



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 07:10 AM EDT

PDB ID : 1NCA
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 : 2.50 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

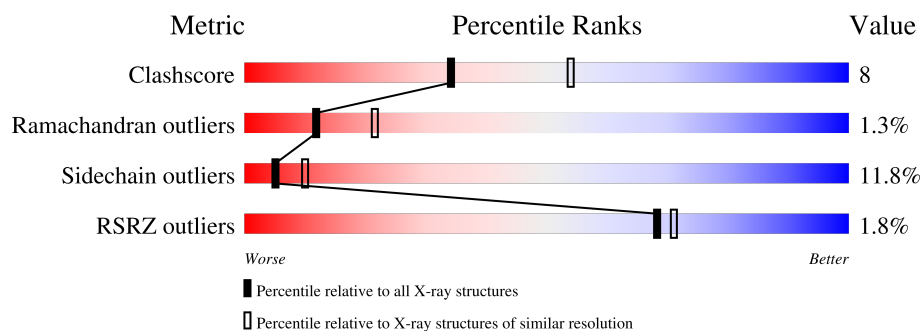
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	
2	L	214	
3	H	221	
4	A	6	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6577 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	539	593	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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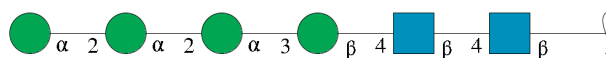
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Chain	Residue	Modelled	Actual	Comment	Reference
L	94	PRO	TYR	conflict	EMBL Y11589

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

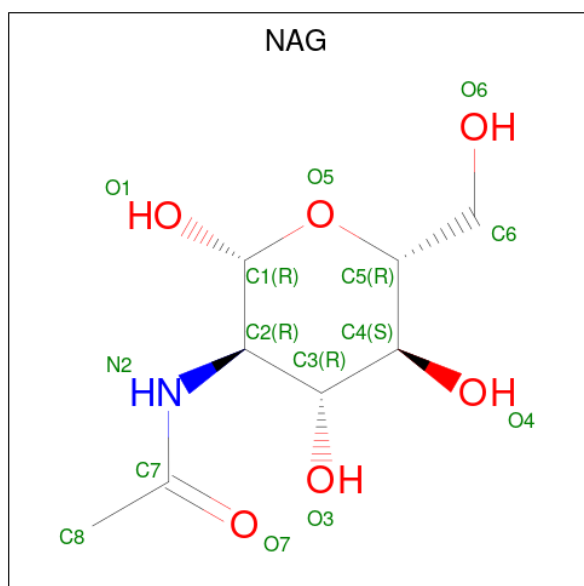
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1662	1048	273	334	7			

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

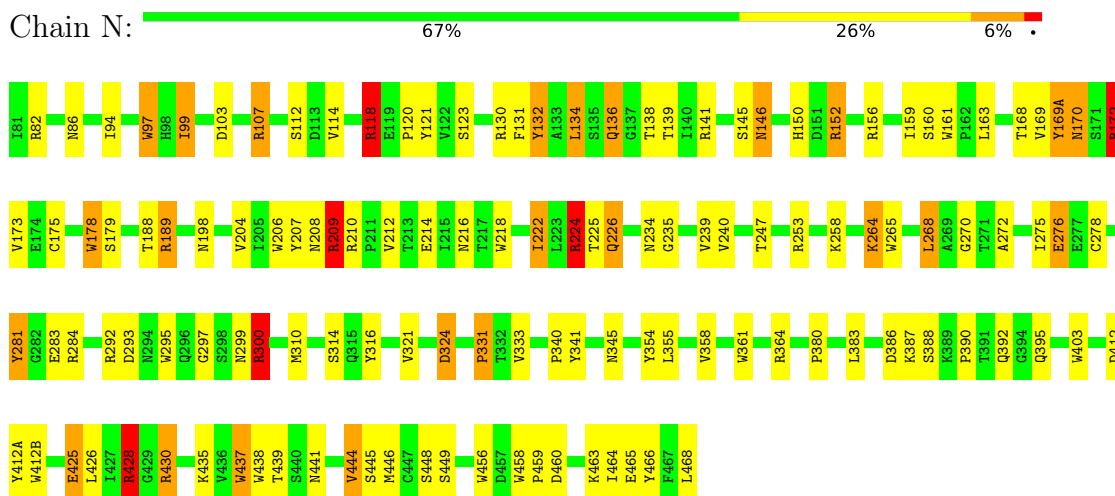
- Molecule 7 is water.

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

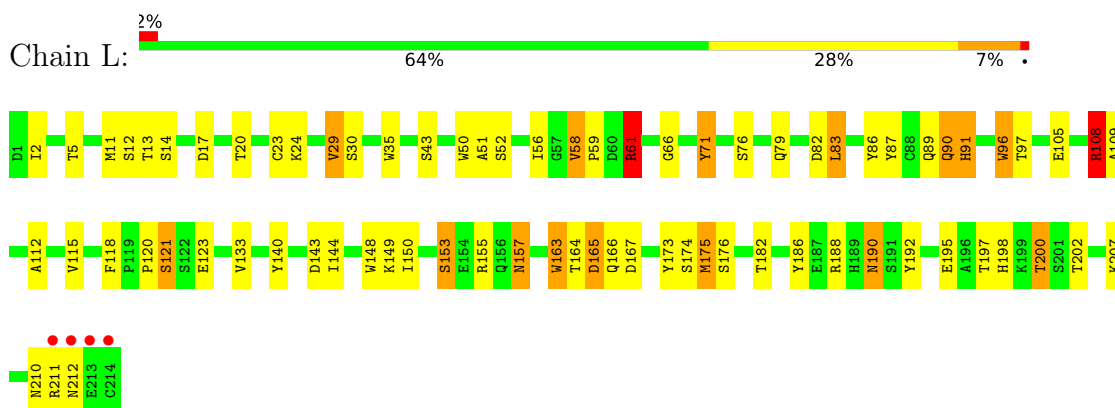
3 Residue-property plots

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.

