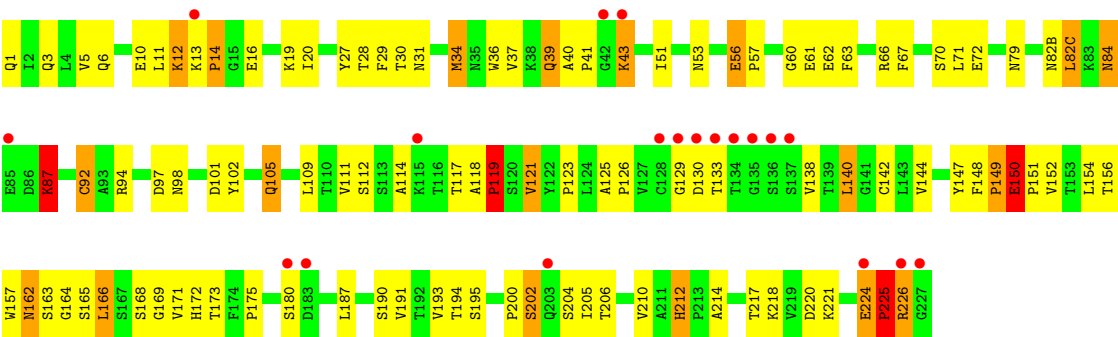


• Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)

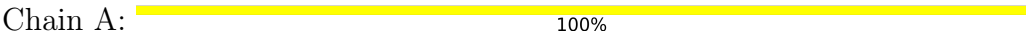


• Molecule 3: IGG2A-KAPPA NC41 FAB (HEAVY CHAIN)





● Molecule 4: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



● Molecule 5: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -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)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 31.8 (8.00-2.50)	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}	0.165 , (Not available) 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.7	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	0.89	EDS
Total number of atoms	6594	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 3.31% 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: MAN, NAG, 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	1.25	17/3158 (0.5%)	2.14	134/4301 (3.1%)
2	L	1.10	7/1708 (0.4%)	2.09	67/2323 (2.9%)
3	H	1.04	6/1707 (0.4%)	2.06	55/2326 (2.4%)
All	All	1.16	30/6573 (0.5%)	2.11	256/8950 (2.9%)

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	5
2	L	0	2
All	All	0	7

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	297	GLY	C-O	7.92	1.32	1.23
2	L	198	HIS	CD2-NE2	-7.59	1.29	1.37
1	N	312	HIS	CD2-NE2	-7.06	1.30	1.37
1	N	144	HIS	CD2-NE2	-7.00	1.30	1.37
1	N	347	ASN	C-O	6.95	1.32	1.24
2	L	91	HIS	CD2-NE2	-6.88	1.30	1.37
1	N	274	HIS	CD2-NE2	-6.80	1.30	1.37
1	N	184	HIS	CD2-NE2	-6.68	1.30	1.37
1	N	254	ILE	CA-CB	6.65	1.61	1.54
2	L	56	ILE	CA-CB	6.58	1.63	1.54
1	N	150	HIS	CD2-NE2	-6.31	1.30	1.37
2	L	189	HIS	CD2-NE2	-6.26	1.30	1.37
1	N	98	HIS	CD2-NE2	-6.10	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5	VAL	CA-CB	5.95	1.62	1.54
1	N	466	TYR	C-N	-5.89	1.25	1.33
3	H	175	PRO	CA-CB	-5.87	1.45	1.53
3	H	212	HIS	CD2-NE2	-5.87	1.31	1.37
1	N	144	HIS	CG-ND1	-5.75	1.31	1.38
2	L	55	HIS	CD2-NE2	-5.70	1.31	1.37
1	N	113	ASP	CA-CB	5.51	1.59	1.52
1	N	162	PRO	CA-CB	-5.39	1.46	1.53
2	L	91	HIS	CG-ND1	-5.39	1.32	1.38
3	H	172	HIS	CD2-NE2	-5.36	1.31	1.37
1	N	233	HIS	CD2-NE2	-5.34	1.31	1.37
1	N	312	HIS	CG-ND1	-5.33	1.32	1.38
3	H	20	ILE	CA-CB	5.27	1.59	1.53
2	L	189	HIS	CG-ND1	-5.10	1.32	1.38
3	H	34	MET	CA-CB	-5.08	1.46	1.53
1	N	167	PRO	CA-CB	-5.03	1.47	1.53
1	N	184	HIS	CG-ND1	-5.01	1.32	1.38

