



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:53 AM GMT

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

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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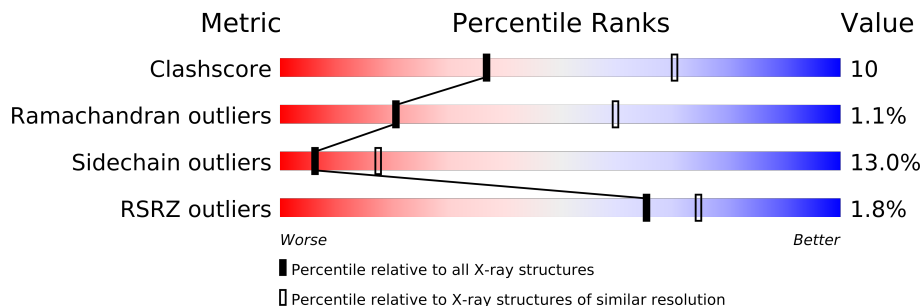
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	N	389	
2	L	214	
3	H	221	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6585 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

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

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

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

There are 21 discrepancies between the modelled and reference sequences:

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

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

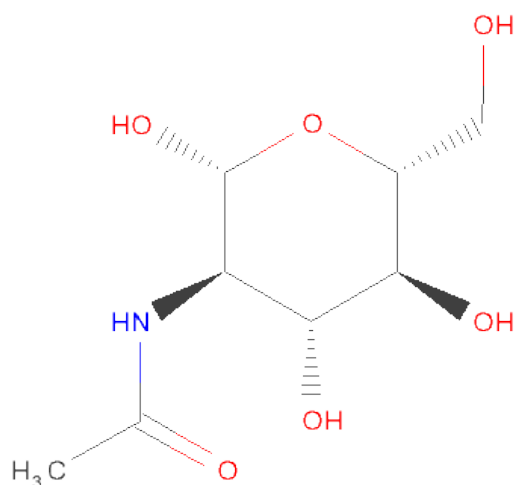
- Molecule 3 is a protein called IGG2A-KAPPA NC41 FAB (HEAVY CHAIN).

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

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

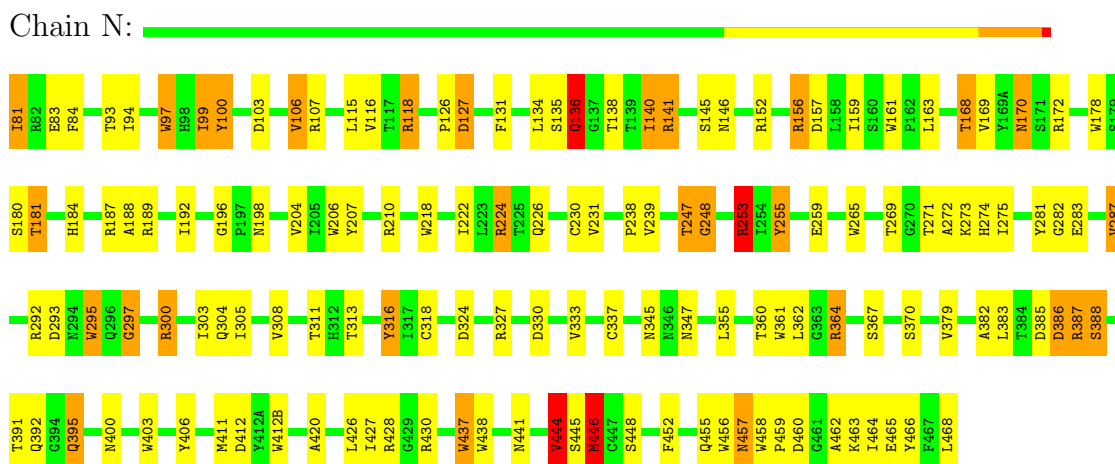
- Molecule 8 is water.