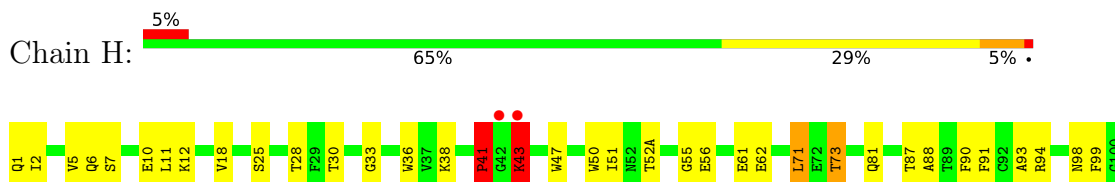
• Molecule 1: INFLUENZA A SUBTYPE N9 NEURAMINIDASE

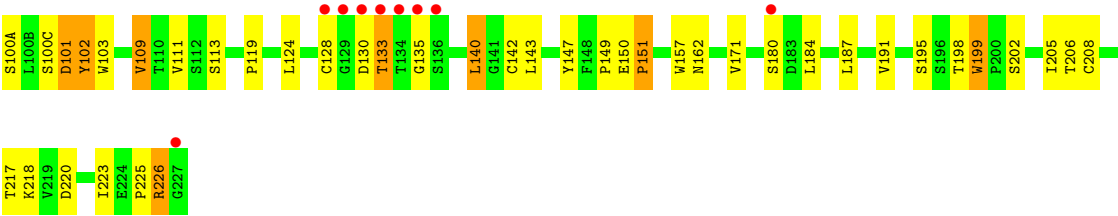


• Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)



• 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

Chain A: 100%

NAG1
NAG2
BR43
MAN4
MAN5
MAN6

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 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 50.2 (8.00-2.90)	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}	0.191 , (Not available) 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 28.9	EDS
L-test for twinning ¹	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6577	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 3.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG, CA

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	1.04	1/3158 (0.0%)	1.93	106/4301 (2.5%)
2	L	0.88	0/1708	1.81	36/2323 (1.5%)
3	H	0.89	0/1704	1.69	28/2323 (1.2%)
All	All	0.96	1/6570 (0.0%)	1.84	170/8947 (1.9%)

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	7
2	L	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	425	GLU	CD-OE2	-5.47	1.19	1.25

