



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:20 PM UTC

PDB ID : 1NCC / pdb_00001ncc
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.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

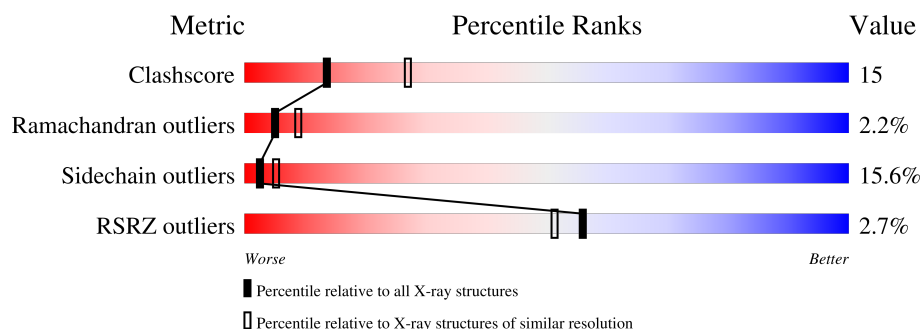
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	 2% 42% 41% 14%
2	L	214	 2% 45% 35% 18%
3	H	221	 5% 46% 41% 11%
4	A	6	 67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6508 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
			3078	1920	542	593	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	368	ARG	ILE	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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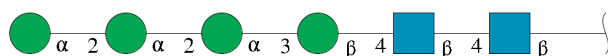
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Chain	Residue	Modelled	Actual	Comment	Reference
L	85	LEU	GLU	conflict	EMBL Y11589
L	87	TYR	PHE	conflict	EMBL Y11589
L	91	HIS	TYR	conflict	EMBL Y11589
L	92	TYR	ASN	conflict	EMBL Y11589
L	93	SER	ARG	conflict	EMBL Y11589
L	94	PRO	TYR	conflict	EMBL Y11589

- 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
			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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

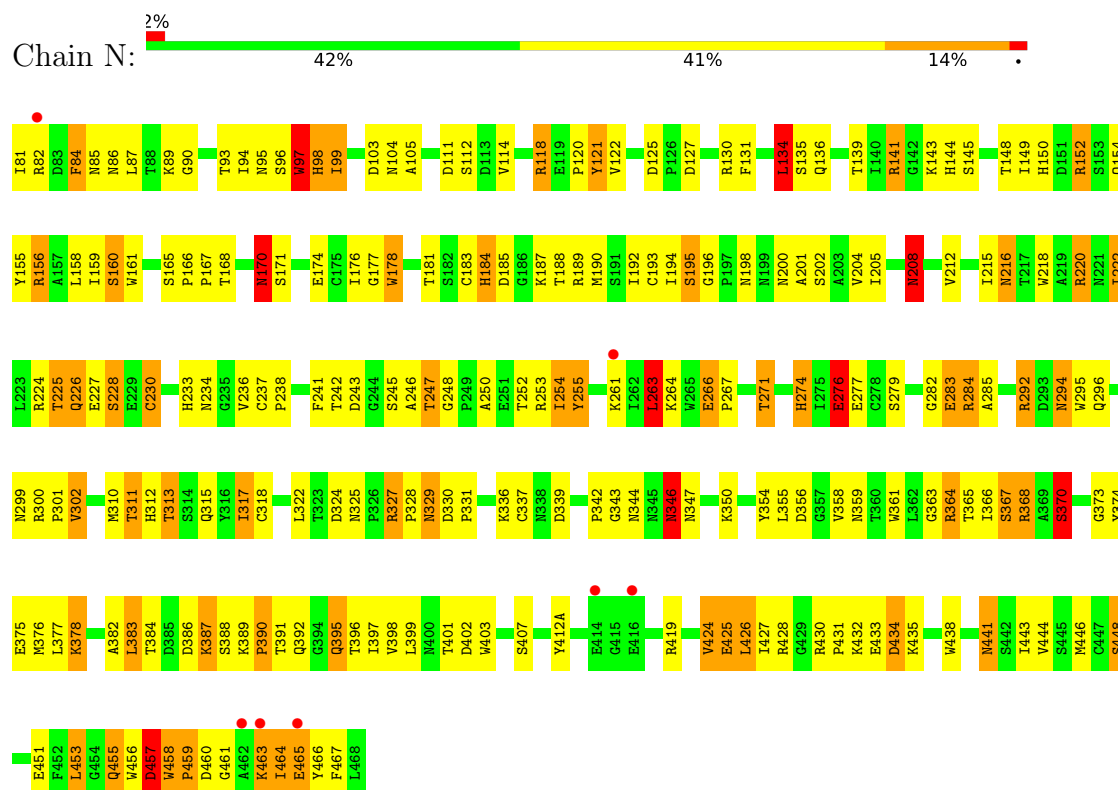
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

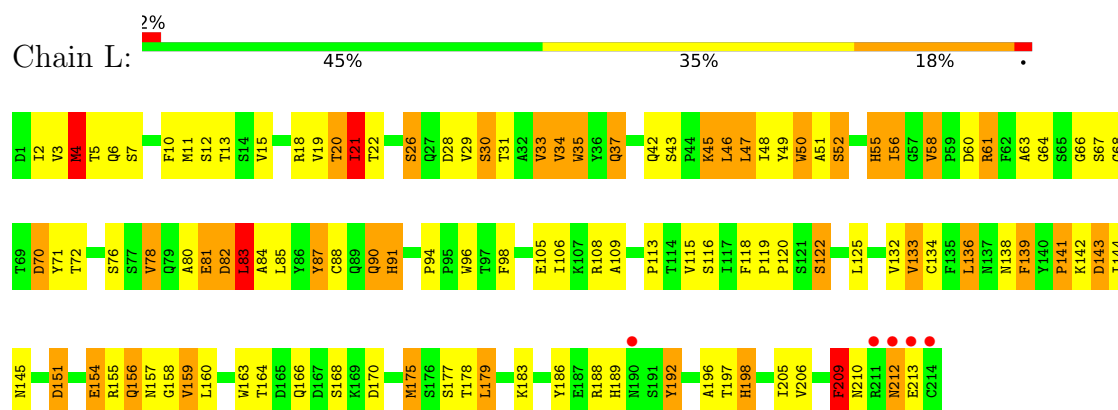
3 Residue-property plots

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.

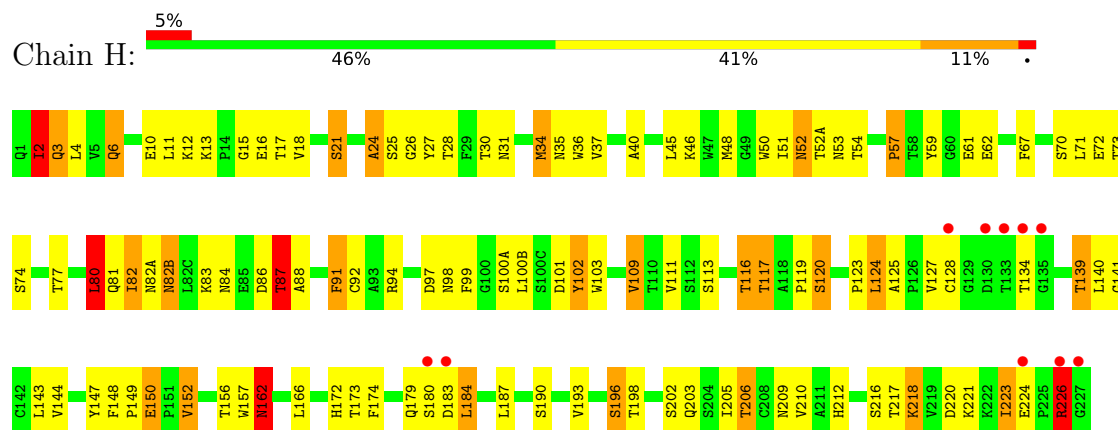
• Molecule 1: INFLUENZA A SUBTYPE N9 NEURAMINIDASE



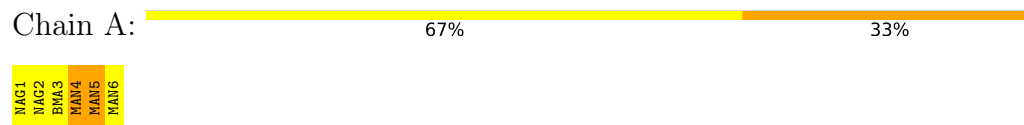
• Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)



● 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



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) 48.0 (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}	0.212 , (Not available) 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 56.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6508	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: BMA, MAN, 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	1.40	24/3161 (0.8%)	2.36	181/4304 (4.2%)
2	L	1.24	9/1708 (0.5%)	2.20	71/2323 (3.1%)
3	H	1.23	6/1704 (0.4%)	2.24	79/2323 (3.4%)
All	All	1.32	39/6573 (0.6%)	2.29	331/8950 (3.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	6
2	L	0	3
All	All	0	9