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

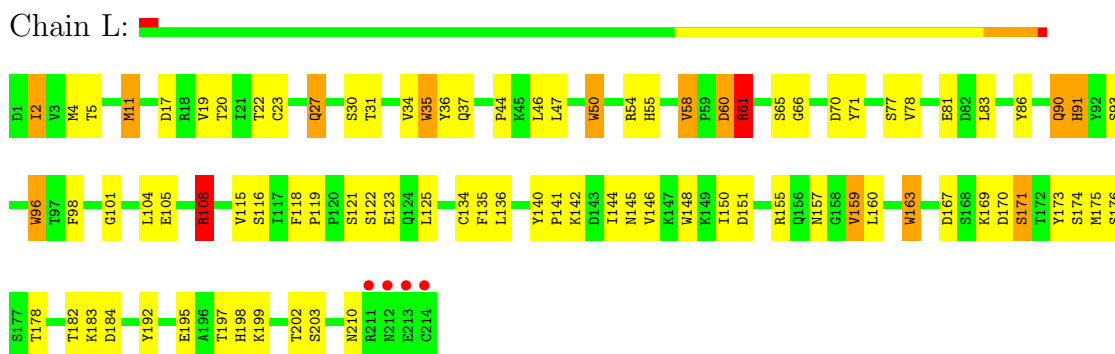
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

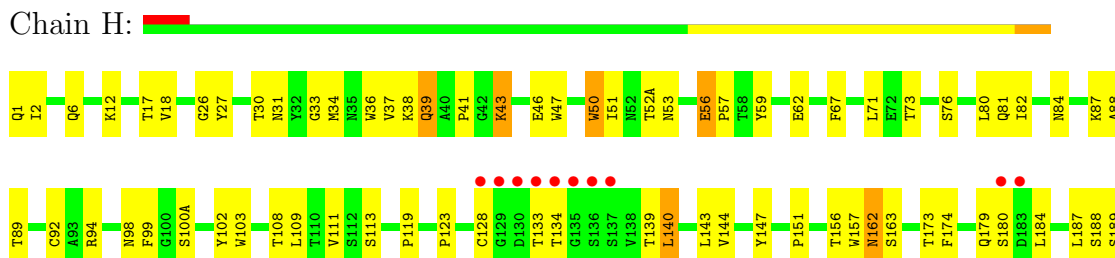
#### • Molecule 1: INFLUENZA A SUBTYPE N9 NEURAMINIDASE



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.00Å 167.00Å 124.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 54.1 (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, $R_{free}$	0.157 , (Not available) 0.234 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 22.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 31846 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	6585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

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



## 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: CA, BMA, NAG, MAN

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	1.02	2/3151 (0.1%)	1.91	92/4292 (2.1%)
2	L	0.89	0/1708	1.72	32/2323 (1.4%)
3	H	0.86	0/1707	1.72	28/2326 (1.2%)
All	All	0.95	2/6566 (0.0%)	1.81	152/8941 (1.7%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	157	ASP	CB-CG	5.82	1.64	1.51
1	N	438	TRP	CD1-NE1	-5.46	1.28	1.38