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	300	ARG	NE-CZ-NH2	-15.62	112.49	120.30
1	N	107	ARG	CD-NE-CZ	-14.89	102.75	123.60
1	N	118	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	N	300	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	N	430	ARG	NE-CZ-NH2	-12.63	113.99	120.30
2	L	188	ARG	NE-CZ-NH2	-12.27	114.16	120.30
1	N	428	ARG	NE-CZ-NH1	-11.62	114.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	188	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	N	107	ARG	CB-CG-CD	-10.38	84.62	111.60
2	L	163	TRP	CD1-CG-CD2	9.68	114.04	106.30
3	H	36	TRP	CD1-CG-CD2	9.64	114.01	106.30
2	L	148	TRP	CD1-CG-CD2	9.36	113.78	106.30
1	N	265	TRP	CD1-CG-CD2	9.32	113.76	106.30
1	N	172	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	N	169(A)	TYR	CB-CG-CD1	-9.01	115.59	121.00
1	N	438	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	N	438	TRP	CG-CD2-CE3	8.70	141.73	133.90
1	N	438	TRP	CB-CG-CD1	-8.55	115.88	127.00
1	N	161	TRP	CG-CD2-CE3	8.49	141.54	133.90
1	N	412(B)	TRP	CD1-CG-CD2	8.41	113.03	106.30
3	H	103	TRP	CD1-CG-CD2	8.39	113.02	106.30
1	N	428	ARG	CD-NE-CZ	-8.35	111.92	123.60
2	L	96	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	N	403	TRP	CD1-CG-CD2	8.29	112.93	106.30
3	H	157	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	N	218	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	N	412(A)	TYR	CB-CG-CD1	-8.17	116.10	121.00
1	N	284	ARG	CB-CG-CD	-8.14	90.44	111.60
1	N	438	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	N	264	LYS	CA-CB-CG	8.09	131.21	113.40
3	H	36	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	N	152	ARG	NE-CZ-NH2	-7.91	116.35	120.30
2	L	96	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	N	107	ARG	CG-CD-NE	7.88	128.34	111.80
1	N	412	ASP	CB-CG-OD1	7.88	125.39	118.30
2	L	163	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	N	361	TRP	CG-CD2-CE3	7.85	140.97	133.90
1	N	161	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	N	403	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	N	239	VAL	CG1-CB-CG2	-7.75	98.51	110.90
1	N	178	TRP	CE2-CD2-CG	-7.70	101.14	107.30
2	L	86	TYR	CB-CG-CD1	-7.66	116.41	121.00
1	N	130	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	N	403	TRP	CG-CD2-CE3	7.63	140.77	133.90
1	N	412(B)	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	N	361	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	N	361	TRP	CE2-CD2-CG	-7.48	101.31	107.30
2	L	87	TYR	CB-CG-CD1	-7.40	116.56	121.00
2	L	148	TRP	CE2-CD2-CG	-7.34	101.43	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	456	TRP	CD1-CG-CD2	7.29	112.13	106.30
2	L	61	ARG	CB-CG-CD	-7.28	92.67	111.60
3	H	50	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	N	178	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	N	97	TRP	CD1-CG-CD2	7.20	112.06	106.30
1	N	295	TRP	CD1-CG-CD2	7.16	112.02	106.30
2	L	50	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	N	428	ARG	CG-CD-NE	7.06	126.63	111.80
2	L	50	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	N	297	GLY	O-C-N	7.02	133.93	122.70
1	N	97	TRP	CE2-CD2-CG	-7.00	101.70	107.30
2	L	61	ARG	CD-NE-CZ	-6.99	113.81	123.60
3	H	199	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	N	297	GLY	CA-C-N	-6.96	101.89	117.20
2	L	210	ASN	CA-CB-CG	-6.94	98.12	113.40
1	N	300	ARG	CD-NE-CZ	-6.90	113.94	123.60
1	N	456	TRP	CE2-CD2-CG	-6.89	101.79	107.30
2	L	35	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	N	428	ARG	NE-CZ-NH2	6.88	123.74	120.30
2	L	83	LEU	CA-CB-CG	6.87	131.11	115.30
1	N	107	ARG	CA-CB-CG	6.87	128.51	113.40
1	N	161	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	N	265	TRP	CE2-CD2-CG	-6.83	101.84	107.30
3	H	103	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	N	218	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	N	361	TRP	CB-CG-CD1	-6.61	118.41	127.00
2	L	35	TRP	CE2-CD2-CG	-6.58	102.04	107.30
3	H	199	TRP	CD1-CG-CD2	6.57	111.56	106.30
3	H	50	TRP	CD1-CG-CD2	6.57	111.55	106.30
1	N	118	ARG	CD-NE-CZ	-6.56	114.41	123.60
1	N	437	TRP	CD1-CG-CD2	6.54	111.54	106.30
3	H	36	TRP	CG-CD2-CE3	6.54	139.78	133.90
3	H	157	TRP	CE2-CD2-CG	-6.53	102.07	107.30
2	L	11	MET	CA-CB-CG	-6.51	102.24	113.30
3	H	47	TRP	CE2-CD2-CG	-6.44	102.15	107.30
2	L	90	GLN	CA-CB-CG	6.38	127.43	113.40
2	L	173	TYR	CB-CG-CD2	-6.36	117.19	121.00
3	H	36	TRP	CG-CD1-NE1	-6.36	103.74	110.10
1	N	172	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	N	247	THR	N-CA-CB	-6.29	98.36	110.30