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	98	HIS	CD2-NE2	-8.55	1.28	1.37
1	N	184	HIS	CD2-NE2	-7.44	1.29	1.37
3	H	212	HIS	CD2-NE2	-7.24	1.29	1.37
1	N	233	HIS	CD2-NE2	-7.13	1.30	1.37
1	N	312	HIS	CD2-NE2	-7.09	1.30	1.37
1	N	150	HIS	CD2-NE2	-6.83	1.30	1.37
2	L	189	HIS	CD2-NE2	-6.81	1.30	1.37
1	N	274	HIS	CD2-NE2	-6.44	1.30	1.37
1	N	184	HIS	CG-ND1	-6.44	1.31	1.38
2	L	91	HIS	CD2-NE2	-6.39	1.30	1.37
2	L	198	HIS	CD2-NE2	-6.39	1.30	1.37
3	H	109	VAL	CA-CB	6.35	1.62	1.54
1	N	233	HIS	CG-ND1	-6.24	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	456	TRP	NE1-CE2	-6.09	1.30	1.37
1	N	97	TRP	CG-CD2	-6.00	1.32	1.43
1	N	144	HIS	CD2-NE2	-6.00	1.31	1.37
2	L	58	VAL	CA-CB	5.93	1.61	1.54
1	N	466	TYR	C-N	-5.89	1.25	1.33
2	L	34	VAL	CA-CB	-5.88	1.46	1.54
2	L	198	HIS	CG-ND1	-5.78	1.31	1.38
1	N	181	THR	CA-CB	5.77	1.63	1.53
1	N	166	PRO	CA-CB	-5.69	1.49	1.54
1	N	327	ARG	CA-CB	-5.63	1.46	1.54
1	N	274	HIS	CG-ND1	-5.47	1.32	1.38
1	N	327	ARG	CZ-NH2	5.46	1.40	1.33
1	N	98	HIS	CG-ND1	-5.43	1.32	1.38
1	N	364	ARG	NE-CZ	5.34	1.39	1.33
3	H	223	ILE	CA-CB	5.30	1.60	1.53
1	N	324	ASP	CA-CB	5.28	1.61	1.53
3	H	172	HIS	CD2-NE2	-5.28	1.32	1.37
2	L	55	HIS	CD2-NE2	-5.27	1.32	1.37
2	L	18	ARG	NE-CZ	5.26	1.38	1.33
3	H	50	TRP	NE1-CE2	-5.26	1.31	1.37
1	N	312	HIS	CG-ND1	-5.25	1.32	1.38
2	L	91	HIS	CG-ND1	-5.24	1.32	1.38
1	N	284	ARG	CZ-NH2	5.18	1.40	1.33
3	H	82	ILE	CA-CB	-5.16	1.47	1.54
1	N	120	PRO	CA-CB	-5.15	1.47	1.53
1	N	276	GLU	N-CA	-5.00	1.39	1.46