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	54	ARG	NE-CZ-NH2	-14.01	113.29	120.30
1	N	224	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	N	107	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	N	300	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	N	210	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	N	438	TRP	CG-CD2-CE3	9.50	142.45	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	156	ARG	NE-CZ-NH2	-9.07	115.77	120.30
2	L	54	ARG	NE-CZ-NH1	9.03	124.81	120.30
2	L	148	TRP	CD1-CG-CD2	8.94	113.45	106.30
1	N	438	TRP	CD1-CG-CD2	8.92	113.44	106.30
1	N	456	TRP	CG-CD2-CE3	8.88	141.90	133.90
1	N	364	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	N	300	ARG	NE-CZ-NH2	-8.86	115.87	120.30
3	H	103	TRP	CD1-CG-CD2	8.86	113.39	106.30
1	N	412(B)	TRP	CE2-CD2-CG	-8.70	100.34	107.30
3	H	157	TRP	CD1-CG-CD2	8.68	113.24	106.30
1	N	456	TRP	CE2-CD2-CG	-8.56	100.45	107.30
1	N	141	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	N	438	TRP	CE2-CD2-CG	-8.53	100.48	107.30
1	N	438	TRP	CB-CG-CD1	-8.50	115.95	127.00
1	N	281	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	N	118	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	N	327	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	N	156	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	N	218	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	N	446	MET	CG-SD-CE	-8.30	86.92	100.20
1	N	265	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	N	178	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	N	292	ARG	NE-CZ-NH1	8.10	124.35	120.30
3	H	27	TYR	CB-CG-CD2	-8.07	116.16	121.00
2	L	163	TRP	CD1-CG-CD2	8.02	112.71	106.30
3	H	50	TRP	CD1-CG-CD2	7.98	112.69	106.30
1	N	161	TRP	CE2-CD2-CG	-7.97	100.93	107.30
1	N	97	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	N	206	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	N	97	TRP	CD1-CG-CD2	7.81	112.55	106.30
2	L	50	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	N	100	TYR	CB-CG-CD2	-7.78	116.33	121.00
1	N	161	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	N	218	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	N	403	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	N	412(B)	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	N	456	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	N	403	TRP	CE2-CD2-CG	-7.63	101.19	107.30
2	L	11	MET	CA-CB-CG	-7.58	100.41	113.30
1	N	295	TRP	CD1-CG-CD2	7.57	112.36	106.30
3	H	157	TRP	CE2-CD2-CG	-7.56	101.25	107.30
2	L	148	TRP	CE2-CD2-CG	-7.47	101.32	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	97	TRP	CG-CD2-CE3	7.46	140.61	133.90
1	N	403	TRP	CG-CD2-CE3	7.46	140.61	133.90
2	L	61	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	N	297	GLY	CA-C-N	-7.41	100.91	117.20
3	H	103	TRP	CE2-CD2-CG	-7.38	101.39	107.30
2	L	35	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	N	403	TRP	CB-CG-CD1	-7.32	117.49	127.00
2	L	50	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	N	361	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	N	178	TRP	CD1-CG-CD2	7.18	112.04	106.30
2	L	61	ARG	NE-CZ-NH2	-7.13	116.73	120.30
2	L	155	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	L	163	TRP	CE2-CD2-CG	-7.11	101.61	107.30
2	L	35	TRP	CD1-CG-CD2	7.08	111.96	106.30
1	N	437	TRP	CE2-CD2-CG	-7.04	101.66	107.30
3	H	36	TRP	CD1-CG-CD2	6.97	111.88	106.30
1	N	295	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	N	253	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	N	161	TRP	CG-CD2-CE3	6.92	140.13	133.90
1	N	437	TRP	CG-CD2-CE3	6.87	140.08	133.90
1	N	206	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	N	136	GLN	CG-CD-NE2	6.76	132.93	116.70
1	N	361	TRP	CE2-CD2-CG	-6.70	101.94	107.30
3	H	50	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	N	172	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	N	406	TYR	CB-CG-CD2	-6.66	117.00	121.00
2	L	96	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	N	226	GLN	N-CA-C	6.59	128.78	111.00
1	N	265	TRP	CG-CD1-NE1	-6.52	103.58	110.10