2	L	148	TRP	CG-CD1-NE1	-6.28	103.82	110.10
1	N	161	TRP	CB-CG-CD1	-6.20	118.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	83	LEU	CB-CG-CD1	-6.14	100.56	111.00
1	N	107	ARG	NH1-CZ-NH2	-6.07	112.73	119.40
1	N	456	TRP	O-C-N	6.06	132.40	122.70
3	H	47	TRP	CD1-CG-CD2	6.02	111.11	106.30
1	N	284	ARG	CA-CB-CG	6.00	126.59	113.40
1	N	430	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	N	206	TRP	CE2-CD2-CG	-5.92	102.56	107.30
1	N	160	SER	N-CA-CB	-5.91	101.63	110.50
2	L	188	ARG	CA-CB-CG	5.89	126.36	113.40
1	N	265	TRP	CG-CD1-NE1	-5.86	104.24	110.10
2	L	108	ARG	CG-CD-NE	-5.83	99.56	111.80
1	N	99	ILE	CB-CA-C	-5.79	100.01	111.60
1	N	121	TYR	CA-CB-CG	5.79	124.41	113.40
2	L	71	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	N	146	ASN	OD1-CG-ND2	-5.76	108.64	121.90
1	N	468	LEU	CA-C-O	-5.75	108.01	120.10
2	L	167	ASP	CB-CG-OD1	5.73	123.46	118.30
1	N	206	TRP	CD1-CG-CD2	5.71	110.87	106.30
1	N	97	TRP	CB-CG-CD1	-5.68	119.61	127.00
3	H	101	ASP	N-CA-C	-5.67	95.68	111.00
1	N	438	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	N	169(A)	TYR	CB-CG-CD2	5.67	124.40	121.00
1	N	224	ARG	CA-CB-CG	5.65	125.84	113.40
3	H	56	GLU	CB-CA-C	-5.63	99.14	110.40
2	L	82	ASP	CB-CG-OD1	5.62	123.36	118.30
1	N	295	TRP	CE2-CD2-CG	-5.58	102.84	107.30
3	H	36	TRP	CB-CG-CD1	-5.58	119.75	127.00
3	H	30	THR	CA-CB-CG2	5.57	120.19	112.40
1	N	150	HIS	O-C-N	5.55	131.59	122.70
1	N	281	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	N	150	HIS	CA-C-N	-5.54	105.01	117.20
1	N	209	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	N	412(B)	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	N	107	ARG	NE-CZ-NH2	5.49	123.05	120.30
2	L	29	VAL	CA-CB-CG2	-5.49	102.66	110.90
1	N	132	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	N	444	VAL	CA-C-N	5.47	129.24	117.20
3	H	55	GLY	CA-C-N	5.45	129.18	117.20
1	N	97	TRP	NE1-CE2-CZ2	-5.42	124.44	130.40
3	H	103	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	N	293	ASP	CA-C-N	-5.40	105.31	117.20
1	N	403	TRP	CG-CD1-NE1	-5.40	104.70	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	226	GLN	N-CA-C	5.39	125.56	111.00
1	N	103	ASP	N-CA-CB	-5.39	100.91	110.60
3	H	109	VAL	CA-CB-CG1	5.38	118.98	110.90
1	N	456	TRP	CG-CD2-CE3	5.37	138.74	133.90
3	H	30	THR	CA-CB-OG1	-5.36	97.74	109.00
1	N	403	TRP	CB-CG-CD1	-5.35	120.04	127.00
1	N	324	ASP	CB-CG-OD1	5.32	123.09	118.30
1	N	412(B)	TRP	CB-CG-CD1	-5.32	120.08	127.00
2	L	190	ASN	CA-C-N	5.32	128.91	117.20
1	N	136	GLN	CG-CD-NE2	5.29	129.38	116.70
1	N	466	TYR	CB-CG-CD2	-5.28	117.83	121.00
2	L	163	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	N	354	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	N	216	ASN	O-C-N	-5.25	114.30	122.70
1	N	437	TRP	CE2-CD2-CG	-5.19	103.15	107.30
1	N	268	LEU	CA-CB-CG	5.16	127.17	115.30
1	N	428	ARG	CB-CG-CD	-5.16	98.18	111.60
3	H	157	TRP	CG-CD1-NE1	-5.15	104.95	110.10
3	H	50	TRP	CG-CD2-CE3	5.14	138.53	133.90
3	H	133	THR	CA-CB-CG2	-5.13	105.22	112.40
3	H	43	LYS	N-CA-C	5.13	124.85	111.00
1	N	293	ASP	CA-C-O	5.13	130.86	120.10
1	N	118	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	N	218	TRP	CG-CD1-NE1	-5.12	104.98	110.10
3	H	73	THR	CA-C-N	-5.11	105.95	117.20
1	N	412(B)	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	N	146	ASN	CB-CG-ND2	5.09	128.93	116.70
2	L	24	LYS	CA-CB-CG	5.09	124.61	113.40
2	L	56	ILE	CA-C-N	-5.04	106.11	116.20
2	L	148	TRP	CB-CG-CD1	-5.04	120.44	127.00
3	H	199	TRP	CG-CD2-CE3	5.04	138.44	133.90
2	L	165	ASP	CB-CG-OD1	5.03	122.83	118.30
2	L	91	HIS	CA-CB-CG	5.03	122.15	113.60
1	N	210	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	N	439	THR	N-CA-C	-5.02	97.43	111.00
1	N	189	ARG	CA-C-N	-5.02	106.15	117.20
1	N	341	TYR	CB-CG-CD1	-5.01	117.99	121.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	108	ARG	Sidechain
2	L	140	TYR	Sidechain
2	L	61	ARG	Sidechain
1	N	107	ARG	Sidechain
1	N	118	ARG	Sidechain
1	N	172	ARG	Sidechain
1	N	209	ARG	Sidechain
1	N	224	ARG	Sidechain
1	N	300	ARG	Sidechain
1	N	428	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	N	3075	0	2903	51	0
2	L	1667	0	1598	23	0
3	H	1662	0	1611	28	0
4	A	72	0	61	0	0
5	N	28	0	26	0	0
6	N	1	0	0	0	0
7	H	4	0	0	0	0
7	L	2	0	0	0	0
7	N	66	0	0	2	0
All	All	6577	0	6199	100	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 8.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:150:GLU:HG2	3:H:151:PRO:HA	1.58	0.85
3:H:87:THR:HG22	3:H:111:VAL:H	1.44	0.83
3:H:11:LEU:HD22	3:H:149:PRO:HG3	1.61	0.80
1:N:146:ASN:OD1	1:N:437:TRP:HB3	1.83	0.77