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	127	ASP	N-CA-C	12.98	125.51	111.36
1	N	293	ASP	CA-C-O	11.44	132.44	120.54
3	H	165	SER	N-CA-C	11.18	123.04	111.07
3	H	220	ASP	CA-CB-CG	11.17	123.77	112.60
1	N	82	ARG	N-CA-C	-11.04	97.20	110.44
3	H	101	ASP	CA-CB-CG	10.78	123.38	112.60
1	N	297	GLY	O-C-N	10.72	133.90	122.96
1	N	185	ASP	CA-CB-CG	10.43	123.03	112.60
1	N	346	ASN	OD1-CG-ND2	-10.35	112.25	122.60
1	N	170	ASN	OD1-CG-ND2	-10.01	112.59	122.60
2	L	210	ASN	CA-CB-CG	-9.64	102.96	112.60
2	L	91	HIS	CA-CB-CG	9.55	123.35	113.80
2	L	29	VAL	N-CA-CB	-9.41	99.77	112.28
3	H	105	GLN	CG-CD-NE2	9.28	130.32	116.40
3	H	6	GLN	OE1-CD-NE2	-8.91	113.69	122.60
1	N	184	HIS	CB-CG-CD2	-8.60	120.01	131.20
1	N	381	ASN	N-CA-C	8.41	123.01	112.24
3	H	67	PHE	CA-CB-CG	-8.38	105.42	113.80
2	L	157	ASN	CA-CB-CG	8.30	120.90	112.60
3	H	150	GLU	CA-C-O	-8.24	113.27	120.19
3	H	94	ARG	CB-CG-CD	-8.13	92.59	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	63	PHE	CA-CB-CG	-8.12	105.69	113.80
2	L	79	GLN	CA-CB-CG	8.11	130.32	114.10
3	H	105	GLN	OE1-CD-NE2	-8.08	114.52	122.60
2	L	210	ASN	OD1-CG-ND2	-8.02	114.58	122.60
1	N	189	ARG	N-CA-C	7.90	122.36	109.72
2	L	3	VAL	N-CA-CB	-7.82	102.08	111.00
2	L	170	ASP	CA-CB-CG	7.75	120.34	112.60
1	N	116	VAL	N-CA-C	-7.73	97.45	108.58
2	L	189	HIS	N-CA-C	7.72	120.81	109.69
1	N	299	ASN	CA-CB-CG	7.71	120.31	112.60
2	L	30	SER	N-CA-C	7.63	121.92	111.54
2	L	205	ILE	N-CA-C	-7.60	96.19	107.51
1	N	198	ASN	OD1-CG-ND2	-7.52	115.08	122.60
2	L	79	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	N	184	HIS	CB-CG-ND1	7.46	133.88	122.70
1	N	151	ASP	N-CA-C	7.45	119.40	111.28
1	N	127	ASP	N-CA-CB	-7.40	99.21	110.16
2	L	198	HIS	CB-CG-CD2	-7.35	121.65	131.20
1	N	285	ALA	N-CA-C	7.33	121.58	111.90
3	H	101	ASP	N-CA-C	-7.32	98.31	109.95
2	L	31	THR	N-CA-CB	-7.29	101.26	113.15
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
3	H	121	VAL	N-CA-CB	-7.26	102.72	111.00
1	N	398	VAL	N-CA-C	-7.25	98.03	108.48
1	N	299	ASN	N-CA-C	-7.24	99.20	110.42
2	L	94	PRO	N-CA-C	7.23	119.52	110.70
1	N	204	VAL	CA-C-O	7.23	128.02	120.36
1	N	170	ASN	CB-CG-ND2	7.20	127.20	116.40
3	H	194	THR	N-CA-C	-7.20	100.83	110.55
1	N	110	GLU	N-CA-C	-7.08	104.12	112.89
2	L	70	ASP	CA-CB-CG	-7.06	105.54	112.60
1	N	99	ILE	CB-CA-C	-7.01	100.16	111.59
1	N	363	GLY	O-C-N	7.00	131.80	122.70
3	H	92	CYS	N-CA-C	-6.99	98.34	109.59
3	H	118	ALA	CA-C-N	6.94	127.39	120.52
3	H	118	ALA	C-N-CA	6.94	127.39	120.52
1	N	386	ASP	N-CA-C	6.91	120.30	112.97
1	N	243	ASP	CA-CB-CG	6.89	119.50	112.60
1	N	125	ASP	CA-CB-CG	6.86	119.46	112.60
3	H	3	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	N	176	ILE	N-CA-CB	-6.83	103.22	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	56	GLU	N-CA-C	6.82	118.72	109.24
1	N	168	THR	N-CA-CB	-6.79	100.39	110.17
1	N	438	TRP	CG-CD2-CE3	6.76	140.66	133.90
1	N	136	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	N	383	LEU	N-CA-C	-6.74	103.55	111.03
3	H	13	LYS	CA-C-N	6.72	128.24	119.84
3	H	13	LYS	C-N-CA	6.72	128.24	119.84
3	H	105	GLN	N-CA-C	6.62	120.81	112.87
1	N	415	GLY	N-CA-C	6.62	119.56	110.56
2	L	138	ASN	N-CA-C	6.61	120.20	111.28
1	N	146	ASN	CA-CB-CG	6.60	119.20	112.60
1	N	121	TYR	CA-CB-CG	6.56	125.71	113.90
1	N	346	ASN	CB-CG-ND2	6.52	126.18	116.40
2	L	31	THR	CA-CB-OG1	-6.47	99.89	109.60
2	L	21	ILE	N-CA-CB	-6.47	103.33	111.41
1	N	226	GLN	N-CA-C	6.46	124.57	110.80
2	L	29	VAL	CB-CA-C	6.45	120.03	111.85
1	N	136	GLN	CG-CD-NE2	6.44	126.06	116.40
3	H	19	LYS	CA-C-N	6.43	130.54	122.43
3	H	19	LYS	C-N-CA	6.43	130.54	122.43
1	N	458	TRP	O-C-N	6.40	127.14	121.32
1	N	333	VAL	CA-C-O	-6.39	114.51	121.28
2	L	121	SER	N-CA-C	-6.38	101.51	110.50
3	H	98	ASN	CA-C-O	-6.37	114.02	121.16
1	N	412	ASP	CA-CB-CG	6.36	118.96	112.60
1	N	198	ASN	CB-CG-ND2	6.36	125.94	116.40
1	N	146	ASN	N-CA-C	6.34	118.78	108.63
2	L	189	HIS	CA-CB-CG	-6.32	107.48	113.80
1	N	102	LYS	CA-C-N	6.30	131.08	120.88
1	N	102	LYS	C-N-CA	6.30	131.08	120.88
3	H	57	PRO	O-C-N	6.29	131.58	122.78
1	N	456	TRP	O-C-N	6.28	130.56	123.27
1	N	264	LYS	CA-CB-CG	6.15	126.40	114.10
1	N	290	THR	N-CA-C	-6.14	99.23	109.24
1	N	218	TRP	CG-CD2-CE3	6.14	140.04	133.90
3	H	162	ASN	CA-CB-CG	6.12	118.72	112.60
2	L	1	ASP	CA-CB-CG	6.11	118.71	112.60
1	N	190	MET	CA-CB-CG	-6.11	101.89	114.10
2	L	210	ASN	N-CA-C	-6.10	100.03	109.24
2	L	81	GLU	CB-CG-CD	6.09	122.95	112.60
1	N	329	ASP	CA-CB-CG	6.08	118.68	112.60
1	N	350	LYS	CA-C-O	-6.05	114.53	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	461	GLY	O-C-N	-6.05	115.52	122.42
3	H	40	ALA	N-CA-C	-6.02	102.49	110.07
1	N	386	ASP	CA-CB-CG	6.01	118.61	112.60
2	L	91	HIS	CB-CG-CD2	-6.00	123.40	131.20
2	L	89	GLN	N-CA-C	-5.98	100.25	109.52
1	N	225	THR	N-CA-C	5.93	116.92	108.74
1	N	103	ASP	N-CA-C	5.91	118.87	111.24
1	N	330	ASP	CA-C-N	5.88	127.20	119.84
1	N	330	ASP	C-N-CA	5.88	127.20	119.84
3	H	212	HIS	CB-CG-CD2	-5.88	123.55	131.20
2	L	91	HIS	CB-CG-ND1	5.88	131.52	122.70
3	H	97	ASP	CA-CB-CG	5.86	118.46	112.60
1	N	384	THR	N-CA-C	5.83	120.54	112.90
3	H	12	LYS	CA-CB-CG	5.83	125.77	114.10
1	N	347	ASN	CA-C-O	5.82	128.83	120.51
3	H	225	PRO	N-CA-C	5.82	124.45	112.47
2	L	194	CYS	N-CA-C	-5.81	97.75	107.80
3	H	226	ARG	N-CA-C	5.81	123.17	110.80
1	N	125	ASP	N-CA-C	-5.80	103.46	110.13
1	N	274	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	N	233	HIS	CB-CG-CD2	-5.79	123.67	131.20
2	L	201	SER	O-C-N	5.79	129.89	123.52
2	L	119	PRO	N-CA-C	5.78	117.76	110.70
1	N	140	ILE	CB-CA-C	-5.78	104.48	111.88
1	N	294	ASN	CA-CB-CG	-5.77	106.83	112.60
1	N	213	THR	CA-CB-OG1	-5.76	100.96	109.60
1	N	438	TRP	CB-CG-CD1	-5.75	118.27	126.90
2	L	61	ARG	CB-CG-CD	-5.75	98.08	111.30
1	N	153	SER	CA-C-N	-5.74	114.00	122.83