3	H	199	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	N	265	TRP	CE2-CD2-CG	-6.42	102.17	107.30
1	N	387	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	N	295	TRP	CG-CD2-CE3	6.31	139.58	133.90
3	H	36	TRP	CE2-CD2-CG	-6.27	102.29	107.30
3	H	199	TRP	CD1-CG-CD2	6.23	111.28	106.30
1	N	97	TRP	CB-CG-CD1	-6.18	118.96	127.00
2	L	163	TRP	CG-CD2-CE3	6.18	139.46	133.90
1	N	161	TRP	CB-CG-CD1	-6.17	118.97	127.00
3	H	59	TYR	CB-CG-CD1	-6.17	117.30	121.00
1	N	157	ASP	CA-CB-CG	6.16	126.95	113.40
3	H	157	TRP	CA-C-N	-6.15	103.68	117.20
2	L	96	TRP	CD1-CG-CD2	6.11	111.19	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	438	TRP	CG-CD1-NE1	-6.11	103.99	110.10
1	N	412(B)	TRP	CG-CD2-CE3	6.07	139.36	133.90
1	N	437	TRP	CD1-CG-CD2	6.06	111.15	106.30
2	L	91	HIS	CA-CB-CG	6.04	123.86	113.60
1	N	99	ILE	CB-CA-C	-6.03	99.53	111.60
3	H	47	TRP	CE2-CD2-CG	-6.01	102.49	107.30
1	N	178	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	N	106	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	N	385	ASP	CA-C-N	5.84	130.06	117.20
2	L	169	LYS	N-CA-C	-5.80	95.34	111.00
1	N	412	ASP	CB-CG-OD1	5.78	123.50	118.30
2	L	210	ASN	CA-CB-CG	-5.76	100.73	113.40
2	L	148	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	N	468	LEU	CA-C-O	-5.75	108.01	120.10
1	N	198	ASN	CB-CG-ND2	5.73	130.45	116.70
1	N	308	VAL	CA-CB-CG1	-5.73	102.31	110.90
1	N	178	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	N	457	ASN	C-N-CA	5.69	135.92	121.70
3	H	202	SER	N-CA-CB	-5.68	101.98	110.50
2	L	50	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	N	444	VAL	CB-CA-C	-5.60	100.75	111.40
3	H	140	LEU	CA-CB-CG	5.60	128.18	115.30
3	H	47	TRP	CD1-CG-CD2	5.60	110.78	106.30
1	N	412(B)	TRP	CB-CG-CD1	-5.59	119.73	127.00
3	H	37	VAL	CG1-CB-CG2	-5.59	101.95	110.90
3	H	103	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	N	127	ASP	N-CA-CB	-5.51	100.69	110.60
1	N	316	TYR	CB-CG-CD2	-5.50	117.70	121.00
3	H	157	TRP	CB-CG-CD1	-5.49	119.87	127.00
1	N	255	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	H	103	TRP	CG-CD1-NE1	-5.48	104.62	110.10
3	H	39	GLN	N-CA-C	-5.48	96.22	111.00
1	N	152	ARG	CA-CB-CG	5.47	125.44	113.40
1	N	218	TRP	CG-CD2-CE3	5.46	138.81	133.90
2	L	36	TYR	CB-CG-CD2	-5.46	117.73	121.00
2	L	148	TRP	CG-CD2-CE3	5.42	138.77	133.90
3	H	162	ASN	CA-CB-CG	-5.42	101.48	113.40
1	N	206	TRP	CG-CD1-NE1	-5.41	104.69	110.10
3	H	50	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	N	347	ASN	CA-CB-CG	5.33	125.12	113.40
2	L	163	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	N	247	THR	N-CA-CB	-5.31	100.21	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	173	TYR	CB-CG-CD1	-5.31	117.81	121.00
3	H	94	ARG	CB-CG-CD	-5.31	97.79	111.60
3	H	223	ILE	N-CA-C	-5.28	96.75	111.00
1	N	466	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	N	253	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	L	163	TRP	CB-CG-CD1	-5.28	120.14	127.00
2	L	35	TRP	CG-CD1-NE1	-5.18	104.92	110.10
2	L	171	SER	N-CA-CB	-5.18	102.73	110.50
2	L	104	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	N	206	TRP	CG-CD2-CE3	5.17	138.55	133.90
3	H	128	CYS	CA-C-N	5.13	126.46	116.20
1	N	239	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	N	297	GLY	O-C-N	5.12	130.89	122.70
1	N	386	ASP	CA-CB-CG	5.11	124.63	113.40
2	L	108	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	L	50	TRP	CG-CD1-NE1	-5.04	105.06	110.10
3	H	157	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	N	218	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	N	224	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	N	265	TRP	CG-CD2-CE3	5.01	138.41	133.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	3069	0	2886	62	0
2	L	1667	0	1598	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1665	0	1612	34	0
4	N	72	0	61	0	0
5	N	14	0	13	0	0
6	N	28	0	25	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	63	0	0	0	0
All	All	6585	0	6195	129	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (129) close contacts within the same asymmetric unit are listed below.