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:140:LEU:HD12	3:H:223:ILE:HG21	1.76	0.67
2:L:61:ARG:HD2	2:L:76:SER:O	1.96	0.66
3:H:6:GLN:HE22	3:H:91:PHE:HA	1.62	0.65
1:N:276:GLU:HB3	1:N:292:ARG:HD3	1.79	0.65
3:H:41:PRO:HD3	3:H:88:ALA:HA	1.79	0.64
3:H:162:ASN:ND2	3:H:206:THR:H	1.96	0.64
1:N:97:TRP:H	1:N:395:GLN:HE22	1.49	0.59
3:H:199:TRP:CH2	3:H:225:PRO:HA	2.38	0.59
1:N:152:ARG:HD2	1:N:198:ASN:HD21	1.67	0.58
3:H:171:VAL:HG22	3:H:191:VAL:HG23	1.86	0.57
1:N:152:ARG:HB2	1:N:178:TRP:CG	2.40	0.57
1:N:118:ARG:HA	1:N:441:ASN:ND2	2.21	0.56
2:L:163:TRP:CZ2	2:L:175:MET:HE2	2.41	0.56
1:N:333:VAL:HG22	1:N:387:LYS:HE3	1.88	0.56
1:N:226:GLN:NE2	1:N:240:VAL:H	2.04	0.55
1:N:168:THR:HG22	1:N:169(A):TYR:H	1.71	0.55
2:L:164:THR:HG22	2:L:165:ASP:O	2.07	0.54
2:L:96:TRP:HZ2	3:H:99:PHE:HB3	1.72	0.54
1:N:299:ASN:HA	7:N:64:HOH:O	2.08	0.53
2:L:83:LEU:HD11	2:L:166:GLN:HB3	1.91	0.52
2:L:150:ILE:HD12	2:L:155:ARG:HH11	1.75	0.52
3:H:199:TRP:CZ2	3:H:225:PRO:HA	2.45	0.52
1:N:188:THR:HG21	1:N:208:ASN:HB2	1.92	0.52
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.91	0.51
2:L:144:ILE:HB	2:L:198:HIS:HD2	1.76	0.51
2:L:115:VAL:O	2:L:207:LYS:HE3	2.10	0.51
1:N:428:ARG:HD2	1:N:460:ASP:OD2	2.11	0.51
1:N:426:LEU:HD11	1:N:444:VAL:CG2	2.41	0.51
1:N:118:ARG:HD3	1:N:425:GLU:OE2	2.11	0.50
1:N:138:THR:HG21	1:N:145:SER:HA	1.93	0.50
3:H:11:LEU:HD22	3:H:149:PRO:CG	2.38	0.50
1:N:152:ARG:HD2	1:N:198:ASN:ND2	2.26	0.50
1:N:226:GLN:HG2	1:N:278:CYS:O	2.12	0.50
1:N:123:SER:HB3	1:N:132:TYR:CE1	2.47	0.49
1:N:430:ARG:HD2	1:N:437:TRP:HA	1.93	0.49
1:N:94:ILE:HG23	1:N:448:SER:HB3	1.94	0.49
2:L:149:LYS:HA	2:L:153:SER:O	2.12	0.49
1:N:168:THR:HB	1:N:170:ASN:ND2	2.27	0.49
1:N:173:VAL:O	1:N:209:ARG:NH2	2.45	0.49
2:L:12:SER:HA	2:L:105:GLU:O	2.12	0.49
1:N:333:VAL:HA	1:N:386:ASP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:121:SER:OG	2:L:123:GLU:HG2	2.13	0.48
3:H:2:ILE:HA	3:H:25:SER:O	2.13	0.48
2:L:155:ARG:HD2	2:L:155:ARG:HA	1.71	0.48
2:L:89:GLN:NE2	2:L:96:TRP:HB3	2.28	0.48
1:N:300:ARG:NH1	1:N:324:ASP:HA	2.28	0.48
3:H:199:TRP:CD1	3:H:205:ILE:HG12	2.49	0.48
3:H:10:GLU:OE2	3:H:12:LYS:NZ	2.46	0.48
1:N:281:TYR:HA	7:N:59:HOH:O	2.14	0.47
1:N:264:LYS:NZ	1:N:310:MET:O	2.47	0.47
1:N:134:LEU:HB3	1:N:156:ARG:NH1	2.29	0.47
1:N:355:LEU:HD13	1:N:383:LEU:HD13	1.97	0.47
3:H:18:VAL:O	3:H:81:GLN:HA	2.14	0.47
2:L:108:ARG:HD3	2:L:109:ALA:O	2.14	0.47
1:N:270:GLY:HA3	1:N:314:SER:H	1.80	0.46
3:H:119:PRO:HD2	3:H:217:THR:HG21	1.98	0.46
2:L:155:ARG:NE	2:L:157:ASN:OD1	2.47	0.46
1:N:97:TRP:N	1:N:395:GLN:HE22	2.13	0.46
3:H:93:ALA:HB1	3:H:100(C):SER:HB3	1.97	0.46
1:N:168:THR:HG22	1:N:169:VAL:N	2.31	0.46
1:N:316:TYR:CZ	1:N:340:PRO:HD3	2.50	0.45
1:N:159:ILE:HG22	1:N:173:VAL:HG22	1.98	0.45
1:N:463:LYS:C	1:N:465:GLU:H	2.19	0.45
1:N:207:TYR:HB3	1:N:212:VAL:HG21	1.99	0.45
2:L:2:ILE:O	2:L:97:THR:HG21	2.17	0.45
3:H:52(A):THR:HA	3:H:71:LEU:HD21	1.99	0.45
1:N:321:VAL:HG21	1:N:390:PRO:HD3	1.97	0.45
3:H:33:GLY:HA2	3:H:52(A):THR:HG23	1.99	0.45
2:L:58:VAL:HA	2:L:59:PRO:HD2	1.80	0.45
1:N:131:PHE:CE1	1:N:163:LEU:HD12	2.53	0.43
3:H:124:LEU:HD11	3:H:143:LEU:HB2	2.00	0.43
1:N:426:LEU:HD11	1:N:444:VAL:HG23	2.01	0.43
1:N:358:VAL:HA	1:N:380:PRO:HB3	2.01	0.43
2:L:91:HIS:HB2	3:H:100(A):SER:HB2	2.01	0.43
1:N:235:GLY:O	1:N:258:LYS: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:CD1	2.53	0.43
2:L:118:PHE:HB2	2:L:133:VAL:HB	2.01	0.43
3:H:2:ILE:HD12	3:H:102:TYR:CD2	2.53	0.43
1:N:463:LYS:C	1:N:465:GLU:N	2.72	0.43
2:L:186:TYR:HA	2:L:192:TYR:OH	2.20	0.42
1:N:458:TRP:HA	1:N:459:PRO:HD2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:LYS:O	3:H:111:VAL:HA	2.19	0.41
3:H:94:ARG:HD3	3:H:101:ASP:OD1	2.20	0.41
1:N:114:VAL:O	1:N:139:THR:HA	2.21	0.41
1:N:272:ALA:HA	1:N:316:TYR:CE1	2.56	0.41
1:N:355:LEU:HD22	1:N:383:LEU:HB2	2.02	0.41
2:L:175:MET:HG2	2:L:176:SER:N	2.36	0.41
1:N:168:THR:H	1:N:170:ASN:HD21	1.68	0.41
1:N:226:GLN:HE21	1:N:240:VAL:H	1.67	0.41
3:H:162:ASN:ND2	3:H:206:THR:N	2.66	0.41
1:N:222:ILE:O	1:N:224:ARG:HD2	2.21	0.40
1:N:86:ASN:OD1	1:N:234:ASN:HB2	2.22	0.40
3:H:38:LYS:HG3	3:H:90:PHE:CE1	2.57	0.40
1:N:179:SER:OG	1:N:225:THR:HG22	2.22	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%)	362 (94%)	23 (6%)	2 (0%)	29	48
2	L	212/214 (99%)	197 (93%)	14 (7%)	1 (0%)	29	48
3	H	219/221 (99%)	195 (89%)	16 (7%)	8 (4%)	3	4
All	All	818/824 (99%)	754 (92%)	53 (6%)	11 (1%)	12	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	43	LYS
3	H	102	TYR
3	H	226	ARG
3	H	41	PRO