1	N	153	SER	C-N-CA	-5.74	114.00	122.83
2	L	201	SER	CA-C-O	5.73	126.79	120.31
1	N	148	THR	CA-C-O	5.73	126.36	119.43
3	H	3	GLN	CA-CB-CG	5.72	125.54	114.10
1	N	455	GLN	N-CA-C	5.68	118.99	109.95
3	H	125	ALA	N-CA-C	-5.66	102.47	110.29
1	N	220	ARG	N-CA-C	5.66	119.77	112.86
2	L	164	THR	N-CA-CB	-5.63	101.69	109.97
1	N	452	PHE	CA-CB-CG	-5.62	108.19	113.80
1	N	218	TRP	CG-CD1-NE1	-5.61	102.90	110.20
1	N	226	GLN	CA-CB-CG	5.61	125.32	114.10
2	L	140	TYR	CA-CB-CG	-5.61	103.81	113.90
2	L	52	SER	CA-CB-OG	-5.60	99.90	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	201	ALA	CA-C-O	-5.60	114.83	121.66
1	N	99	ILE	N-CA-CB	5.58	117.61	110.13
3	H	119	PRO	N-CA-C	5.58	119.45	111.13
3	H	87	LYS	N-CA-C	-5.58	100.02	108.67
3	H	31	ASN	OD1-CG-ND2	-5.57	117.03	122.60
3	H	121	VAL	CB-CA-C	5.57	117.69	110.96
2	L	54	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	N	317	ILE	N-CA-C	-5.55	99.60	107.98
1	N	170	ASN	CA-CB-CG	5.51	118.11	112.60
2	L	107	LYS	CA-C-O	5.47	127.52	121.39
1	N	284	ARG	NE-CZ-NH1	5.47	126.97	121.50
3	H	112	SER	N-CA-C	5.46	117.40	108.55
2	L	33	VAL	CA-CB-CG2	-5.46	101.12	110.40
1	N	428	ARG	CA-CB-CG	-5.45	103.19	114.10
3	H	166	LEU	N-CA-C	-5.45	100.22	108.67
2	L	164	THR	N-CA-C	-5.45	102.21	110.28
2	L	27	GLN	CB-CG-CD	-5.45	103.34	112.60
2	L	171	SER	N-CA-C	5.44	122.39	110.80
2	L	96	TRP	CE2-CD2-CG	-5.43	100.69	107.20
2	L	151	ASP	CA-CB-CG	-5.43	107.17	112.60
1	N	161	TRP	CA-C-N	5.42	126.62	119.84
1	N	161	TRP	C-N-CA	5.42	126.62	119.84
1	N	374	TYR	N-CA-C	-5.42	99.77	108.55
1	N	209	ARG	CB-CG-CD	5.42	123.76	111.30
3	H	3	GLN	CG-CD-NE2	5.42	124.53	116.40
1	N	85	ASN	CB-CG-ND2	5.41	124.51	116.40
1	N	361	TRP	CA-C-N	5.41	131.90	122.81
1	N	361	TRP	C-N-CA	5.41	131.90	122.81
2	L	187	GLU	CB-CG-CD	5.41	121.80	112.60
3	H	202	SER	N-CA-C	5.41	117.62	111.02
1	N	344	ASN	CA-C-O	5.40	128.03	120.52
1	N	144	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	N	218	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	N	397	ILE	O-C-N	-5.40	115.83	122.57
2	L	20	THR	CA-CB-OG1	-5.39	101.52	109.60
2	L	107	LYS	O-C-N	5.37	129.18	122.63
3	H	82(B)	ASN	OD1-CG-ND2	-5.37	117.23	122.60
2	L	167	ASP	CA-CB-CG	5.36	117.96	112.60
1	N	192	ILE	N-CA-CB	-5.35	104.54	111.82
1	N	354	TYR	CA-CB-CG	-5.34	104.28	113.90
1	N	160	SER	CA-CB-OG	5.33	121.76	111.10
3	H	150	GLU	N-CA-C	-5.33	103.36	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	135	SER	CA-CB-OG	5.31	121.72	111.10
3	H	165	SER	O-C-N	-5.31	116.60	122.07
2	L	6	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	N	208	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	N	242	THR	CA-CB-OG1	-5.30	101.64	109.60
1	N	213	THR	CA-CB-CG2	5.30	119.51	110.50
1	N	330	ASP	CA-CB-CG	5.30	117.90	112.60
2	L	58	VAL	N-CA-C	-5.29	97.44	108.88
1	N	142	GLY	O-C-N	-5.29	116.40	122.91
2	L	198	HIS	CB-CG-ND1	5.29	130.64	122.70
1	N	306	ASP	CA-C-N	5.29	124.79	119.19
1	N	306	ASP	C-N-CA	5.29	124.79	119.19
3	H	60	GLY	N-CA-C	-5.28	104.62	113.02
2	L	48	ILE	N-CA-CB	-5.28	101.59	111.62
2	L	163	TRP	CG-CD2-CE3	5.27	139.17	133.90
2	L	20	THR	CB-CA-C	5.27	118.57	110.14
1	N	105	ALA	N-CA-C	5.27	117.43	111.11
1	N	156	ARG	CB-CG-CD	-5.27	99.18	111.30
1	N	459	PRO	CB-CA-C	-5.26	104.22	111.21
1	N	81	ILE	N-CA-C	-5.25	96.29	111.00
1	N	226	GLN	OE1-CD-NE2	-5.25	117.35	122.60
2	L	176	SER	N-CA-C	-5.25	101.72	110.17
2	L	3	VAL	CA-CB-CG2	-5.25	101.48	110.40
1	N	145	SER	N-CA-C	-5.24	106.84	113.18
1	N	125	ASP	CA-C-N	5.23	125.28	119.32
1	N	125	ASP	C-N-CA	5.23	125.28	119.32
3	H	117	THR	N-CA-C	-5.23	100.88	109.40
1	N	345	ASN	CA-C-N	5.23	130.36	122.68
1	N	345	ASN	C-N-CA	5.23	130.36	122.68
1	N	180	SER	CA-C-O	5.22	127.36	121.51
2	L	79	GLN	CB-CG-CD	5.22	121.48	112.60
1	N	345	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	N	361	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	N	324	ASP	CA-CB-CG	5.18	117.78	112.60
3	H	162	ASN	OD1-CG-ND2	-5.18	117.42	122.60
2	L	20	THR	N-CA-CB	-5.17	102.66	110.77
1	N	218	TRP	CD1-CG-CD2	5.17	114.56	106.30
2	L	202	THR	CA-CB-OG1	-5.16	101.86	109.60
1	N	313	THR	CA-C-O	-5.16	115.93	121.45
2	L	148	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	L	50	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	N	412(B)	TRP	CB-CG-CD1	-5.14	119.19	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	224	GLU	CA-C-N	5.12	126.25	119.84
3	H	224	GLU	C-N-CA	5.12	126.25	119.84
3	H	173	THR	N-CA-C	-5.12	100.95	109.46
2	L	28	ASP	CA-CB-CG	5.12	117.72	112.60
1	N	293	ASP	CA-CB-CG	5.11	117.71	112.60
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
1	N	189	ARG	CA-C-O	5.09	126.87	121.11
1	N	396	THR	O-C-N	5.09	128.99	123.13
1	N	176	ILE	N-CA-C	5.09	115.42	107.99
3	H	56	GLU	CA-CB-CG	-5.07	103.95	114.10
1	N	395	GLN	CB-CG-CD	5.07	121.22	112.60
1	N	281	TYR	CA-C-O	-5.07	115.70	121.58
2	L	148	TRP	CD1-CG-CD2	5.06	114.40	106.30
3	H	152	VAL	CG1-CB-CG2	-5.06	99.67	110.80
1	N	223	LEU	N-CA-C	-5.06	102.37	109.96
2	L	48	ILE	O-C-N	-5.05	117.44	123.00
2	L	39	LYS	CA-C-N	5.05	126.15	119.84
2	L	39	LYS	C-N-CA	5.05	126.15	119.84
1	N	215	ILE	N-CA-C	-5.04	98.86	109.34
3	H	39	GLN	CA-CB-CG	-5.03	104.04	114.10
2	L	150	ILE	N-CA-C	-5.01	101.15	108.17
1	N	428	ARG	CD-NE-CZ	-5.01	117.38	124.40
3	H	84	ASN	N-CA-C	5.01	121.46	110.80
1	N	103	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	140	TYR	Sidechain
2	L	209	PHE	Peptide
1	N	107	ARG	Sidechain
1	N	118	ARG	Sidechain
1	N	210	ARG	Sidechain
1	N	224	ARG	Sidechain
1	N	406	TYR	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	N	3075	0	2902	60	0
2	L	1667	0	1598	33	0
3	H	1665	0	1612	35	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
8	N	66	0	0	3	0
All	All	6594	0	6211	125	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 (125) 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:N:97:TRP:H	1:N:395:GLN:HE22	1.32	0.76