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:67:PHE:CE2	3:H:82:ILE:HG12	2.42	0.54
1:N:392:GLN:NE2	1:N:452:PHE:HE2	2.06	0.54
1:N:238:PRO:HB2	1:N:305:ILE:HD13	1.91	0.53
1:N:457:ASN:N	1:N:457:ASN:HD22	2.06	0.53
1:N:146:ASN:OD1	1:N:437:TRP:HB3	2.09	0.52
3:H:18:VAL:O	3:H:81:GLN:HA	2.10	0.52
2:L:23:CYS:HB2	2:L:35:TRP:HH2	1.75	0.52
2:L:115:VAL:HG22	2:L:136:LEU:HD23	1.92	0.52
1:N:275:ILE:HG12	1:N:303:ILE:HD11	1.91	0.52
3:H:162:ASN:OD1	3:H:205:ILE:HA	2.10	0.51
1:N:103:ASP:HB3	1:N:131:PHE:HE2	1.75	0.51
2:L:86:TYR:O	2:L:101:GLY:HA2	2.10	0.51
2:L:160:LEU:HD11	3:H:179:GLN:NE2	2.25	0.51
3:H:224:GLU:HG2	3:H:225:PRO:HD2	1.92	0.51
1:N:181:THR:HG22	1:N:192:ILE:HB	1.93	0.51
3:H:34:MET:O	3:H:50:TRP:HA	2.10	0.51
3:H:144:VAL:HB	3:H:187:LEU:HB3	1.93	0.50
1:N:395:GLN:HA	1:N:455:GLN:NE2	2.25	0.50
1:N:272:ALA:HA	1:N:316:TYR:HE1	1.76	0.50
3:H:39:GLN:O	3:H:88:ALA:HB1	2.11	0.49
1:N:293:ASP:HB3	1:N:297:GLY:HA3	1.94	0.49
3:H:199:TRP:CD1	3:H:205:ILE:HG12	2.46	0.49
2:L:125:LEU:O	2:L:183:LYS:HE2	2.11	0.49
1:N:457:ASN:ND2	1:N:457:ASN:H	2.10	0.49
1:N:333:VAL:HA	1:N:386:ASP:O	2.12	0.49
1:N:106:VAL:HG12	1:N:462:ALA:CB	2.43	0.49
2:L:61:ARG:HG2	2:L:61:ARG:HH11	1.78	0.48
3:H:123:PRO:HD3	3:H:221:LYS:HZ3	1.78	0.48
2:L:34:VAL:HG23	2:L:91:HIS:HD2	1.79	0.47
1:N:100:TYR:CE2	1:N:163:LEU:HD11	2.50	0.47
2:L:141:PRO:HG2	2:L:199:LYS:HD3	1.97	0.47
2:L:121:SER:OG	2:L:123:GLU:HG2	2.13	0.47
1:N:428:ARG:NH1	1:N:460:ASP:OD2	2.47	0.47
1:N:180:SER:HA	1:N:192:ILE:O	2.15	0.47
2:L:30:SER:O	2:L:31:THR:HB	2.14	0.46
3:H:1:GLN:HA	3:H:1:GLN:OE1	2.15	0.46
1:N:430:ARG:HE	1:N:437:TRP:HA	1.81	0.46
2:L:159:VAL:HA	2:L:178:THR:O	2.15	0.46
2:L:17:ASP:O	2:L:78:VAL:HG23	2.15	0.45
1:N:136:GLN:NE2	1:N:156:ARG:HD3	2.31	0.45
1:N:463:LYS:C	1:N:465:GLU:H	2.19	0.45
2:L:31:THR:HG22	2:L:50:TRP:HE3	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:231:VAL:HG11	1:N:282:GLY:HA3	1.97	0.45
2:L:4:MET:HB2	2:L:98:PHE:O	2.17	0.45
2:L:2:ILE:HD13	2:L:90:GLN:HE22	1.79	0.45
2:L:116:SER:O	2:L:134:CYS:HA	2.17	0.45
3:H:6:GLN:NE2	3:H:92:CYS:H	2.15	0.45
2:L:118:PHE:HE2	2:L:135:PHE:CD2	2.36	0.45
1:N:395:GLN:HG2	1:N:455:GLN:HE21	1.82	0.44
2:L:136:LEU:HD13	2:L:146:VAL:HG11	1.99	0.44
1:N:395:GLN:HA	1:N:455:GLN:HE21	1.82	0.44
1:N:360:THR:HG21	1:N:382:ALA:HB3	1.99	0.44
1:N:138:THR:HG21	1:N:145:SER:HA	1.98	0.44
3:H:98:ASN:O	3:H:99:PHE:HB2	2.16	0.44
3:H:2:ILE:HA	3:H:26:GLY:HA3	1.99	0.44