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Mol	Chain	Res	Type
3	H	128	CYS
3	H	130	ASP
3	H	180	SER
1	N	222	ILE
1	N	331	PRO
2	L	51	ALA
3	H	135	GLY

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%)	313 (92%)	29 (8%)	10	21
2	L	190/190 (100%)	161 (85%)	29 (15%)	2	5
3	H	187/187 (100%)	160 (86%)	27 (14%)	3	6
All	All	719/719 (100%)	634 (88%)	85 (12%)	5	10

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	82	ARG
1	N	99	ILE
1	N	112	SER
1	N	118	ARG
1	N	120	PRO
1	N	134	LEU
1	N	136	GLN
1	N	141	ARG
1	N	170	ASN
1	N	172	ARG
1	N	175	CYS
1	N	189	ARG
1	N	204	VAL
1	N	214	GLU
1	N	224	ARG

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Mol	Chain	Res	Type
1	N	253	ARG
1	N	268	LEU
1	N	275	ILE
1	N	276	GLU
1	N	283	GLU
1	N	331	PRO
1	N	345	ASN
1	N	364	ARG
1	N	388	SER
1	N	392	GLN
1	N	435	LYS
1	N	445	SER
1	N	446	MET
1	N	449	SER
2	L	5	THR
2	L	13	THR
2	L	14	SER
2	L	17	ASP
2	L	20	THR
2	L	23	CYS
2	L	29	VAL
2	L	30	SER
2	L	43	SER
2	L	52	SER
2	L	58	VAL
2	L	79	GLN
2	L	90	GLN
2	L	108	ARG
2	L	120	PRO
2	L	121	SER
2	L	143	ASP
2	L	153	SER
2	L	157	ASN
2	L	174	SER
2	L	175	MET
2	L	182	THR
2	L	190	ASN
2	L	195	GLU
2	L	197	THR
2	L	200	THR
2	L	202	THR
2	L	211	ARG

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Mol	Chain	Res	Type
2	L	212	ASN
3	H	1	GLN
3	H	5	VAL
3	H	7	SER
3	H	28	THR
3	H	41	PRO
3	H	43	LYS
3	H	51	ILE
3	H	61	GLU
3	H	62	GLU
3	H	71	LEU
3	H	73	THR
3	H	98	ASN
3	H	109	VAL
3	H	113	SER
3	H	133	THR
3	H	140	LEU
3	H	142	CYS
3	H	151	PRO
3	H	184	LEU
3	H	187	LEU
3	H	195	SER
3	H	198	THR
3	H	202	SER
3	H	208	CYS
3	H	218	LYS
3	H	220	ASP
3	H	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	136	GLN
1	N	144	HIS
1	N	170	ASN
1	N	198	ASN
1	N	226	GLN
1	N	345	ASN
1	N	381	ASN
1	N	395	GLN
1	N	441	ASN
1	N	455	GLN

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Mol	Chain	Res	Type
2	L	138	ASN
3	H	6	GLN
3	H	53	ASN
3	H	79	ASN
3	H	98	ASN
3	H	162	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 ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1	4,1	14,14,15	0.57	0	17,19,21	1.17	1 (5%)
4	NAG	A	2	4	14,14,15	1.10	1 (7%)	17,19,21	1.32	1 (5%)
4	BMA	A	3	4	11,11,12	1.08	1 (9%)	15,15,17	1.30	2 (13%)
4	MAN	A	4	4	11,11,12	0.34	0	15,15,17	1.17	1 (6%)
4	MAN	A	5	4	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
4	MAN	A	6	4	11,11,12	0.83	0	15,15,17	1.67	1 (6%)

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	-	0/6/23/26	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
4	MAN	A	6	4	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	NAG	C4-C3	2.47	1.58	1.52
4	A	3	BMA	C6-C5	2.02	1.58	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6	MAN	C1-O5-C5	5.93	120.23	112.19
4	A	2	NAG	C4-C3-C2	-3.17	106.37	111.02
4	A	3	BMA	C6-C5-C4	3.12	120.31	113.00
4	A	4	MAN	O2-C2-C1	-2.38	104.29	109.15
4	A	3	BMA	O5-C5-C4	-2.30	105.23	110.83
4	A	5	MAN	C6-C5-C4	-2.23	107.77	113.00
4	A	1	NAG	C1-C2-N2	-2.05	106.98	110.49
4	A	5	MAN	O5-C1-C2	2.04	113.93	110.77

There are no chirality outliers.