1:N:442:SER:HB2	1:N:460:ASP:OD1	1.94	0.66
1:N:192:ILE:HG12	1:N:205:ILE:HG13	1.78	0.66
1:N:272:ALA:HA	1:N:316:TYR:CE1	2.30	0.66
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.80	0.63
2:L:38:GLN:HE22	3:H:39:GLN:HE22	1.46	0.62
1:N:152:ARG:HD2	1:N:198:ASN:HD21	1.65	0.61
2:L:195:GLU:HB2	2:L:206:VAL:HG13	1.81	0.60
2:L:46:LEU:HD22	2:L:55:HIS:HB2	1.84	0.60
3:H:140:LEU:HD11	3:H:205:ILE:HD12	1.84	0.59
1:N:97:TRP:N	1:N:395:GLN:HE22	2.01	0.59
1:N:364:ARG:HH11	1:N:377:LEU:HD11	1.68	0.59
3:H:154:LEU:HG	3:H:210:VAL:HG22	1.86	0.58
1:N:430:ARG:HG2	1:N:434:ASP:HA	1.86	0.57
3:H:123:PRO:HD3	3:H:221:LYS:HG3	1.85	0.57
3:H:16:GLU:O	3:H:82(C):LEU:HG	2.05	0.57
1:N:94:ILE:HG23	1:N:448:SER:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:THR:H	1:N:170:ASN:HD21	1.52	0.56
1:N:226:GLN:HE22	1:N:240:VAL:H	1.53	0.56
2:L:159:VAL:HA	2:L:178:THR:O	2.06	0.56
2:L:54:ARG:NE	2:L:60:ASP:HA	2.21	0.56
2:L:115:VAL:O	2:L:207:LYS:HE3	2.06	0.55
1:N:121:TYR:CG	1:N:228:SER:HA	2.42	0.55
1:N:89:LYS:HG2	1:N:417:CYS:HA	1.89	0.54
1:N:281:TYR:HB2	1:N:411:MET:HE2	1.87	0.54
1:N:114:VAL:O	1:N:139:THR:HA	2.07	0.54
1:N:272:ALA:HA	1:N:316:TYR:HE1	1.70	0.53
3:H:200:PRO:HB3	3:H:225:PRO:HG3	1.91	0.53
2:L:30:SER:O	2:L:31:THR:HB	2.08	0.53
1:N:168:THR:HB	1:N:170:ASN:ND2	2.24	0.52
1:N:426:LEU:HB2	1:N:442:SER:HB3	1.91	0.52
1:N:411:MET:SD	1:N:418:TYR:HB3	2.50	0.51
1:N:199:ASN:HA	1:N:220:ARG:O	2.11	0.51
1:N:276:GLU:HB2	1:N:292:ARG:HD3	1.91	0.51
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.93	0.51
1:N:94:ILE:HG12	1:N:359:ASN:ND2	2.26	0.51
1:N:152:ARG:HD2	1:N:198:ASN:ND2	2.26	0.51
2:L:38:GLN:HE22	3:H:39:GLN:NE2	2.09	0.51
1:N:463:LYS:C	1:N:465:GLU:H	2.19	0.50
3:H:121:VAL:HG22	3:H:144:VAL:HG13	1.94	0.50
3:H:84:ASN:HA	3:H:111:VAL:HG11	1.94	0.49
1:N:115:LEU:HD12	1:N:159:ILE:HD13	1.94	0.49
1:N:276:GLU:HB2	1:N:292:ARG:HB3	1.95	0.49
3:H:87:LYS:HA	3:H:109:LEU:O	2.13	0.49
1:N:392:GLN:HE22	1:N:452:PHE:HE1	1.60	0.49
3:H:30:THR:HG22	3:H:53:ASN:HD22	1.78	0.48
3:H:166:LEU:HD23	3:H:191:VAL:HG21	1.96	0.48
3:H:12:LYS:O	3:H:111:VAL:HA	2.14	0.48
1:N:463:LYS:C	1:N:465:GLU:N	2.72	0.47
2:L:17:ASP:O	2:L:78:VAL:HG23	2.14	0.47
2:L:13:THR:HG21	2:L:78:VAL:HG21	1.95	0.47
1:N:110:GLU:HB2	1:N:467:PHE:CZ	2.50	0.47
1:N:144:HIS:HD2	8:N:39:HOH:O	1.98	0.47
1:N:81:ILE:HG23	1:N:83:ASP:O	2.15	0.47
1:N:426:LEU:O	1:N:441:ASN:HA	2.15	0.47
1:N:281:TYR:CE1	1:N:288:THR:HB	2.51	0.46
2:L:48:ILE:HA	2:L:53:THR:O	2.14	0.46
3:H:150:GLU:OE1	3:H:151:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:156:THR:HB	3:H:164:GLY:H	1.81	0.46
2:L:115:VAL:HG22	2:L:136:LEU:HG	1.97	0.46
3:H:169:GLY:O	3:H:191:VAL:HA	2.16	0.46
2:L:38:GLN:NE2	3:H:39:GLN:HE22	2.11	0.46
2:L:136:LEU:HD23	2:L:144:ILE:HD13	1.98	0.46
2:L:66:GLY:HA3	2:L:71:TYR:CD1	2.51	0.46
2:L:32:ALA:HA	2:L:91:HIS:CE1	2.52	0.45
1:N:149:ILE:HD11	1:N:431:PRO:HD3	1.98	0.45
1:N:81:ILE:HG13	1:N:82:ARG:H	1.83	0.44
3:H:212:HIS:HB3	3:H:217:THR:HB	1.99	0.44
1:N:436:VAL:CG1	1:N:464:ILE:HD12	2.47	0.44
2:L:108:ARG:HG2	2:L:109:ALA:N	2.33	0.44
1:N:97:TRP:HB3	1:N:446:MET:HG2	1.99	0.44
1:N:100:TYR:CE2	1:N:163:LEU:HD11	2.53	0.43
2:L:16:GLY:HA2	2:L:77:SER:HA	1.99	0.43
1:N:99:ILE:H	1:N:99:ILE:HG13	1.52	0.43
2:L:89:GLN:HG2	2:L:90:GLN:N	2.33	0.43
1:N:281:TYR:HA	8:N:57:HOH:O	2.18	0.43
1:N:89:LYS:HG2	1:N:416:GLU:O	2.18	0.43
1:N:277:GLU:HG3	8:N:32:HOH:O	2.18	0.43
3:H:11:LEU:HD11	3:H:148:PHE:HE2	1.83	0.43
3:H:11:LEU:HD13	3:H:149:PRO:HB3	2.01	0.43
3:H:212:HIS:CE1	3:H:214:ALA:HB3	2.53	0.43
2:L:18:ARG:HH11	2:L:18:ARG:HG3	1.84	0.43
1:N:436:VAL:HG11	1:N:464:ILE:HD12	2.00	0.43
1:N:464:ILE:O	1:N:464:ILE:CG2	2.66	0.43
2:L:19:VAL:O	2:L:74:THR:HA	2.19	0.43
3:H:1:GLN:HA	3:H:1:GLN:OE1	2.18	0.43
3:H:27:TYR:CE1	3:H:29:PHE:HA	2.53	0.43
3:H:34:MET:HB2	3:H:51:ILE:HG22	2.00	0.43
1:N:323:THR:HA	1:N:364:ARG:HB3	2.00	0.43
2:L:11:MET:HE1	2:L:20:THR:O	2.18	0.43
2:L:55:HIS:CE1	2:L:56:ILE:HG22	2.53	0.43
1:N:89:LYS:HB2	1:N:418:TYR:CE2	2.54	0.43
1:N:235:GLY:O	1:N:258:LYS:HA	2.19	0.43
3:H:138:VAL:HG13	3:H:193:VAL:HG23	2.00	0.43
1:N:135:SER:O	1:N:156:ARG:HA	2.19	0.42
3:H:162:ASN:ND2	3:H:206:THR:H	2.17	0.42
1:N:81:ILE:N	1:N:126:PRO:HG2	2.34	0.42
1:N:321:VAL:HG21	1:N:390:PRO:HD3	2.00	0.42
1:N:188:THR:HG22	1:N:207:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:226:GLN:HG3	1:N:278:CYS:O	2.19	0.42
1:N:161:TRP:CH2	1:N:167:PRO:HB3	2.55	0.42
1:N:152:ARG:HH11	1:N:198:ASN:HD21	1.66	0.42
1:N:458:TRP:HA	1:N:459:PRO:HD2	1.80	0.42
3:H:43:LYS:HD2	3:H:43:LYS:HA	1.96	0.41
3:H:114:ALA:HB3	3:H:148:PHE:CE2	2.55	0.41
2:L:195:GLU:HG3	2:L:204:PRO:HB3	2.01	0.41
1:N:102:LYS:O	1:N:164:SER:HB3	2.20	0.41
2:L:29:VAL:HG21	2:L:90:GLN:HG2	2.03	0.41
2:L:32:ALA:HB1	2:L:91:HIS:ND1	2.36	0.41
1:N:94:ILE:HG12	1:N:359:ASN:HD21	1.86	0.41
1:N:277:GLU:HB3	1:N:350:LYS:HD2	2.03	0.41
2:L:108:ARG:HG2	2:L:109:ALA:H	1.86	0.41
3:H:140:LEU:HD23	3:H:140:LEU:N	2.36	0.41
3:H:142:CYS:HB2	3:H:157:TRP:CH2	2.56	0.41
3:H:171:VAL:HG22	3:H:191:VAL:HG23	2.03	0.41
3:H:66:ARG:HH11	3:H:66:ARG:HD2	1.70	0.41
1:N:168:THR:H	1:N:170:ASN:ND2	2.18	0.40
2:L:159:VAL:HG22	2:L:179:LEU:HD12	2.03	0.40
3:H:36:TRP:CZ3	3:H:92:CYS:HB3	2.55	0.40
3:H:140:LEU:HD21	3:H:193:VAL:HG22	2.03	0.40
2:L:39:LYS:HG3	2:L:40:PRO:HD2	2.02	0.40
2:L:86:TYR:O	2:L:101:GLY:HA2	2.21	0.40
1:N:152:ARG:HB2	1:N:178:TRP:CG	2.56	0.40
2:L:4:MET:HE3	2:L:23:CYS:SG	2.62	0.40
2:L:125:LEU:O	2:L:183:LYS:HD2	2.21	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%)	343 (89%)	40 (10%)	4 (1%)	12	24
2	L	212/214 (99%)	190 (90%)	14 (7%)	8 (4%)	2	3
3	H	219/221 (99%)	191 (87%)	16 (7%)	12 (6%)	1	1
All	All	818/824 (99%)	724 (88%)	70 (9%)	24 (3%)	3	5