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	189	HIS	CA-CB-CG	-15.29	98.51	113.80
1	N	226	GLN	N-CA-C	13.68	129.26	111.75
1	N	104	ASN	OD1-CG-ND2	-13.64	108.95	122.60
3	H	98	ASN	OD1-CG-ND2	-12.13	110.47	122.60
1	N	284	ARG	CD-NE-CZ	-12.03	107.56	124.40
1	N	127	ASP	CA-CB-CG	-11.82	100.78	112.60
3	H	101	ASP	CA-CB-CG	11.82	124.42	112.60
1	N	111	ASP	O-C-N	-10.99	110.28	121.93
3	H	86	ASP	CA-CB-CG	10.88	123.48	112.60
1	N	198	ASN	OD1-CG-ND2	-10.60	112.00	122.60
1	N	312	HIS	N-CA-C	10.41	125.21	108.76
1	N	198	ASN	CB-CG-ND2	10.18	131.67	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	455	GLN	OE1-CD-NE2	-10.07	112.53	122.60
1	N	337	CYS	N-CA-C	9.97	123.39	111.82
3	H	220	ASP	CA-CB-CG	9.59	122.19	112.60
2	L	98	PHE	CA-CB-CG	9.42	123.22	113.80
1	N	104	ASN	CB-CG-ND2	9.41	130.51	116.40
2	L	210	ASN	CA-CB-CG	-9.39	103.21	112.60
2	L	20	THR	N-CA-CB	-9.24	94.58	111.13
3	H	98	ASN	CB-CG-ND2	9.06	129.99	116.40
1	N	178	TRP	N-CA-C	9.02	124.02	112.92
3	H	174	PHE	CA-CB-CG	-9.02	104.78	113.80
1	N	226	GLN	OE1-CD-NE2	-8.98	113.62	122.60
1	N	367	SER	CA-C-N	8.89	132.92	120.29
1	N	367	SER	C-N-CA	8.89	132.92	120.29
1	N	457	ASP	O-C-N	-8.87	111.99	123.16
1	N	312	HIS	CB-CG-CD2	-8.80	119.75	131.20
2	L	26	SER	N-CA-C	8.59	120.26	111.07
1	N	253	ARG	N-CA-CB	-8.55	96.49	110.59
3	H	30	THR	CA-CB-OG1	-8.43	96.96	109.60
1	N	266	GLU	CA-C-N	8.28	128.22	120.03
1	N	266	GLU	C-N-CA	8.28	128.22	120.03
3	H	82(A)	ASN	OD1-CG-ND2	-8.23	114.37	122.60
3	H	203	GLN	OE1-CD-NE2	-8.18	114.42	122.60
3	H	24	ALA	N-CA-C	8.18	121.72	108.63
1	N	85	ASN	CA-CB-CG	8.12	120.72	112.60
3	H	30	THR	N-CA-CB	-8.06	97.78	110.28
1	N	184	HIS	CA-C-O	-8.05	111.66	120.43
3	H	109	VAL	CA-C-O	8.00	129.83	120.72
2	L	118	PHE	CA-C-N	7.96	125.39	119.66
2	L	118	PHE	C-N-CA	7.96	125.39	119.66
2	L	143	ASP	CA-CB-CG	7.95	120.55	112.60
1	N	271	THR	N-CA-C	7.95	122.80	113.18
1	N	99	ILE	CB-CA-C	-7.85	100.94	111.15
1	N	97	TRP	CE2-CD2-CE3	7.81	126.61	118.80
1	N	103	ASP	CA-CB-CG	7.81	120.41	112.60
1	N	456	TRP	CG-CD2-CE3	7.77	141.67	133.90
1	N	344	ASN	CA-CB-CG	-7.77	104.83	112.60
1	N	216	ASN	OD1-CG-ND2	-7.77	114.83	122.60
3	H	97	ASP	CA-CB-CG	7.77	120.37	112.60
3	H	36	TRP	CG-CD2-CE3	7.75	141.65	133.90
1	N	98	HIS	CB-CG-CD2	-7.73	121.15	131.20
1	N	185	ASP	CA-CB-CG	7.72	120.33	112.60
1	N	277	GLU	N-CA-C	7.72	121.90	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	34	MET	CG-SD-CE	-7.72	83.92	100.90
2	L	70	ASP	N-CA-C	7.66	120.89	108.41
1	N	311	THR	CA-CB-OG1	-7.62	98.16	109.60
1	N	324	ASP	CA-CB-CG	7.55	120.16	112.60
3	H	72	GLU	N-CA-C	-7.53	97.93	108.54
1	N	253	ARG	CA-CB-CG	7.48	129.06	114.10
1	N	99	ILE	N-CA-CB	7.46	118.66	110.53
2	L	20	THR	CA-CB-OG1	-7.44	98.45	109.60
1	N	253	ARG	CB-CA-C	7.40	121.05	110.24
2	L	138	ASN	CA-CB-CG	-7.40	105.20	112.60
2	L	96	TRP	CB-CG-CD1	-7.40	115.81	126.90
1	N	226	GLN	CG-CD-NE2	7.30	127.35	116.40
1	N	327	ARG	N-CA-CB	-7.29	98.06	111.19
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
1	N	277	GLU	N-CA-CB	-7.20	100.28	111.65
2	L	151	ASP	CA-CB-CG	-7.20	105.40	112.60
2	L	82	ASP	CA-CB-CG	7.20	119.80	112.60
1	N	196	GLY	CA-C-N	7.20	127.62	119.92
1	N	196	GLY	C-N-CA	7.20	127.62	119.92
3	H	139	THR	CA-CB-OG1	-7.19	98.82	109.60
1	N	86	ASN	CA-CB-CG	-7.18	105.42	112.60
1	N	143	LYS	N-CA-C	7.14	121.62	112.34
1	N	95	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	N	236	VAL	N-CA-C	7.06	118.04	107.80
3	H	53	ASN	N-CA-C	-7.06	102.66	112.12
1	N	234	ASN	CA-CB-CG	7.00	119.60	112.60
3	H	94	ARG	N-CA-C	-6.93	97.61	108.90
2	L	96	TRP	CG-CD2-CE3	6.92	140.82	133.90
2	L	136	LEU	N-CA-C	-6.88	97.19	108.41
2	L	22	THR	N-CA-C	6.85	119.65	109.59
1	N	389	LYS	O-C-N	-6.80	116.25	121.55
1	N	208	ASN	CA-C-O	6.79	129.48	121.40
2	L	164	THR	N-CA-C	-6.79	100.43	110.48
1	N	181	THR	N-CA-C	-6.77	96.38	110.80
1	N	247	THR	CA-CB-OG1	-6.77	99.44	109.60
1	N	121	TYR	CA-CB-CG	6.74	126.04	113.90
2	L	138	ASN	N-CA-C	6.73	120.85	112.24
1	N	456	TRP	O-C-N	6.71	131.87	123.15
1	N	150	HIS	CA-C-N	6.68	129.53	120.38
1	N	150	HIS	C-N-CA	6.68	129.53	120.38
3	H	100(A)	SER	CA-CB-OG	6.66	124.42	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	30	SER	N-CA-C	6.61	120.51	111.39
1	N	327	ARG	CB-CA-C	6.57	119.76	108.91
1	N	456	TRP	N-CA-C	-6.57	99.33	109.52
2	L	90	GLN	N-CA-CB	-6.57	100.31	110.29
1	N	438	TRP	CG-CD2-CE3	6.55	140.45	133.90
2	L	20	THR	CB-CA-C	6.54	122.65	109.38
2	L	61	ARG	N-CA-C	6.54	120.97	113.19
3	H	120	SER	N-CA-C	-6.52	98.58	109.07
1	N	356	ASP	CA-C-O	6.51	128.87	121.32
3	H	99	PHE	N-CA-CB	6.51	121.49	110.49
1	N	97	TRP	CD2-CE3-CZ3	-6.51	110.14	118.60
1	N	144	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	N	237	CYS	CA-C-N	6.50	126.26	119.76
1	N	237	CYS	C-N-CA	6.50	126.26	119.76
3	H	173	THR	N-CA-C	-6.49	98.66	109.24
3	H	3	GLN	OE1-CD-NE2	-6.49	116.11	122.60
1	N	99	ILE	O-C-N	6.49	130.01	122.81
1	N	234	ASN	CB-CA-C	-6.48	101.48	111.66
1	N	198	ASN	CA-CB-CG	6.48	119.08	112.60
1	N	443	ILE	CA-C-N	6.47	132.03	122.71
1	N	443	ILE	C-N-CA	6.47	132.03	122.71
1	N	200	ASN	CA-C-O	6.47	126.05	119.97
1	N	208	ASN	OD1-CG-ND2	-6.47	116.13	122.60
3	H	80	LEU	N-CA-C	-6.43	99.72	109.95
1	N	127	ASP	N-CA-C	6.42	121.27	113.38
1	N	313	THR	OG1-CB-CG2	6.40	122.10	109.30
1	N	458	TRP	O-C-N	6.40	127.14	121.32
2	L	170	ASP	CA-CB-CG	6.39	119.00	112.60
1	N	165	SER	N-CA-C	-6.39	102.03	110.40
1	N	370	SER	CA-CB-OG	6.38	123.86	111.10
2	L	210	ASN	OD1-CG-ND2	-6.38	116.22	122.60
3	H	36	TRP	CB-CG-CD1	-6.37	117.34	126.90
1	N	225	THR	CA-CB-OG1	-6.37	100.05	109.60
2	L	156	GLN	CB-CG-CD	6.34	123.38	112.60
1	N	382	ALA	N-CA-C	6.31	118.96	111.71
1	N	457	ASP	CA-C-N	6.30	131.61	122.98
1	N	457	ASP	C-N-CA	6.30	131.61	122.98
1	N	84	PHE	CA-CB-CG	6.30	120.10	113.80
2	L	156	GLN	OE1-CD-NE2	-6.22	116.38	122.60
3	H	2	ILE	N-CA-C	-6.21	101.56	109.58
3	H	36	TRP	CE2-CD2-CG	-6.20	99.76	107.20
2	L	157	ASN	CA-CB-CG	6.19	118.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	152	ARG	CG-CD-NE	-6.18	98.40	112.00
2	L	83	LEU	O-C-N	6.18	130.53	122.93
1	N	170	ASN	OD1-CG-ND2	-6.18	116.42	122.60
3	H	82(B)	ASN	CA-C-N	-6.18	103.61	117.20
2	L	30	SER	N-CA-CB	-6.17	102.58	111.70
2	L	21	ILE	CA-C-O	6.16	128.47	120.78
1	N	170	ASN	CB-CG-ND2	6.15	125.63	116.40
1	N	356	ASP	N-CA-CB	-6.15	102.41	111.51
1	N	136	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	N	230	CYS	O-C-N	-6.13	115.51	122.68
2	L	29	VAL	N-CA-CB	-6.12	103.15	112.15
3	H	172	HIS	N-CA-C	-6.12	97.21	107.80
1	N	90	GLY	N-CA-C	-6.11	102.00	112.64
2	L	83	LEU	N-CA-C	-6.11	100.80	109.96
3	H	103	TRP	O-C-N	-6.10	115.30	123.23
3	H	216	SER	N-CA-C	6.09	120.51	113.38
1	N	158	LEU	N-CA-C	-6.09	99.28	108.96
1	N	145	SER	N-CA-C	-6.09	105.86	113.28
2	L	37	GLN	N-CA-C	-6.08	99.09	109.24
2	L	212	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	N	301	PRO	CB-CA-C	6.05	119.26	111.21
1	N	461	GLY	O-C-N	-6.05	115.52	122.42
1	N	299	ASN	N-CA-C	-6.04	101.26	109.95
2	L	3	VAL	CA-C-O	6.02	126.21	120.31
2	L	96	TRP	CE2-CD2-CG	-6.02	99.98	107.20
1	N	276	GLU	CA-CB-CG	-6.00	102.10	114.10
1	N	263	LEU	N-CA-C	-6.00	104.08	111.40
3	H	6	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	N	412(A)	TYR	CA-CB-CG	-5.98	103.14	113.90
3	H	62	GLU	CA-CB-CG	5.97	126.03	114.10