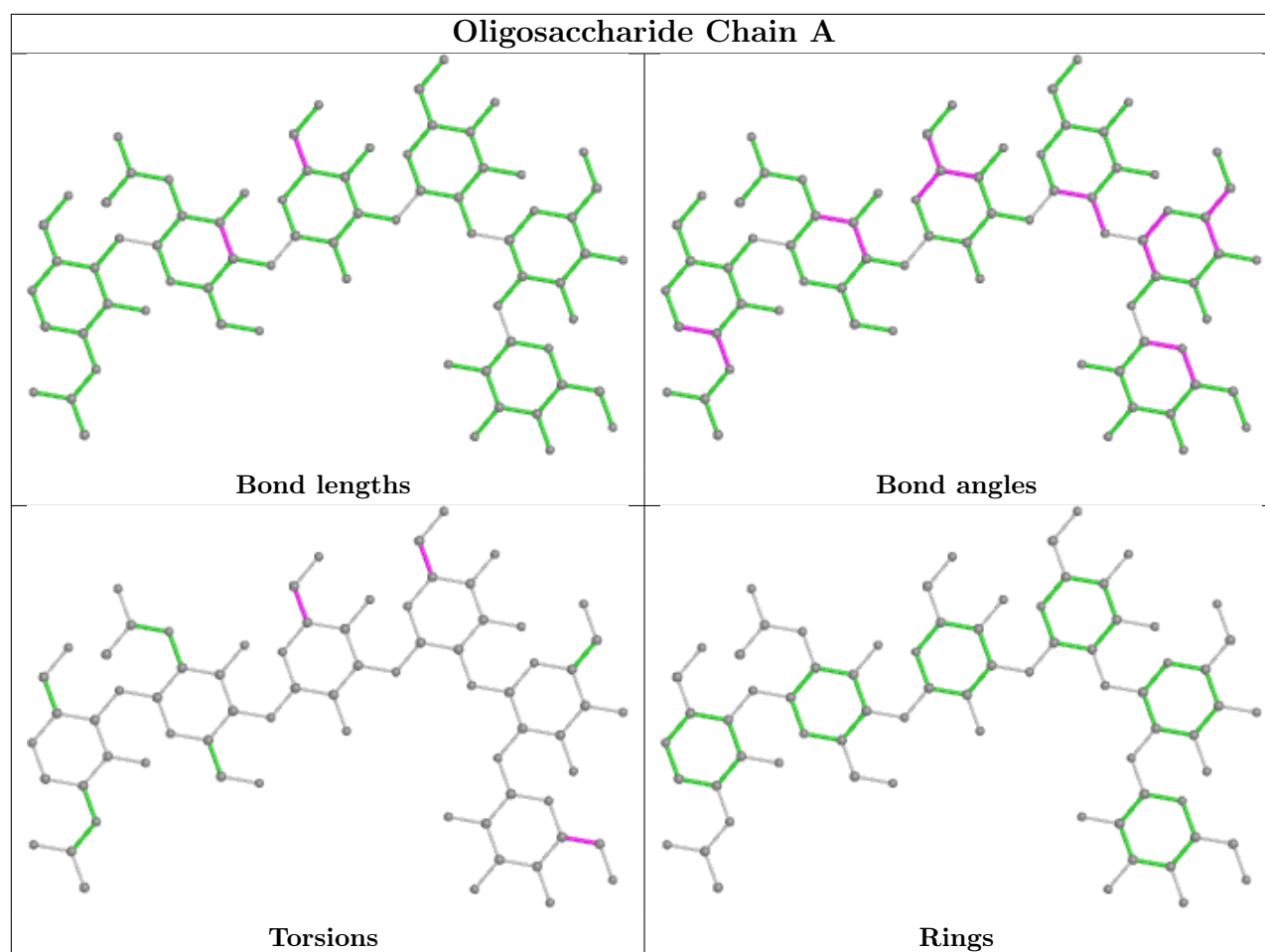
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3	BMA	C4-C5-C6-O6
4	A	6	MAN	O5-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	6	MAN	C4-C5-C6-O6
4	A	4	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
5	NAG	N	475(A)	1	14,14,15	0.97	0	17,19,21	1.38	2 (11%)
5	NAG	N	476(A)	1	14,14,15	1.15	1 (7%)	17,19,21	1.91	5 (29%)