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	222	ILE
2	L	157	ASN
2	L	171	SER
3	H	163	SER
3	H	226	ARG
2	L	60	ASP
3	H	62	GLU
3	H	102	TYR
1	N	226	GLN
2	L	204	PRO
3	H	14	PRO
3	H	41	PRO
3	H	43	LYS
3	H	180	SER
1	N	359	ASN
3	H	82(C)	LEU
3	H	130	ASP
3	H	225	PRO
2	L	40	PRO
2	L	119	PRO
2	L	187	GLU
3	H	129	GLY
2	L	68	GLY
1	N	349	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	N	342/342 (100%)	301 (88%)	41 (12%)	5	10
2	L	190/190 (100%)	152 (80%)	38 (20%)	1	2
3	H	187/187 (100%)	161 (86%)	26 (14%)	3	7
All	All	719/719 (100%)	614 (85%)	105 (15%)	3	6

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	81	ILE
1	N	87	LEU
1	N	89	LYS
1	N	99	ILE
1	N	118	ARG
1	N	120	PRO
1	N	127	ASP
1	N	134	LEU
1	N	136	GLN
1	N	141	ARG
1	N	149	ILE
1	N	154	GLN
1	N	162	PRO
1	N	168	THR
1	N	170	ASN
1	N	204	VAL
1	N	214	GLU
1	N	224	ARG
1	N	226	GLN
1	N	227	GLU
1	N	253	ARG
1	N	264	LYS
1	N	268	LEU
1	N	271	THR
1	N	276	GLU
1	N	283	GLU
1	N	284	ARG
1	N	287	ILE
1	N	323	THR
1	N	329	ASP
1	N	330	ASP
1	N	345	ASN
1	N	364	ARG
1	N	368	ILE