1	N	456	TRP	CA-C-N	-5.96	113.27	122.87
1	N	456	TRP	C-N-CA	-5.96	113.27	122.87
2	L	177	SER	CA-CB-OG	5.95	123.00	111.10
1	N	322	LEU	O-C-N	-5.94	116.09	123.04
1	N	441	ASN	N-CA-C	5.94	116.40	108.38
1	N	312	HIS	CB-CG-ND1	5.93	131.60	122.70
1	N	243	ASP	CA-CB-CG	5.93	118.53	112.60
2	L	83	LEU	N-CA-CB	5.92	118.66	109.85
1	N	234	ASN	OD1-CG-ND2	5.89	128.49	122.60
1	N	339	ASP	O-C-N	-5.89	117.70	121.88
3	H	81	GLN	OE1-CD-NE2	-5.87	116.73	122.60
3	H	162	ASN	OD1-CG-ND2	-5.87	116.73	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	317	ILE	N-CA-C	-5.86	101.15	108.89
3	H	35	ASN	CA-C-O	-5.86	114.50	120.71
3	H	40	ALA	N-CA-C	-5.86	101.52	110.07
1	N	152	ARG	N-CA-C	5.85	118.44	108.90
2	L	139	PHE	CA-CB-CG	5.85	119.65	113.80
1	N	285	ALA	N-CA-C	5.84	119.71	112.24
2	L	91	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	N	354	TYR	CA-C-O	5.82	126.59	120.36
3	H	99	PHE	CB-CA-C	-5.82	98.84	110.42
2	L	58	VAL	CA-C-N	5.81	125.76	119.78
2	L	58	VAL	C-N-CA	5.81	125.76	119.78
1	N	363	GLY	O-C-N	5.80	130.17	123.21
1	N	402	ASP	N-CA-C	-5.80	101.34	109.69
1	N	184	HIS	O-C-N	-5.79	116.73	123.27
3	H	101	ASP	O-C-N	-5.79	115.81	122.93
1	N	118	ARG	CA-CB-CG	-5.78	102.53	114.10
1	N	432	LYS	N-CA-C	5.78	118.80	111.69
2	L	206	VAL	O-C-N	-5.77	117.08	123.03
1	N	279	SER	CB-CA-C	5.77	120.69	109.33
2	L	33	VAL	N-CA-CB	-5.77	103.10	111.52
1	N	264	LYS	CA-CB-CG	5.76	125.63	114.10
1	N	294	ASN	CB-CG-ND2	5.76	125.04	116.40
2	L	84	ALA	O-C-N	-5.75	117.85	123.26
2	L	6	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	N	365	THR	CA-C-O	-5.73	115.47	121.55
1	N	230	CYS	CA-C-O	-5.71	115.21	121.89
1	N	148	THR	CA-C-O	5.70	128.01	119.23
1	N	392	GLN	OE1-CD-NE2	-5.70	116.91	122.60
3	H	179	GLN	CA-C-O	5.70	127.19	120.70
1	N	208	ASN	CA-CB-CG	5.68	118.28	112.60
2	L	209	PHE	N-CA-C	5.68	116.05	108.38
2	L	188	ARG	N-CA-C	-5.67	106.71	113.97
1	N	443	ILE	O-C-N	5.67	129.15	122.69
2	L	163	TRP	CE2-CD2-CE3	5.65	124.45	118.80
1	N	218	TRP	CE2-CD2-CG	-5.63	100.44	107.20
3	H	53	ASN	CA-CB-CG	-5.63	106.97	112.60
3	H	77	THR	CA-CB-OG1	-5.62	101.17	109.60
1	N	144	HIS	CB-CG-ND1	5.61	131.12	122.70
1	N	378	LYS	CB-CG-CD	5.61	124.20	111.30
2	L	192	TYR	N-CA-C	-5.60	98.50	108.13
3	H	87	THR	O-C-N	-5.60	115.14	122.59
3	H	209	ASN	OD1-CG-ND2	-5.59	117.01	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	10	PHE	CA-CB-CG	5.55	119.35	113.80
1	N	302	VAL	CG1-CB-CG2	-5.55	98.58	110.80
1	N	279	SER	N-CA-CB	-5.53	101.62	111.08
1	N	426	LEU	CA-C-O	-5.53	115.17	120.92
1	N	434	ASP	N-CA-C	5.53	119.77	113.19
3	H	209	ASN	CA-CB-CG	5.53	118.13	112.60
1	N	438	TRP	CE2-CD2-CG	-5.52	100.58	107.20
1	N	112	SER	N-CA-C	-5.51	102.31	110.46
1	N	131	PHE	CA-CB-CG	5.51	119.31	113.80
2	L	81	GLU	CB-CG-CD	5.50	121.95	112.60
2	L	19	VAL	CA-C-O	5.49	126.85	121.19
1	N	122	VAL	N-CA-C	-5.49	100.16	108.17
3	H	212	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	N	296	GLN	CA-C-O	-5.48	114.97	121.32
2	L	163	TRP	CE2-CD2-CG	-5.48	100.63	107.20
3	H	100(A)	SER	N-CA-C	-5.47	104.18	111.24
3	H	88	ALA	N-CA-C	5.47	115.46	108.24
1	N	347	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	N	364	ARG	CA-CB-CG	5.46	125.02	114.10
3	H	30	THR	CA-C-N	-5.45	113.93	122.65
3	H	30	THR	C-N-CA	-5.45	113.93	122.65
3	H	34	MET	N-CA-C	5.43	118.40	109.76
1	N	98	HIS	CA-C-O	-5.43	115.54	121.89
1	N	444	VAL	CA-C-O	-5.42	114.79	120.76
1	N	325	ASN	OD1-CG-ND2	-5.42	117.18	122.60
3	H	157	TRP	CE2-CD2-CG	-5.42	100.70	107.20
2	L	20	THR	OG1-CB-CG2	5.40	120.09	109.30
3	H	30	THR	OG1-CB-CG2	5.36	120.03	109.30
1	N	283	GLU	N-CA-C	-5.36	100.30	108.76
1	N	195	SER	CA-CB-OG	-5.35	100.39	111.10
2	L	106	ILE	N-CA-C	-5.34	100.19	107.99
1	N	274	HIS	CA-CB-CG	5.33	119.13	113.80
2	L	4	MET	CA-CB-CG	-5.32	103.45	114.10
3	H	196	SER	N-CA-CB	-5.32	102.02	110.22
2	L	210	ASN	N-CA-C	-5.32	100.23	108.42
1	N	339	ASP	CA-C-N	5.32	126.49	119.84
1	N	339	ASP	C-N-CA	5.32	126.49	119.84
1	N	279	SER	CA-CB-OG	5.31	121.71	111.10
3	H	206	THR	N-CA-C	5.30	117.81	108.75
1	N	254	ILE	O-C-N	-5.29	116.90	122.83
1	N	134	LEU	O-C-N	-5.29	116.86	123.04
2	L	134	CYS	N-CA-C	-5.28	100.42	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	103	TRP	CG-CD1-NE1	-5.28	103.34	110.20
3	H	206	THR	CA-CB-OG1	-5.27	101.69	109.60
1	N	185	ASP	N-CA-C	5.26	119.34	113.02
1	N	228	SER	CA-CB-OG	5.26	121.62	111.10
1	N	407	SER	CA-C-O	5.26	126.63	120.43
1	N	459	PRO	CB-CA-C	-5.26	104.22	111.21
1	N	327	ARG	NE-CZ-NH1	-5.25	116.25	121.50
2	L	35	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	N	105	ALA	N-CA-C	5.24	117.67	111.33
1	N	136	GLN	CG-CD-NE2	5.24	124.26	116.40
1	N	368	ARG	CA-C-N	5.24	132.59	122.53
1	N	368	ARG	C-N-CA	5.24	132.59	122.53
3	H	36	TRP	CD1-CG-CD2	5.24	114.68	106.30
2	L	91	HIS	CA-CB-CG	5.24	119.04	113.80
3	H	54	THR	CA-C-O	5.24	124.90	119.14
3	H	152	VAL	N-CA-C	-5.22	101.37	108.06
1	N	218	TRP	CG-CD1-NE1	-5.22	103.41	110.20
3	H	220	ASP	CB-CA-C	-5.20	104.41	111.95
3	H	103	TRP	CG-CD2-CE3	5.19	139.09	133.90
3	H	92	CYS	N-CA-C	-5.19	100.71	109.07
2	L	189	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	N	241	PHE	CA-CB-CG	5.18	118.98	113.80
1	N	424	VAL	CA-C-N	5.18	128.70	121.24
1	N	424	VAL	C-N-CA	5.18	128.70	121.24
1	N	81	ILE	N-CA-C	-5.17	96.51	111.00
2	L	35	TRP	CG-CD2-CE3	5.17	139.07	133.90
3	H	172	HIS	CB-CG-ND1	5.17	130.45	122.70
1	N	150	HIS	O-C-N	5.17	129.74	122.77
1	N	346	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	N	370	SER	N-CA-C	5.15	116.82	109.14
3	H	157	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	N	456	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	L	63	ALA	CA-C-N	-5.14	116.58	121.57
2	L	63	ALA	C-N-CA	-5.14	116.58	121.57
3	H	150	GLU	N-CA-C	-5.14	102.69	109.84
2	L	175	MET	N-CA-CB	-5.13	103.60	111.56
3	H	150	GLU	N-CA-CB	5.13	117.78	110.03
1	N	125	ASP	N-CA-C	-5.13	102.58	110.58
3	H	91	PHE	CA-C-N	-5.13	115.92	123.00
3	H	91	PHE	C-N-CA	-5.13	115.92	123.00
1	N	327	ARG	O-C-N	-5.13	118.24	121.88
1	N	329	ASN	OD1-CG-ND2	-5.13	117.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	218	TRP	CD1-CG-CD2	5.12	114.49	106.30
2	L	159	VAL	N-CA-CB	-5.12	101.54	110.49
3	H	157	TRP	N-CA-C	-5.11	101.38	109.96
1	N	292	ARG	CA-C-N	-5.11	115.21	122.77
1	N	292	ARG	C-N-CA	-5.11	115.21	122.77
3	H	10	GLU	CA-CB-CG	-5.11	103.89	114.10
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	390	PRO	CA-C-O	-5.10	115.78	121.23
1	N	139	THR	CA-C-O	-5.09	115.72	121.72
1	N	425	GLU	CB-CG-CD	5.09	121.25	112.60
3	H	21	SER	N-CA-C	5.07	118.01	109.95
1	N	311	THR	N-CA-CB	-5.06	103.20	111.66
3	H	116	THR	N-CA-C	-5.06	101.52	109.25
2	L	28	ASP	CA-CB-CG	5.05	117.65	112.60
3	H	18	VAL	N-CA-CB	-5.04	103.17	111.44
1	N	443	ILE	N-CA-C	-5.04	101.17	108.97
3	H	30	THR	CA-CB-CG2	5.04	119.06	110.50
1	N	403	TRP	CG-CD1-NE1	-5.03	103.66	110.20
1	N	390	PRO	O-C-N	-5.02	117.23	123.01
2	L	133	VAL	O-C-N	-5.02	117.01	122.83
3	H	52	ASN	OD1-CG-ND2	-5.00	117.60	122.60
3	H	174	PHE	CA-C-N	5.00	124.98	120.03
3	H	174	PHE	C-N-CA	5.00	124.98	120.03
2	L	50	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	56	ILE	Mainchain
2	L	87	TYR	Sidechain
2	L	94	PRO	Peptide
1	N	155	TYR	Sidechain
1	N	248	GLY	Peptide
1	N	255	TYR	Sidechain
1	N	284	ARG	Sidechain
1	N	327	ARG	Sidechain
1	N	457	ASP	Mainchain