2:L:144:ILE:HG13	2:L:198:HIS:HB2	2.00	0.44
2:L:150:ILE:HG23	2:L:192:TYR:CE1	2.52	0.44
3:H:38:LYS:HB3	3:H:46:GLU:HB3	1.99	0.44
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.99	0.44
2:L:19:VAL:HG22	2:L:20:THR:N	2.33	0.43
3:H:123:PRO:HD3	3:H:221:LYS:HZ1	1.82	0.43
2:L:27:GLN:HE21	2:L:27:GLN:HB3	1.65	0.43
1:N:367:SER:HB3	1:N:370:SER:O	2.19	0.43
2:L:37:GLN:O	2:L:44:PRO:HA	2.19	0.43
3:H:30:THR:HG22	3:H:53:ASN:HD22	1.83	0.43
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.99	0.43
1:N:464:ILE:O	1:N:464:ILE:CG2	2.66	0.43
2:L:2:ILE:HD12	2:L:2:ILE:N	2.32	0.43
1:N:463:LYS:C	1:N:465:GLU:N	2.72	0.43
1:N:400:ASN:HB3	3:H:31:ASN:O	2.19	0.42
3:H:17:THR:HA	3:H:82:ILE:O	2.18	0.42
1:N:106:VAL:HG12	1:N:462:ALA:HB2	2.00	0.42
1:N:116:VAL:HG22	1:N:140:ILE:HA	2.01	0.42
1:N:355:LEU:HD13	1:N:383:LEU:HD13	2.01	0.42
2:L:2:ILE:HD11	2:L:93:SER:HB2	2.02	0.42
1:N:248:GLY:O	1:N:274:HIS:HD2	2.01	0.42
3:H:56:GLU:HA	3:H:57:PRO:HD3	1.70	0.42
1:N:430:ARG:NE	1:N:437:TRP:HA	2.34	0.42
1:N:379:VAL:CG1	1:N:388:SER:HB2	2.49	0.42
1:N:458:TRP:HA	1:N:459:PRO:HD2	1.80	0.42
1:N:188:ALA:HB3	1:N:207:TYR:CZ	2.55	0.42
2:L:174:SER:C	3:H:174:PHE:HE1	2.22	0.41
1:N:115:LEU:HD21	1:N:169:VAL:HG22	2.01	0.41
1:N:271:THR:O	1:N:273:LYS:HD2	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:126:PRO:HD2	1:N:184:HIS:CD2	2.55	0.41
3:H:33:GLY:HA2	3:H:52(A):THR:HG23	2.03	0.41
3:H:139:THR:HA	3:H:191:VAL:O	2.21	0.41
1:N:94:ILE:HD12	1:N:420:ALA:HB3	2.03	0.41
1:N:168:THR:HB	1:N:170:ASN:HD21	1.82	0.41
1:N:253:ARG:HG3	1:N:255:TYR:HE1	1.86	0.41
1:N:318:CYS:SG	1:N:383:LEU:O	2.79	0.41
1:N:140:ILE:HD13	1:N:140:ILE:HG21	1.80	0.40
1:N:94:ILE:HG21	1:N:97:TRP:CZ2	2.55	0.40
2:L:167:ASP:O	2:L:171:SER:HA	2.21	0.40
2:L:118:PHE:HA	2:L:119:PRO:HD2	1.79	0.40
3:H:34:MET:HB2	3:H:51:ILE:HG22	2.02	0.40
1:N:207:TYR:CE2	1:N:259:GLU:HG2	2.57	0.40
1:N:84:PHE:CE1	1:N:187:ARG:HD3	2.56	0.40
3:H:109:LEU:HD12	3:H:109:LEU:HA	1.83	0.40
1:N:81:ILE:HG13	1:N:83:GLU:N	2.30	0.40
1:N:427:ILE:O	1:N:428:ARG:HD2	2.21	0.40
2:L:175:MET:HG2	2:L:176:SER:N	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	387/389 (100%)	352 (91%)	33 (8%)	2 (0%)	38	79
2	L	212/214 (99%)	197 (93%)	14 (7%)	1 (0%)	38	79
3	H	219/221 (99%)	192 (88%)	21 (10%)	6 (3%)	8	30
All	All	818/824 (99%)	741 (91%)	68 (8%)	9 (1%)	21	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	295	TRP