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Mol	Chain	Res	Type
1	N	384	THR
1	N	388	SER
1	N	399	LEU
1	N	445	SER
1	N	446	MET
1	N	463	LYS
1	N	464	ILE
2	L	5	THR
2	L	11	MET
2	L	13	THR
2	L	15	VAL
2	L	17	ASP
2	L	20	THR
2	L	33	VAL
2	L	39	LYS
2	L	46	LEU
2	L	48	ILE
2	L	53	THR
2	L	65	SER
2	L	76	SER
2	L	77	SER
2	L	78	VAL
2	L	79	GLN
2	L	83	LEU
2	L	91	HIS
2	L	103	LYS
2	L	116	SER
2	L	123	GLU
2	L	138	ASN
2	L	146	VAL
2	L	151	ASP
2	L	160	LEU
2	L	163	TRP
2	L	164	THR
2	L	175	MET
2	L	181	LEU
2	L	182	THR
2	L	190	ASN
2	L	191	SER
2	L	195	GLU
2	L	197	THR
2	L	200	THR

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Mol	Chain	Res	Type
2	L	204	PRO
2	L	206	VAL
2	L	207	LYS
3	H	10	GLU
3	H	14	PRO
3	H	28	THR
3	H	37	VAL
3	H	56	GLU
3	H	61	GLU
3	H	70	SER
3	H	71	LEU
3	H	72	GLU
3	H	79	ASN
3	H	87	LYS
3	H	105	GLN
3	H	119	PRO
3	H	126	PRO
3	H	133	THR
3	H	140	LEU
3	H	149	PRO
3	H	150	GLU
3	H	168	SER
3	H	187	LEU
3	H	190	SER
3	H	195	SER
3	H	202	SER
3	H	204	SER
3	H	218	LYS
3	H	224	GLU

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

Mol	Chain	Res	Type
1	N	95	ASN
1	N	136	GLN
1	N	144	HIS
1	N	154	GLN
1	N	170	ASN
1	N	198	ASN
1	N	208	ASN
1	N	226	GLN
1	N	315	GLN

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Mol	Chain	Res	Type
1	N	325	ASN
1	N	381	ASN
1	N	392	GLN
1	N	395	GLN
1	N	441	ASN
2	L	55	HIS
3	H	6	GLN
3	H	39	GLN
3	H	53	ASN
3	H	162	ASN
3	H	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,4	14,14,15	0.69	0	17,19,21	1.02	1 (5%)
4	NAG	A	2	4	14,14,15	1.04	0	17,19,21	1.77	2 (11%)
4	BMA	A	3	4	11,11,12	0.93	1 (9%)	15,15,17	1.06	2 (13%)
4	MAN	A	4	4	11,11,12	0.56	0	15,15,17	1.11	1 (6%)
4	MAN	A	5	4	11,11,12	1.17	2 (18%)	15,15,17	1.26	3 (20%)
4	MAN	A	6	4	11,11,12	1.14	0	15,15,17	1.55	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1	1,5	14,14,15	0.53	0	17,19,21	1.59	3 (17%)
5	NAG	B	2	5	14,14,15	0.96	1 (7%)	17,19,21	1.34	2 (11%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	NAG	C1-C2	2.36	1.55	1.52
4	A	5	MAN	O5-C5	2.25	1.47	1.43
4	A	3	BMA	O2-C2	-2.04	1.39	1.43
4	A	5	MAN	C2-C3	2.02	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	NAG	C1-O5-C5	5.87	120.05	112.19
5	B	1	NAG	C2-N2-C7	4.09	128.38	122.90
5	B	2	NAG	C4-C3-C2	-3.39	106.05	111.02
5	B	1	NAG	C6-C5-C4	2.81	119.92	113.02
4	A	6	MAN	C1-O5-C5	2.79	115.93	112.19
4	A	4	MAN	O2-C2-C1	-2.73	102.98	109.22
4	A	6	MAN	O5-C5-C6	2.71	112.94	107.66
5	B	2	NAG	O5-C1-C2	-2.45	107.50	111.29
4	A	5	MAN	C6-C5-C4	-2.45	107.01	113.02
4	A	2	NAG	C4-C3-C2	-2.45	107.43	111.02
4	A	5	MAN	C3-C4-C5	2.29	114.38	110.23
4	A	3	BMA	C1-O5-C5	2.22	115.16	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3	BMA	O5-C5-C4	-2.15	105.59	110.83
4	A	6	MAN	O5-C5-C4	-2.15	105.60	110.83
4	A	1	NAG	O5-C1-C2	-2.06	108.11	111.29
5	B	1	NAG	C1-C2-N2	2.06	113.67	110.43
4	A	5	MAN	O3-C3-C4	-2.05	105.55	110.38

There are no chirality outliers.

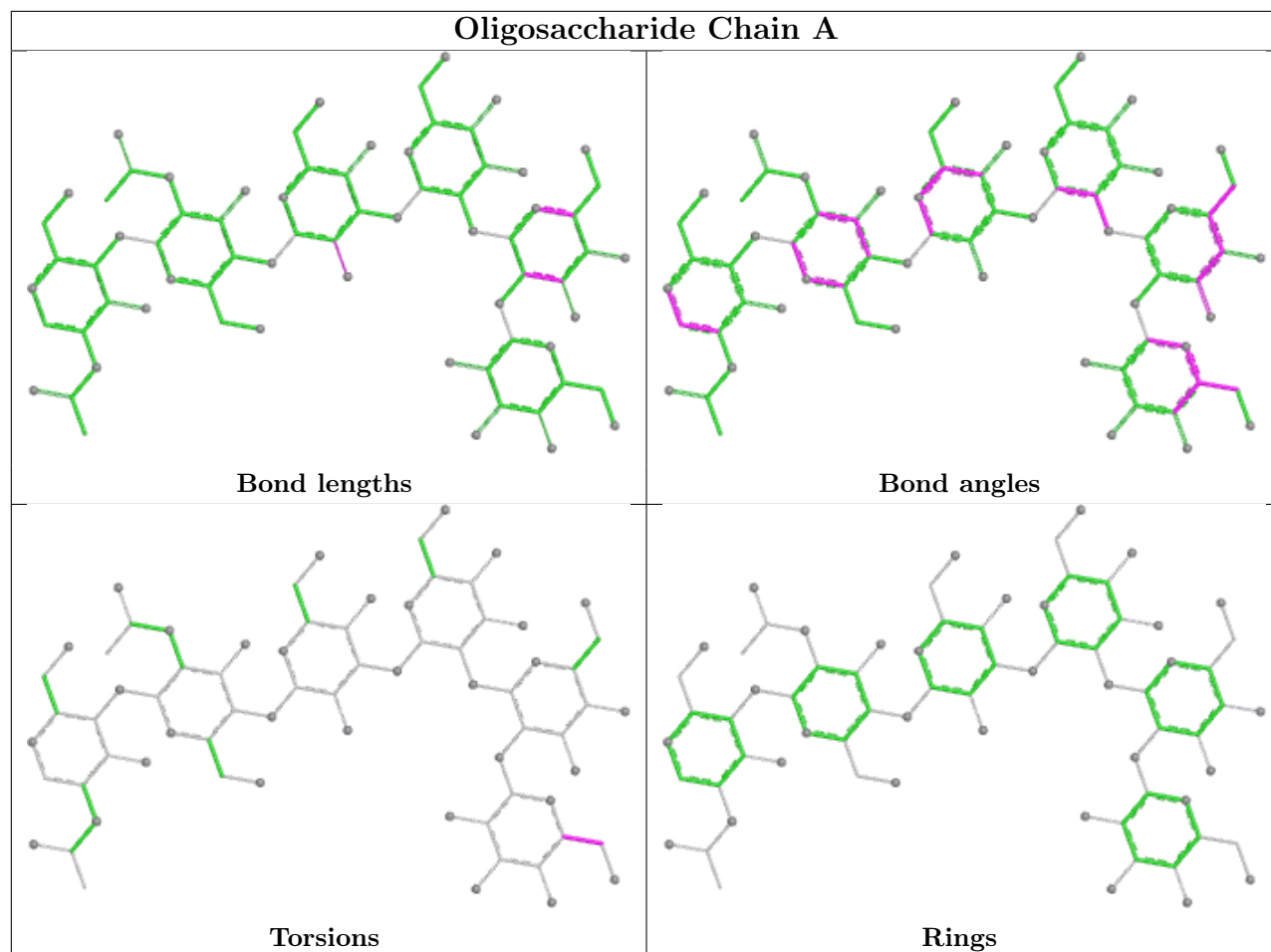
All (7) torsion outliers are listed below:

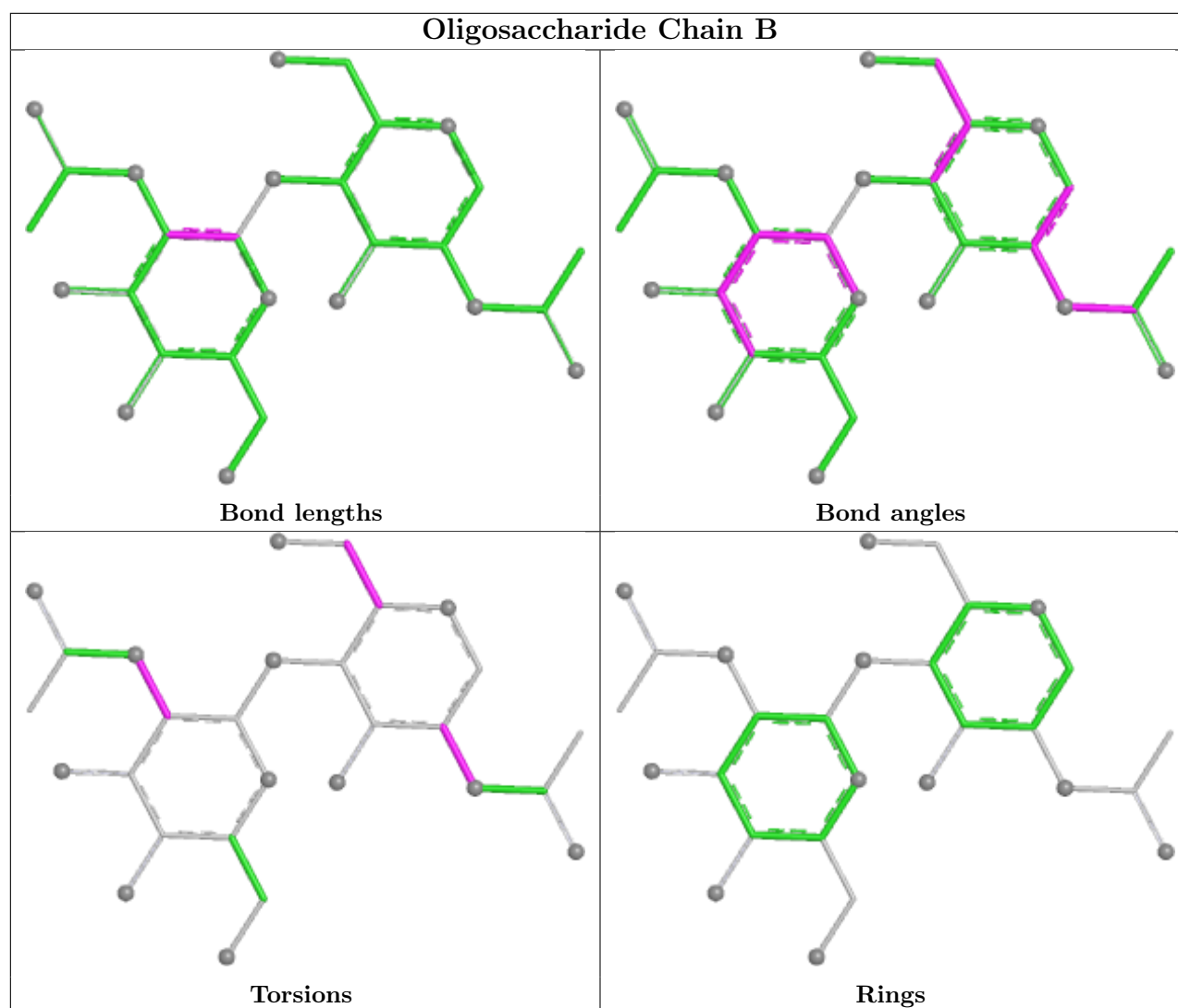
Mol	Chain	Res	Type	Atoms
4	A	6	MAN	O5-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
4	A	6	MAN	C4-C5-C6-O6
5	B	1	NAG	C4-C5-C6-O6
5	B	1	NAG	C1-C2-N2-C7
5	B	2	NAG	C1-C2-N2-C7
5	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

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	0.85	0	17,19,21	1.73	3 (17%)

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	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	475(A)	NAG	C1-O5-C5	4.46	118.16	112.19
6	N	475(A)	NAG	C4-C3-C2	-2.79	106.93	111.02
6	N	475(A)	NAG	C8-C7-N2	2.10	119.60	116.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	475(A)	NAG	O5-C5-C6-O6
6	N	475(A)	NAG	C4-C5-C6-O6