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	3078	0	2905	103	0
2	L	1667	0	1598	43	0
3	H	1662	0	1611	47	0
4	A	72	0	61	1	0
5	N	28	0	26	1	0
6	N	1	0	0	0	0
All	All	6508	0	6201	185	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 15.

All (185) 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:426:LEU:HD23	1:N:460:ASP:HB2	1.40	1.03
2:L:145:ASN:HB3	2:L:197:THR:HB	1.53	0.91
1:N:426:LEU:HD23	1:N:460:ASP:CB	2.00	0.91
1:N:188:THR:HG21	1:N:208:ASN:HB2	1.60	0.82
1:N:426:LEU:HD23	1:N:460:ASP:CA	2.10	0.81
3:H:2:ILE:HA	3:H:26:GLY:HA3	1.64	0.80
1:N:141:ARG:HH21	1:N:467:PHE:HA	1.47	0.77
1:N:401:THR:HB	3:H:52:ASN:ND2	2.00	0.76
1:N:373:GLY:HA2	1:N:398:VAL:HG13	1.70	0.72
1:N:426:LEU:CD2	1:N:460:ASP:CA	2.68	0.72
1:N:194:ILE:HD11	1:N:225:THR:HB	1.75	0.69
3:H:11:LEU:HD22	3:H:149:PRO:HG3	1.75	0.69
3:H:6:GLN:HE22	3:H:91:PHE:HA	1.58	0.68
1:N:387:LYS:HB2	1:N:387:LYS:NZ	2.11	0.66
2:L:4:MET:SD	2:L:90:GLN:HB2	2.36	0.66
1:N:361:TRP:HE1	1:N:378:LYS:HZ1	1.44	0.65
1:N:399:LEU:HD12	1:N:457:ASP:OD2	1.98	0.63
3:H:210:VAL:O	3:H:218:LYS:HA	1.98	0.63
3:H:84:ASN:HA	3:H:111:VAL:HB	1.81	0.63
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.80	0.62
3:H:117:THR:O	3:H:147:TYR:HA	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:361:TRP:HE1	1:N:378:LYS:NZ	1.98	0.62
3:H:123:PRO:HD3	3:H:221:LYS:HG3	1.82	0.61
2:L:133:VAL:HG22	2:L:178:THR:HG23	1.83	0.61
3:H:34:MET:HB2	3:H:51:ILE:HG22	1.82	0.61
1:N:374:TYR:HB3	1:N:397:ILE:HB	1.83	0.61
1:N:168:THR:H	1:N:170:ASN:HD21	1.49	0.60
3:H:184:LEU:H	3:H:184:LEU:HD22	1.65	0.60
1:N:328:PRO:HG3	1:N:343:GLY:HA3	1.84	0.60
2:L:34:VAL:HG23	2:L:91:HIS:CD2	2.37	0.60
1:N:368:ARG:HH12	2:L:55:HIS:CD2	2.19	0.59
1:N:426:LEU:CD2	1:N:460:ASP:N	2.65	0.59
3:H:48:MET:HE1	3:H:80:LEU:HD11	1.85	0.59
1:N:426:LEU:CD2	1:N:460:ASP:HA	2.33	0.59
1:N:97:TRP:HZ3	1:N:361:TRP:CE3	2.21	0.58
3:H:12:LYS:O	3:H:111:VAL:HA	2.03	0.58
1:N:149:ILE:HD12	1:N:430:ARG:HB3	1.87	0.57
3:H:2:ILE:HD12	3:H:27:TYR:HB3	1.86	0.57
1:N:118:ARG:HA	1:N:441:ASN:ND2	2.19	0.56
2:L:83:LEU:HD13	2:L:166:GLN:HB3	1.87	0.56
2:L:141:PRO:HD2	2:L:198:HIS:CE1	2.40	0.56
3:H:144:VAL:HB	3:H:187:LEU:HB3	1.88	0.56
3:H:15:GLY:O	3:H:82(B):ASN:HA	2.04	0.56
1:N:94:ILE:HD12	1:N:359:ASN:HD21	1.71	0.56
2:L:144:ILE:HD12	2:L:198:HIS:HB2	1.88	0.56
3:H:148:PHE:CE2	3:H:149:PRO:HB3	2.41	0.56
1:N:149:ILE:HD11	1:N:431:PRO:HD3	1.87	0.56
1:N:401:THR:HB	3:H:52:ASN:HD21	1.70	0.56
3:H:17:THR:HA	3:H:82:ILE:O	2.06	0.56
2:L:122:SER:HA	2:L:125:LEU:HD12	1.87	0.56
3:H:2:ILE:HB	3:H:102:TYR:CD2	2.41	0.56
1:N:118:ARG:HA	1:N:441:ASN:HD22	1.71	0.55
1:N:135:SER:HB2	1:N:159:ILE:HD13	1.88	0.55
1:N:152:ARG:HG2	1:N:178:TRP:CG	2.40	0.55
3:H:34:MET:HB2	3:H:51:ILE:CG2	2.36	0.55
1:N:428:ARG:HH21	1:N:464:ILE:HG12	1.71	0.55
1:N:168:THR:H	1:N:170:ASN:ND2	2.05	0.55
3:H:2:ILE:HG23	3:H:27:TYR:HD1	1.72	0.55
1:N:451:GLU:HB2	1:N:453:LEU:HD21	1.88	0.54
2:L:125:LEU:O	2:L:183:LYS:HD3	2.08	0.54
2:L:45:LYS:HD2	2:L:46:LEU:N	2.23	0.54
1:N:366:ILE:HD13	3:H:31:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:426:LEU:HD23	1:N:460:ASP:N	2.23	0.53
1:N:205:ILE:HD11	1:N:215:ILE:HD12	1.89	0.53
1:N:170:ASN:HD22	1:N:171:SER:N	2.07	0.53
3:H:162:ASN:OD1	3:H:205:ILE:HA	2.07	0.53
1:N:97:TRP:H	1:N:395:GLN:HE21	1.55	0.53
1:N:188:THR:CG2	1:N:208:ASN:HB2	2.37	0.53
1:N:294:ASN:O	1:N:346:ASN:HA	2.09	0.53
2:L:66:GLY:HA3	2:L:71:TYR:CD1	2.44	0.52
2:L:108:ARG:HG2	2:L:109:ALA:H	1.72	0.52
1:N:121:TYR:CB	1:N:228:SER:HA	2.39	0.52
1:N:84:PHE:O	5:N:475(A):NAG:H82	2.08	0.52
1:N:378:LYS:O	1:N:390:PRO:HA	2.09	0.52
1:N:176:ILE:O	1:N:193:CYS:HB3	2.09	0.52
1:N:263:LEU:HD22	1:N:310:MET:HE1	1.92	0.52
1:N:96:SER:OG	1:N:453:LEU:HG	2.10	0.52
1:N:386:ASP:OD1	1:N:387:LYS:NZ	2.43	0.51
3:H:125:ALA:HB2	3:H:223:ILE:HG23	1.91	0.51
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.45	0.51
3:H:116:THR:HG22	3:H:149:PRO:HD3	1.92	0.51
1:N:387:LYS:HB2	1:N:387:LYS:HZ3	1.74	0.51
1:N:161:TRP:CE3	1:N:167:PRO:HB3	2.46	0.51
1:N:376:MET:O	1:N:377:LEU:HD23	2.11	0.51
3:H:124:LEU:HB2	3:H:141:GLY:C	2.36	0.51
1:N:226:GLN:O	1:N:350:LYS:NZ	2.45	0.50
1:N:97:TRP:N	1:N:395:GLN:HE21	2.08	0.50
3:H:4:LEU:CD2	3:H:24:ALA:HA	2.42	0.50
1:N:463:LYS:C	1:N:465:GLU:H	2.19	0.50
3:H:83:LYS:O	3:H:111:VAL:HG21	2.12	0.50
2:L:83:LEU:O	2:L:83:LEU:HG	2.11	0.49
1:N:271:THR:OG1	1:N:315:GLN:HA	2.12	0.49