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Mol	Chain	Res	Type
2	L	60	ASP
3	H	216	SER
3	H	226	ARG
1	N	222	ILE
3	H	43	LYS
3	H	102	TYR
3	H	180	SER
3	H	41	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	341/341 (100%)	303 (89%)	38 (11%)	9	26
2	L	190/190 (100%)	160 (84%)	30 (16%)	4	11
3	H	187/187 (100%)	162 (87%)	25 (13%)	6	15
All	All	718/718 (100%)	625 (87%)	93 (13%)	6	17

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	81	ILE
1	N	93	THR
1	N	99	ILE
1	N	118	ARG
1	N	127	ASP
1	N	134	LEU
1	N	136	GLN
1	N	140	ILE
1	N	141	ARG
1	N	168	THR
1	N	170	ASN
1	N	181	THR
1	N	189	ARG
1	N	204	VAL
1	N	224	ARG

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Mol	Chain	Res	Type
1	N	230	CYS
1	N	247	THR
1	N	253	ARG
1	N	269	THR
1	N	283	GLU
1	N	287	VAL
1	N	304	GLN
1	N	311	THR
1	N	313	THR
1	N	330	ASP
1	N	337	CYS
1	N	345	ASN
1	N	362	LEU
1	N	364	ARG
1	N	387	ARG
1	N	388	SER
1	N	391	THR
1	N	395	GLN
1	N	411	MET
1	N	441	ASN
1	N	444	VAL
1	N	445	SER
1	N	446	MET
2	L	2	ILE
2	L	5	THR
2	L	11	MET
2	L	22	THR
2	L	27	GLN
2	L	58	VAL
2	L	60	ASP
2	L	61	ARG
2	L	65	SER
2	L	70	ASP
2	L	77	SER
2	L	81	GLU
2	L	83	LEU
2	L	90	GLN
2	L	105	GLU
2	L	108	ARG
2	L	122	SER
2	L	142	LYS
2	L	145	ASN

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Mol	Chain	Res	Type
2	L	151	ASP
2	L	157	ASN
2	L	159	VAL
2	L	163	TRP
2	L	170	ASP
2	L	182	THR
2	L	184	ASP
2	L	195	GLU
2	L	197	THR
2	L	202	THR
2	L	203	SER
3	H	43	LYS
3	H	56	GLU
3	H	62	GLU
3	H	71	LEU
3	H	73	THR
3	H	76	SER
3	H	80	LEU
3	H	87	LYS
3	H	89	THR
3	H	108	THR
3	H	113	SER
3	H	133	THR
3	H	134	THR
3	H	140	LEU
3	H	151	PRO
3	H	156	THR
3	H	163	SER
3	H	184	LEU
3	H	194	THR
3	H	198	THR
3	H	202	SER
3	H	209	ASN
3	H	218	LYS
3	H	220	ASP
3	H	224	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	95	ASN
1	N	136	GLN

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Mol	Chain	Res	Type
1	N	144	HIS
1	N	170	ASN
1	N	226	GLN
1	N	315	GLN
1	N	345	ASN
1	N	346	ASN
1	N	395	GLN
1	N	441	ASN
1	N	455	GLN
1	N	457	ASN
2	L	27	GLN
2	L	38	GLN
2	L	138	ASN
3	H	6	GLN
3	H	39	GLN
3	H	53	ASN
3	H	82(B)	ASN
3	H	172	HIS
3	H	179	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	N	469(A)	1,4	12,14,15	0.85	0	15,19,21	1.37	2 (13%)
4	NAG	N	470(B)	4	12,14,15	0.72	0	15,19,21	1.53	2 (13%)
4	BMA	N	471(C)	4	10,11,12	1.20	1 (10%)	11,15,17	2.36	4 (36%)
4	MAN	N	472(D)	4	10,11,12	1.05	0	11,15,17	1.44	2 (18%)
4	MAN	N	473(E)	4	10,11,12	1.18	1 (10%)	11,15,17	1.41	1 (9%)
4	MAN	N	474(F)	4	10,11,12	1.24	2 (20%)	11,15,17	0.95	0
6	NAG	N	476(A)	1,6	12,14,15	0.84	0	15,19,21	1.45	3 (20%)
6	NAG	N	477(B)	6	12,14,15	0.84	0	15,19,21	2.29	4 (26%)