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
5	NAG	N	475(A)	1	-	1/6/23/26	0/1/1/1
5	NAG	N	476(A)	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	476(A)	NAG	C1-C2	3.42	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	476(A)	NAG	C4-C3-C2	-5.35	103.18	111.02
5	N	475(A)	NAG	C1-O5-C5	3.81	117.35	112.19
5	N	476(A)	NAG	C8-C7-N2	3.10	121.34	116.10
5	N	476(A)	NAG	O3-C3-C4	2.67	116.52	110.35
5	N	476(A)	NAG	C6-C5-C4	2.45	118.75	113.00
5	N	475(A)	NAG	C1-C2-N2	2.40	114.59	110.49
5	N	476(A)	NAG	O7-C7-C8	-2.12	118.12	122.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	476(A)	NAG	O5-C5-C6-O6
5	N	475(A)	NAG	O5-C5-C6-O6
5	N	476(A)	NAG	C1-C2-N2-C7
5	N	476(A)	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	N	389/389 (100%)	-0.83	0 100 100	2, 8, 23, 48	5 (1%)
2	L	214/214 (100%)	-0.10	4 (1%) 66 69	4, 27, 44, 48	11 (5%)
3	H	221/221 (100%)	0.00	11 (4%) 28 30	5, 28, 41, 45	22 (9%)
All	All	824/824 (100%)	-0.42	15 (1%) 68 71	2, 18, 40, 48	38 (4%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	214	CYS	14.9
3	H	129	GLY	11.2
2	L	212	ASN	10.2
2	L	213	GLU	7.9
3	H	133	THR	7.9
3	H	134	THR	7.8
3	H	128	CYS	6.1
3	H	130	ASP	6.0
3	H	135	GLY	5.5
3	H	136	SER	5.5
3	H	43	LYS	4.2
3	H	180	SER	4.2
3	H	42	GLY	4.1
2	L	211	ARG	3.8
3	H	227	GLY	3.7

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

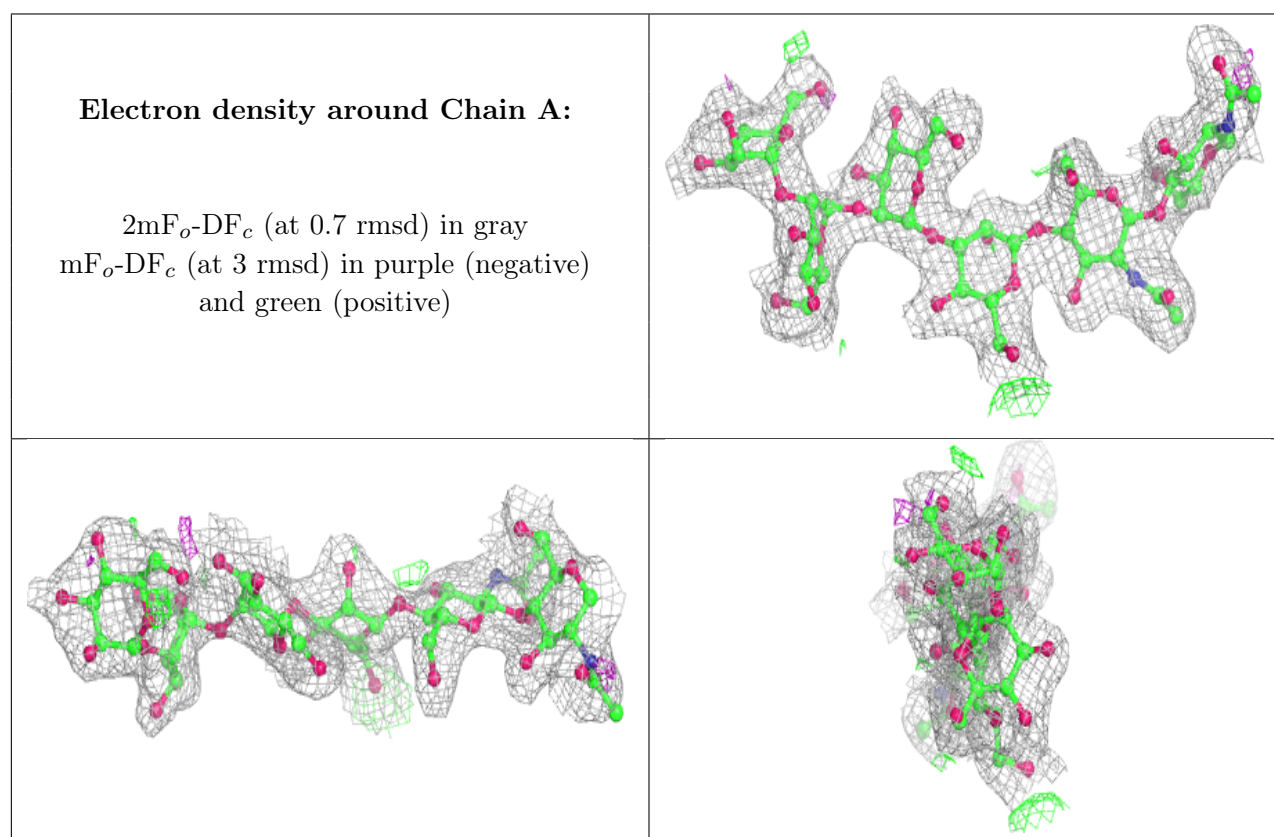
There are no non-standard protein/DNA/RNA residues in this entry.

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	MAN	A	5	11/12	0.94	0.13	11,15,19,19	0
4	MAN	A	4	11/12	0.95	0.13	9,12,14,18	0
4	NAG	A	1	14/15	0.95	0.14	8,13,22,22	0
4	NAG	A	2	14/15	0.96	0.12	12,14,18,24	0
4	BMA	A	3	11/12	0.96	0.10	6,10,12,12	0
4	MAN	A	6	11/12	0.96	0.12	11,14,15,16	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(\AA^2)	Q<0.9
5	NAG	N	476(A)	14/15	0.84	0.24	40,44,54,57	0
5	NAG	N	475(A)	14/15	0.92	0.18	38,41,43,43	0
6	CA	N	1	1/1	0.94	0.15	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.