2:L:196:ALA:HB3	2:L:205:ILE:HB	1.93	0.49
3:H:183:ASP:HB3	3:H:184:LEU:HD13	1.94	0.49
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.94	0.49
2:L:52:SER:HA	2:L:64:GLY:HA3	1.95	0.49
1:N:97:TRP:H	1:N:395:GLN:NE2	2.11	0.49
1:N:121:TYR:CG	1:N:228:SER:HA	2.48	0.49
2:L:154:GLU:CD	2:L:154:GLU:H	2.20	0.49
3:H:2:ILE:HG23	3:H:27:TYR:CD1	2.47	0.49
1:N:130:ARG:HE	1:N:160:SER:HB2	1.78	0.48
2:L:34:VAL:HA	2:L:48:ILE:O	2.13	0.48
1:N:318:CYS:HB3	1:N:386:ASP:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:3:GLN:HB2	3:H:25:SER:HB2	1.95	0.48
1:N:367:SER:HB3	1:N:370:SER:O	2.14	0.47
2:L:49:TYR:CD1	3:H:100(B):LEU:HD21	2.48	0.47
1:N:184:HIS:HA	1:N:189:ARG:HA	1.96	0.47
1:N:463:LYS:C	1:N:465:GLU:N	2.72	0.47
3:H:67:PHE:CE1	3:H:82:ILE:HG23	2.50	0.47
3:H:37:VAL:HA	3:H:46:LYS:O	2.14	0.47
1:N:84:PHE:CD1	1:N:187:LYS:HG3	2.50	0.47
1:N:114:VAL:HG13	1:N:167:PRO:O	2.15	0.47
1:N:246:ALA:HA	1:N:274:HIS:NE2	2.30	0.46
2:L:37:GLN:HB2	2:L:47:LEU:HD21	1.96	0.46
1:N:195:SER:O	1:N:201:ALA:HA	2.15	0.46
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.97	0.46
1:N:189:ARG:HG2	1:N:190:MET:O	2.16	0.46
1:N:395:GLN:HA	1:N:455:GLN:NE2	2.31	0.46
1:N:224:ARG:HG2	1:N:224:ARG:HH11	1.81	0.46
2:L:34:VAL:HG23	2:L:91:HIS:HD2	1.80	0.46
2:L:45:LYS:HD2	2:L:46:LEU:H	1.80	0.46
2:L:15:VAL:HA	2:L:78:VAL:O	2.16	0.45
1:N:426:LEU:CD2	1:N:460:ASP:HB2	2.29	0.45
3:H:57:PRO:HB2	3:H:59:TYR:CE1	2.51	0.45
2:L:186:TYR:HA	2:L:192:TYR:OH	2.17	0.45
1:N:426:LEU:HD21	1:N:460:ASP:N	2.32	0.45
1:N:216:ASN:ND2	1:N:220:ARG:HH21	2.15	0.45
2:L:46:LEU:HD11	3:H:100(B):LEU:HD23	1.99	0.45
2:L:87:TYR:CD2	3:H:45:LEU:HD12	2.52	0.45
1:N:373:GLY:HA2	1:N:398:VAL:O	2.17	0.44
1:N:366:ILE:HG12	1:N:375:GLU:HG2	1.99	0.44
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.51	0.44
2:L:155:ARG:HG2	2:L:179:LEU:HD11	2.00	0.44
3:H:127:VAL:O	3:H:128:CYS:HB2	2.16	0.44
1:N:428:ARG:NH2	1:N:433:GLU:OE2	2.51	0.44
2:L:49:TYR:HD2	2:L:50:TRP:HD1	1.65	0.44
1:N:134:LEU:HB3	1:N:156:ARG:NH1	2.33	0.44
3:H:166:LEU:HD12	3:H:166:LEU:HA	1.84	0.44
1:N:98:HIS:O	1:N:446:MET:HB3	2.17	0.43
2:L:4:MET:HG2	2:L:88:CYS:SG	2.59	0.43
1:N:121:TYR:HB3	1:N:228:SER:HA	1.99	0.43
1:N:245:SER:O	1:N:250:ALA:HB2	2.19	0.43
1:N:238:PRO:HA	1:N:255:TYR:O	2.18	0.43
1:N:266:GLU:HA	1:N:267:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:355:LEU:HD13	1:N:383:LEU:HD13	2.01	0.43
1:N:464:ILE:O	1:N:464:ILE:CG2	2.66	0.43
1:N:94:ILE:HD12	1:N:359:ASN:ND2	2.33	0.43
2:L:119:PRO:HG3	3:H:226:ARG:NH2	2.34	0.43
3:H:124:LEU:HD21	3:H:143:LEU:HB2	2.00	0.43
1:N:192:ILE:HG12	1:N:205:ILE:HG23	2.00	0.42
1:N:246:ALA:HA	1:N:274:HIS:HE2	1.84	0.42
1:N:425:GLU:OE1	1:N:427:ILE:HD11	2.19	0.42
1:N:453:LEU:HD23	1:N:453:LEU:N	2.34	0.42
2:L:21:ILE:O	2:L:72:THR:HA	2.19	0.42
2:L:12:SER:HA	2:L:105:GLU:O	2.19	0.42
4:A:4:MAN:O3	4:A:5:MAN:C1	2.67	0.42
1:N:130:ARG:HH21	1:N:160:SER:HB2	1.84	0.42
1:N:87:LEU:HD13	1:N:282:GLY:HA3	2.02	0.42
1:N:276:GLU:HB3	1:N:292:ARG:HB3	2.01	0.42
3:H:4:LEU:HD23	3:H:24:ALA:HA	2.01	0.42
1:N:419:ARG:HD2	1:N:448:SER:O	2.20	0.42
1:N:300:ARG:O	1:N:317:ILE:HG12	2.20	0.42
1:N:458:TRP:HA	1:N:459:PRO:HD2	1.80	0.42
1:N:227:GLU:C	1:N:350:LYS:HZ3	2.27	0.41
1:N:176:ILE:HG22	1:N:177:GLY:N	2.36	0.41
1:N:330:ASP:HA	1:N:331:PRO:HD2	1.94	0.41
2:L:115:VAL:HG13	2:L:136:LEU:HG	2.02	0.41
1:N:368:ARG:NH1	2:L:55:HIS:CD2	2.86	0.41
1:N:451:GLU:HB2	1:N:453:LEU:CD2	2.49	0.41
3:H:184:LEU:HD22	3:H:184:LEU:N	2.30	0.41
1:N:430:ARG:HG3	1:N:434:ASP:HA	2.01	0.41
3:H:139:THR:O	3:H:140:LEU:HD23	2.21	0.41
3:H:224:GLU:O	3:H:226:ARG:HG2	2.20	0.41
1:N:373:GLY:CA	1:N:398:VAL:HG13	2.47	0.41
2:L:80:ALA:HB1	2:L:168:SER:O	2.20	0.41
1:N:183:CYS:HB3	1:N:230:CYS:O	2.21	0.41
3:H:87:THR:O	3:H:87:THR:HG23	2.21	0.41
2:L:33:VAL:HG21	2:L:71:TYR:CD2	2.56	0.41
2:L:35:TRP:O	2:L:47:LEU:HB2	2.21	0.41
1:N:161:TRP:CE2	1:N:167:PRO:HD3	2.55	0.40
1:N:216:ASN:HD21	1:N:220:ARG:HH21	1.68	0.40
1:N:242:THR:HA	1:N:252:THR:HA	2.03	0.40
1:N:274:HIS:HE1	1:N:294:ASN:HB3	1.86	0.40
2:L:143:ASP:O	2:L:198:HIS:CD2	2.75	0.40
2:L:159:VAL:HA	2:L:178:THR:O	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%)	336 (87%)	48 (12%)	3 (1%)	16	31
2	L	212/214 (99%)	187 (88%)	19 (9%)	6 (3%)	4	6
3	H	219/221 (99%)	180 (82%)	30 (14%)	9 (4%)	2	3
All	All	818/824 (99%)	703 (86%)	97 (12%)	18 (2%)	5	9