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%)	-0.64	4 (1%) 79 76	2, 8, 24, 48	0
2	L	214/214 (100%)	0.00	10 (4%) 36 32	5, 26, 42, 47	0
3	H	221/221 (100%)	0.28	19 (8%) 16 14	4, 26, 41, 46	0
All	All	824/824 (100%)	-0.22	33 (4%) 42 38	2, 18, 39, 48	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	128	CYS	16.0
2	L	212	ASN	11.2
3	H	180	SER	10.3
3	H	133	THR	10.1
2	L	214	CYS	9.3
3	H	130	ASP	9.1
3	H	227	GLY	9.1
3	H	42	GLY	8.7
3	H	43	LYS	8.0
3	H	134	THR	7.8
3	H	129	GLY	5.7
2	L	211	ARG	5.7
1	N	465	GLU	5.3
2	L	213	GLU	5.2
3	H	135	GLY	5.0
3	H	137	SER	4.4
3	H	85	GLU	4.4
3	H	183	ASP	4.1
3	H	203	GLN	4.0
3	H	136	SER	3.8
1	N	82	ARG	3.8
1	N	261	LYS	3.5
2	L	156	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
3	H	224	GLU	3.4
3	H	226	ARG	3.0
1	N	416	GLU	2.6
3	H	13	LYS	2.6
2	L	105	GLU	2.4
2	L	107	LYS	2.3
2	L	154	GLU	2.2
2	L	7	SER	2.1
3	H	115	LYS	2.1
2	L	188	ARG	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](#)

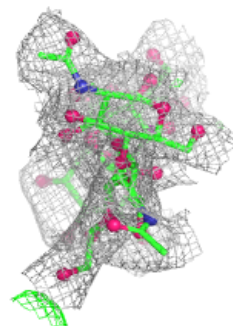
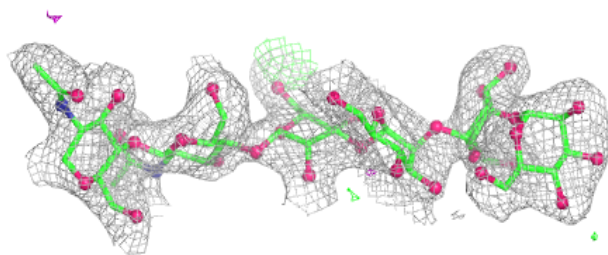
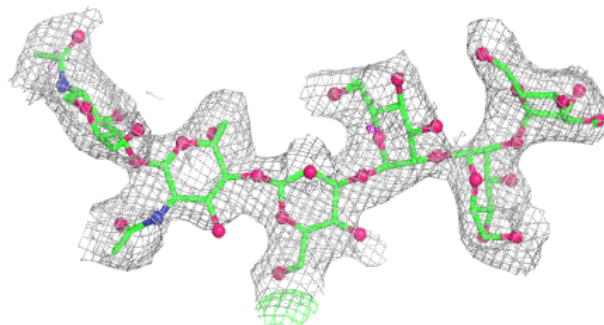
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

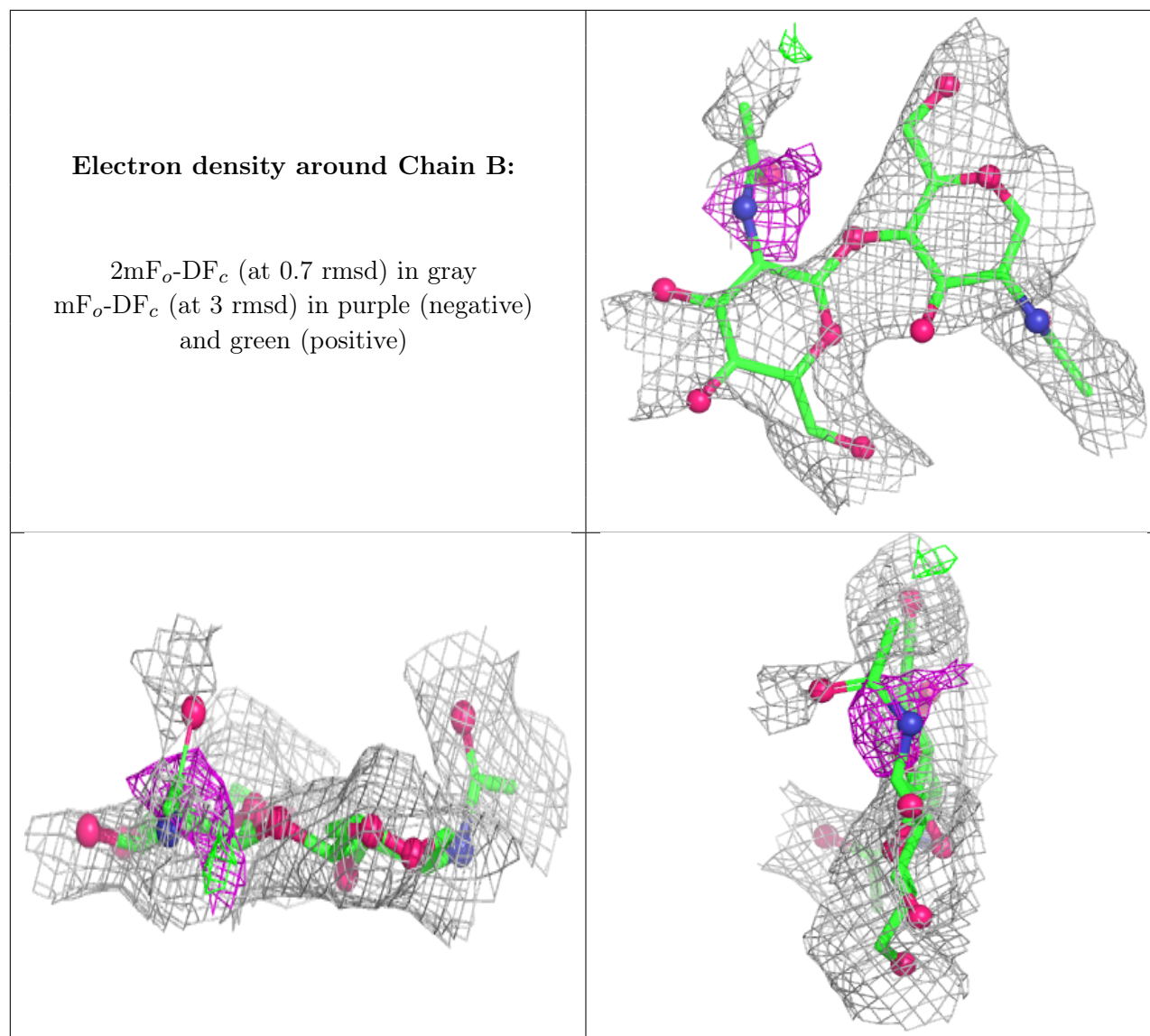
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1	14/15	-	-	6,11,22,24	0
4	NAG	A	2	14/15	-	-	12,14,17,18	0
4	BMA	A	3	11/12	-	-	8,12,14,15	0
4	MAN	A	4	11/12	-	-	8,11,14,18	0
4	MAN	A	5	11/12	-	-	15,17,19,20	0
4	MAN	A	6	11/12	-	-	11,13,15,16	0
5	NAG	B	1	14/15	-	-	42,47,53,56	0
5	NAG	B	2	14/15	-	-	55,57,60,61	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.

Electron density around Chain A:

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





6.4 Ligands [i](#)

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	0.89	0.11	37,40,45,45	0
7	CA	N	0	1/1	0.99	0.14	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.