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	N	469(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	470(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	N	471(C)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	472(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	473(E)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	474(F)	4	-	0/2/19/22	0/1/1/1
6	NAG	N	476(A)	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	477(B)	6	-	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)
4	N	473(E)	MAN	C3-C2	2.77	1.59	1.52
4	N	474(F)	MAN	O3-C3	-2.12	1.37	1.43
4	N	471(C)	BMA	O5-C5	-2.06	1.41	1.45
4	N	474(F)	MAN	C3-C2	-2.01	1.48	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	477(B)	NAG	C3-C2-N2	-5.88	102.81	111.76
4	N	471(C)	BMA	O5-C5-C4	-5.03	104.27	110.65
6	N	477(B)	NAG	C2-N2-C7	3.60	129.13	123.09
4	N	471(C)	BMA	O5-C5-C6	3.46	110.61	106.98
4	N	470(B)	NAG	C3-C2-N2	-3.27	106.79	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	477(B)	NAG	O5-C5-C4	-2.95	106.90	110.65
4	N	469(A)	NAG	O5-C5-C4	-2.88	107.00	110.65
6	N	476(A)	NAG	C6-C5-C4	2.84	119.85	113.00
4	N	470(B)	NAG	C8-C7-N2	2.82	121.62	116.11
4	N	469(A)	NAG	O5-C5-C6	2.70	109.82	106.98
4	N	471(C)	BMA	O4-C4-C3	-2.66	104.38	110.35
6	N	476(A)	NAG	C4-C3-C2	-2.63	104.88	111.32
4	N	473(E)	MAN	O5-C5-C6	2.53	109.63	106.98
6	N	476(A)	NAG	O5-C5-C6	-2.40	104.46	106.98
4	N	472(D)	MAN	O3-C3-C4	-2.24	105.33	110.35
6	N	477(B)	NAG	C3-C4-C5	-2.16	106.34	110.20
4	N	472(D)	MAN	O5-C5-C4	-2.10	107.99	110.65
4	N	471(C)	BMA	C6-C5-C4	2.09	118.04	113.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	477(B)	NAG	C1-C2-N2-C7

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

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
5	NAG	N	475(A)	1	12,14,15	0.83	0	15,19,21	1.41	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
5	NAG	N	475(A)	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	N	475(A)	NAG	C8-C7-N2	3.21	122.37	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	N	389/389 (100%)	-1.01	0 100 100	2, 8, 24, 47	0
2	L	214/214 (100%)	-0.39	4 (1%) 64 72	4, 25, 42, 47	0
3	H	221/221 (100%)	-0.34	11 (4%) 28 33	4, 26, 40, 45	0
All	All	824/824 (100%)	-0.67	15 (1%) 65 74	2, 17, 38, 47	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	128	CYS	8.4
2	L	214	CYS	7.8
3	H	134	THR	6.5
3	H	135	GLY	6.3
3	H	129	GLY	5.7
3	H	130	ASP	5.2
3	H	227	GLY	5.1
2	L	211	ARG	5.1
2	L	213	GLU	5.1
3	H	133	THR	4.3
3	H	180	SER	4.2
2	L	212	ASN	3.7
3	H	183	ASP	2.6
3	H	136	SER	2.6
3	H	137	SER	2.0

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	N	477(B)	14/15	0.23	-	54,57,59,61	0
4	NAG	N	469(A)	14/15	0.11	-	5,11,23,24	0
4	MAN	N	473(E)	11/12	0.15	-	14,17,19,19	0
4	MAN	N	472(D)	11/12	0.12	-	9,11,14,19	0
4	NAG	N	470(B)	14/15	0.11	-	12,14,16,20	0
6	NAG	N	476(A)	14/15	0.23	-	41,46,53,57	0
4	BMA	N	471(C)	11/12	0.12	-	8,11,13,13	0
4	MAN	N	474(F)	11/12	0.12	-	11,13,15,16	0

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	CA	N	0	1/1	0.08	-	20,20,20,20	0
5	NAG	N	475(A)	14/15	0.20	-	37,40,44,46	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.