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	154	GLU
2	L	158	GLY
3	H	16	GLU
3	H	87	THR
3	H	162	ASN
2	L	51	ALA
3	H	102	TYR
3	H	134	THR
3	H	226	ARG
1	N	346	ASN
2	L	60	ASP
2	L	78	VAL
1	N	295	TRP
3	H	52(A)	THR
1	N	222	ILE
3	H	180	SER
3	H	57	PRO
2	L	68	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%)	295 (86%)	47 (14%)	3	7
2	L	190/190 (100%)	153 (80%)	37 (20%)	1	2
3	H	187/187 (100%)	159 (85%)	28 (15%)	3	6
All	All	719/719 (100%)	607 (84%)	112 (16%)	2	5

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	82	ARG
1	N	89	LYS
1	N	93	THR
1	N	97	TRP
1	N	99	ILE
1	N	134	LEU
1	N	141	ARG
1	N	154	GLN
1	N	156	ARG
1	N	160	SER
1	N	170	ASN
1	N	174	GLU
1	N	202	SER
1	N	204	VAL
1	N	208	ASN
1	N	212	VAL
1	N	220	ARG
1	N	222	ILE
1	N	247	THR
1	N	254	ILE
1	N	261	LYS
1	N	263	LEU
1	N	276	GLU
1	N	283	GLU
1	N	302	VAL
1	N	311	THR

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Mol	Chain	Res	Type
1	N	313	THR
1	N	329	ASN
1	N	336	LYS
1	N	342	PRO
1	N	346	ASN
1	N	358	VAL
1	N	364	ARG
1	N	370	SER
1	N	383	LEU
1	N	384	THR
1	N	387	LYS
1	N	388	SER
1	N	391	THR
1	N	395	GLN
1	N	396	THR
1	N	424	VAL
1	N	435	LYS
1	N	448	SER
1	N	453	LEU
1	N	463	LYS
1	N	464	ILE
2	L	2	ILE
2	L	4	MET
2	L	5	THR
2	L	7	SER
2	L	11	MET
2	L	13	THR
2	L	20	THR
2	L	21	ILE
2	L	26	SER
2	L	30	SER
2	L	31	THR
2	L	42	GLN
2	L	43	SER
2	L	45	LYS
2	L	46	LEU
2	L	47	LEU
2	L	52	SER
2	L	56	ILE
2	L	58	VAL
2	L	67	SER
2	L	70	ASP

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Mol	Chain	Res	Type
2	L	76	SER
2	L	81	GLU
2	L	83	LEU
2	L	85	LEU
2	L	116	SER
2	L	122	SER
2	L	141	PRO
2	L	142	LYS
2	L	151	ASP
2	L	156	GLN
2	L	160	LEU
2	L	175	MET
2	L	179	LEU
2	L	209	PHE
2	L	212	ASN
2	L	213	GLU
3	H	2	ILE
3	H	13	LYS
3	H	21	SER
3	H	28	THR
3	H	61	GLU
3	H	70	SER
3	H	71	LEU
3	H	73	THR
3	H	74	SER
3	H	80	LEU
3	H	109	VAL
3	H	113	SER
3	H	117	THR
3	H	120	SER
3	H	124	LEU
3	H	150	GLU
3	H	152	VAL
3	H	156	THR
3	H	184	LEU
3	H	190	SER
3	H	193	VAL
3	H	196	SER
3	H	198	THR
3	H	202	SER
3	H	206	THR
3	H	217	THR

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Mol	Chain	Res	Type
3	H	218	LYS
3	H	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	95	ASN
1	N	170	ASN
1	N	208	ASN
1	N	216	ASN
1	N	296	GLN
1	N	329	ASN
1	N	359	ASN
1	N	392	GLN
1	N	395	GLN
1	N	455	GLN
2	L	38	GLN
2	L	212	ASN
3	H	6	GLN
3	H	39	GLN
3	H	81	GLN
3	H	82(A)	ASN
3	H	82(B)	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1	1,4	14,14,15	0.60	0	17,19,21	1.72	5 (29%)
4	NAG	A	2	4	14,14,15	0.83	1 (7%)	17,19,21	2.05	3 (17%)
4	BMA	A	3	4	11,11,12	1.82	2 (18%)	15,15,17	1.71	5 (33%)
4	MAN	A	4	4	11,11,12	1.17	1 (9%)	15,15,17	3.06	7 (46%)
4	MAN	A	5	4	11,11,12	1.21	2 (18%)	15,15,17	2.83	6 (40%)
4	MAN	A	6	4	11,11,12	1.65	3 (27%)	15,15,17	1.98	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	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	-	2/2/19/22	0/1/1/1
4	MAN	A	4	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5	4	-	2/2/19/22	1/1/1/1
4	MAN	A	6	4	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	BMA	C6-C5	3.85	1.64	1.51
4	A	6	MAN	C1-C2	2.77	1.58	1.52
4	A	6	MAN	C6-C5	2.65	1.60	1.51
4	A	3	BMA	C4-C5	2.61	1.58	1.53
4	A	6	MAN	O5-C5	2.47	1.48	1.43
4	A	5	MAN	C4-C3	2.45	1.58	1.52
4	A	4	MAN	C6-C5	2.16	1.59	1.51
4	A	5	MAN	O5-C5	2.15	1.47	1.43
4	A	2	NAG	C1-C2	2.08	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5	MAN	C1-O5-C5	8.37	123.40	112.19
4	A	4	MAN	C1-O5-C5	7.09	121.69	112.19
4	A	6	MAN	C1-O5-C5	6.82	121.33	112.19
4	A	2	NAG	C8-C7-N2	5.97	126.02	116.12
4	A	4	MAN	C1-C2-C3	5.66	117.89	109.64
4	A	1	NAG	C1-C2-N2	-4.07	104.03	110.43
4	A	4	MAN	O2-C2-C3	-4.05	101.76	110.15
4	A	4	MAN	O4-C4-C3	3.96	119.70	110.38
4	A	2	NAG	O7-C7-C8	-3.80	115.28	122.05
4	A	5	MAN	O5-C1-C2	3.22	118.48	110.79
4	A	3	BMA	O5-C5-C4	-3.06	103.39	110.83
4	A	3	BMA	C1-O5-C5	2.86	116.01	112.19
4	A	2	NAG	C1-O5-C5	2.82	115.96	112.19
4	A	4	MAN	C6-C5-C4	-2.78	106.18	113.02
4	A	3	BMA	C6-C5-C4	2.78	119.85	113.02
4	A	1	NAG	C6-C5-C4	2.74	119.76	113.02
4	A	5	MAN	C2-C3-C4	2.65	115.53	110.86
4	A	1	NAG	C8-C7-N2	2.62	120.47	116.12
4	A	5	MAN	C1-C2-C3	-2.62	105.83	109.64
4	A	1	NAG	C4-C3-C2	-2.59	107.23	111.02
4	A	5	MAN	C3-C4-C5	2.53	114.82	110.23
4	A	5	MAN	O2-C2-C1	2.41	114.75	109.22
4	A	3	BMA	O6-C6-C5	2.32	119.24	111.33
4	A	4	MAN	O3-C3-C2	-2.30	105.35	110.05
4	A	4	MAN	O2-C2-C1	-2.14	104.32	109.22
4	A	3	BMA	O5-C5-C6	2.10	111.74	107.66
4	A	1	NAG	O3-C3-C2	2.09	113.75	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	6	MAN	O5-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	6	MAN	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	5	MAN	C4-C5-C6-O6
4	A	5	MAN	O5-C5-C6-O6

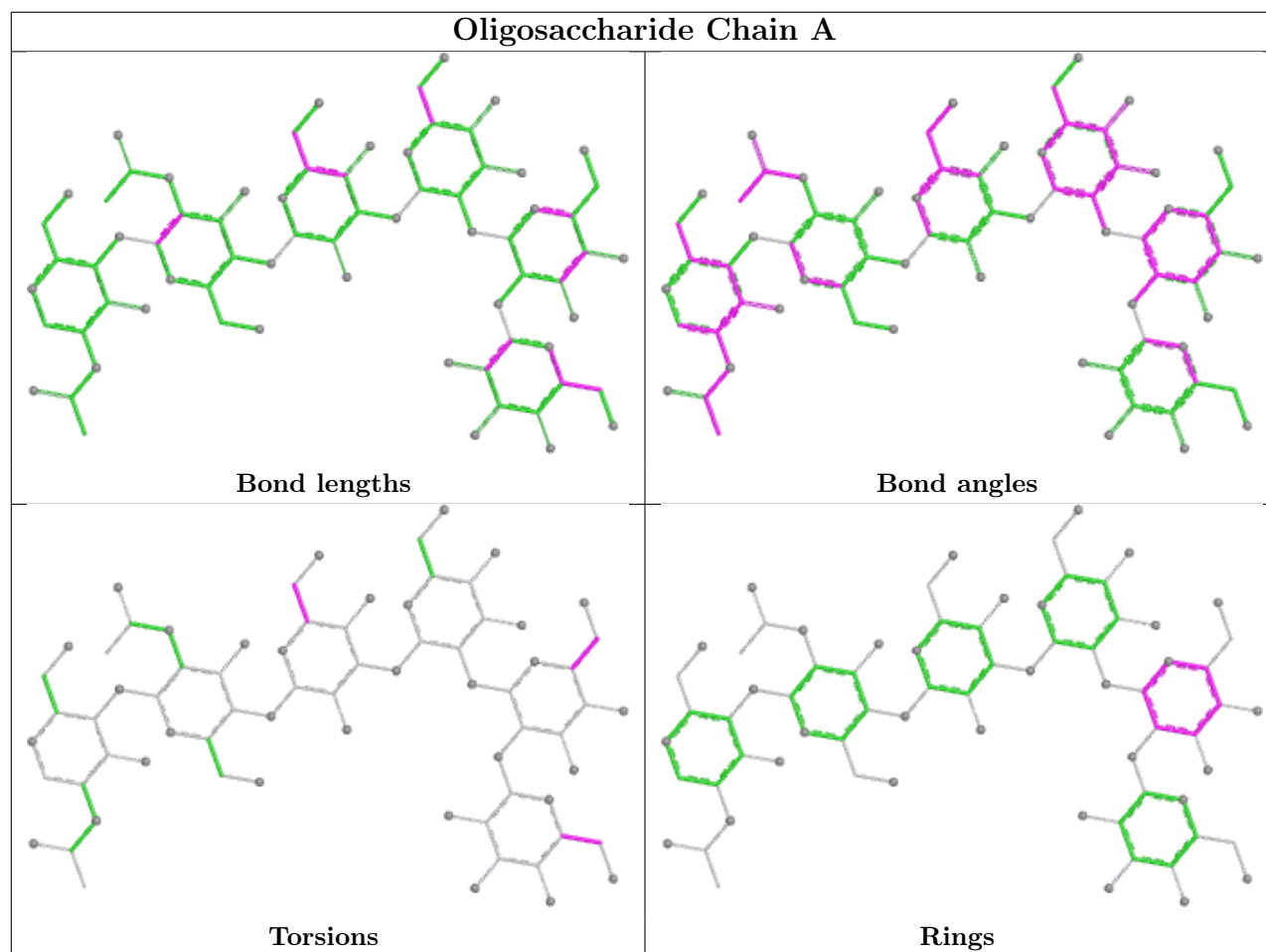
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5	MAN	1	0
4	A	4	MAN	1	0

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	1.45	2 (14%)	17,19,21	1.77	5 (29%)
5	NAG	N	476(A)	1	14,14,15	0.89	0	17,19,21	1.73	6 (35%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	475(A)	NAG	C2-N2	-3.94	1.39	1.46
5	N	475(A)	NAG	O5-C1	2.13	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	476(A)	NAG	C4-C3-C2	-3.54	105.83	111.02
5	N	475(A)	NAG	C8-C7-N2	3.46	121.86	116.12
5	N	475(A)	NAG	C6-C5-C4	2.95	120.27	113.02
5	N	476(A)	NAG	C8-C7-N2	2.79	120.74	116.12
5	N	476(A)	NAG	C1-C2-N2	2.47	114.32	110.43
5	N	475(A)	NAG	O4-C4-C5	2.38	115.19	109.32
5	N	475(A)	NAG	O3-C3-C4	2.36	115.94	110.38
5	N	475(A)	NAG	O5-C5-C6	-2.26	103.26	107.66
5	N	476(A)	NAG	O7-C7-C8	-2.22	118.10	122.05
5	N	476(A)	NAG	O5-C5-C4	-2.08	105.76	110.83
5	N	476(A)	NAG	C2-N2-C7	2.00	125.58	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	475(A)	NAG	1	0

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%)	-0.54	7 (1%) 67 64	2, 3, 18, 39	0
2	L	214/214 (100%)	-0.12	5 (2%) 61 57	2, 19, 38, 68	0
3	H	221/221 (100%)	0.08	10 (4%) 38 33	2, 24, 44, 67	0
All	All	824/824 (100%)	-0.26	22 (2%) 56 51	2, 12, 37, 68	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	135	GLY	6.6
3	H	130	ASP	6.0
3	H	134	THR	5.3
1	N	465	GLU	4.9
2	L	213	GLU	4.7
1	N	261	LYS	4.2
3	H	227	GLY	4.2
3	H	180	SER	4.1
3	H	133	THR	3.8
1	N	416	GLU	3.5
2	L	214	CYS	3.5
1	N	82	ARG	3.2
1	N	414	GLU	3.2
3	H	128	CYS	3.0
1	N	462	ALA	2.9
3	H	224	GLU	2.6
2	L	212	ASN	2.5
3	H	226	ARG	2.3
2	L	211	ARG	2.3
2	L	190	ASN	2.1
1	N	463	LYS	2.0
3	H	183	ASP	2.0

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

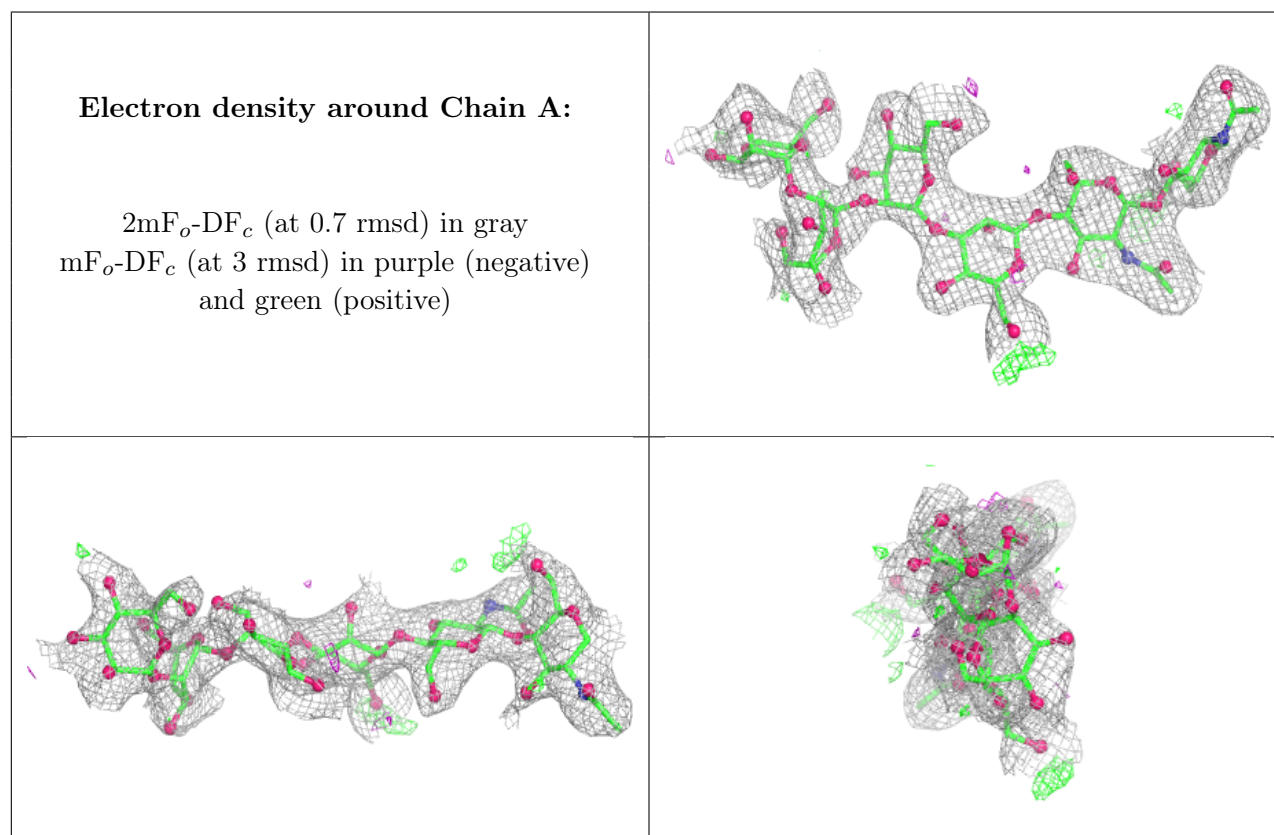
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	A	1	14/15	-	-	8,11,16,17	0
4	NAG	A	2	14/15	-	-	8,11,12,13	0
4	BMA	A	3	11/12	-	-	5,7,8,9	0
4	MAN	A	4	11/12	-	-	6,7,9,11	0
4	MAN	A	5	11/12	-	-	10,13,15,17	0
4	MAN	A	6	11/12	-	-	13,14,15,16	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($\text{\AA}^2$)	Q<0.9
6	CA	N	1	1/1	0.67	0.21	44,44,44,44	0
5	NAG	N	476(A)	14/15	0.92	0.09	20,22,26,27	0
5	NAG	N	475(A)	14/15	0.96	0.07	19,22,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.