



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1NCB
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

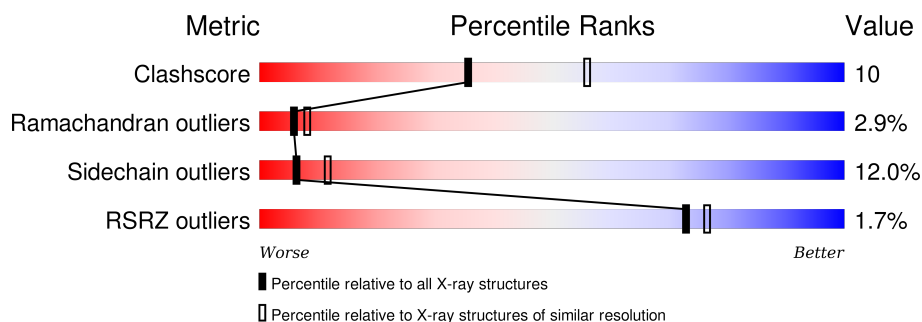
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>65%</div> <div>29%</div> <div>5%</div> </div>
2	L	214	<div> <div>2%</div> <div>58%</div> <div>32%</div> <div>9%</div> </div>
3	H	221	<div> <div>5%</div> <div>58%</div> <div>34%</div> <div>8%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	389	Total	C	N	O	S	0	0	0
			3075	1920	538	594	23			

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 21 discrepancies between the modelled and reference sequences:

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

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

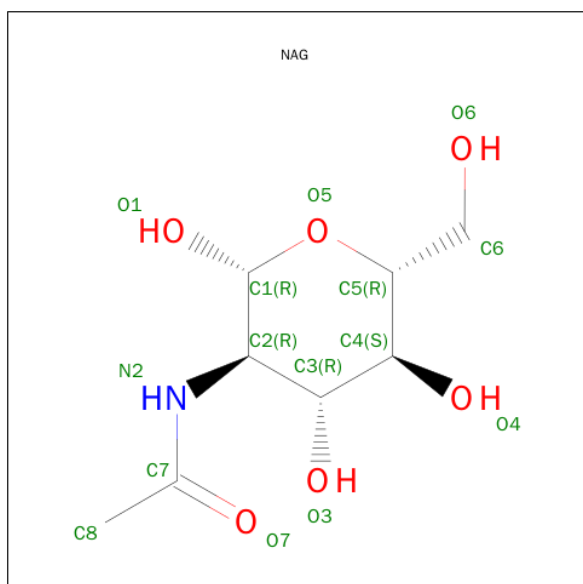
- Molecule 3 is a protein called IGG2A-KAPPA NC41 FAB (HEAVY CHAIN).

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

- Molecule 4 is 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: $C_8H_{15}NO_6$).



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	Ca	0	0
			1	1		

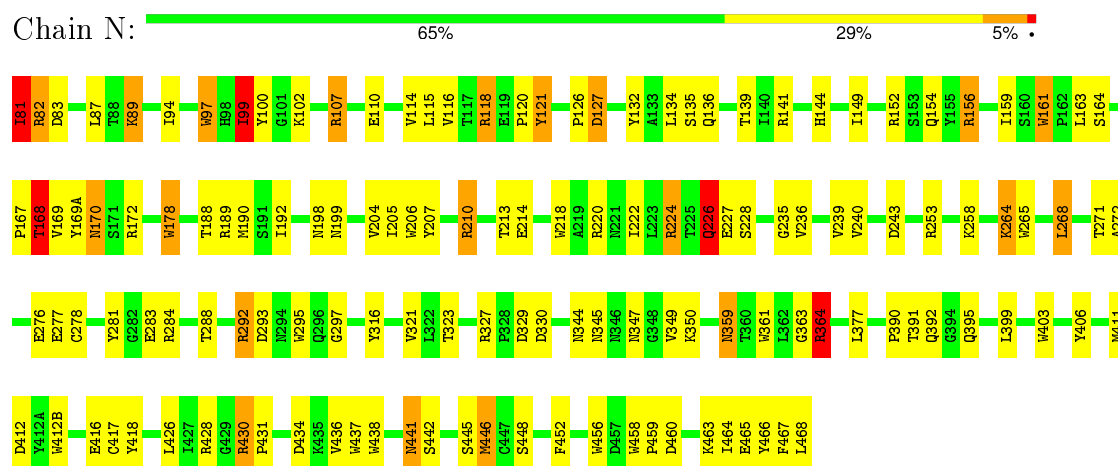
- Molecule 8 is water.

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

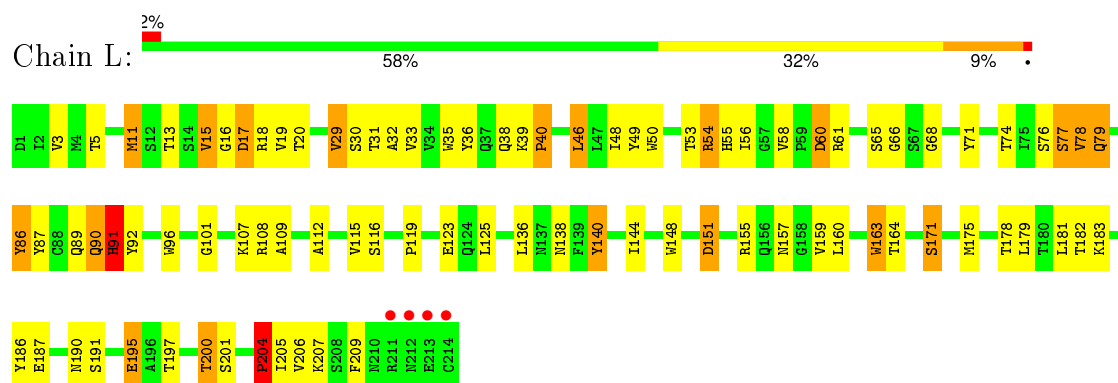
3 Residue-property plots

These plots are drawn for all protein, RNA 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.

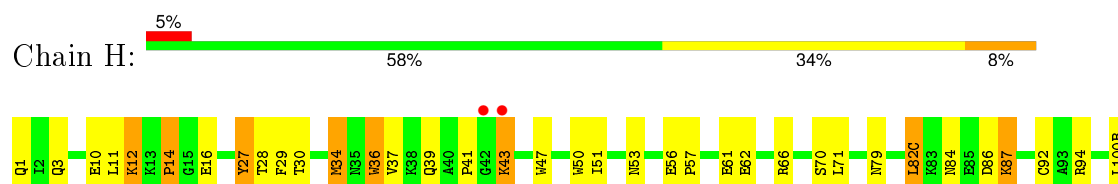
• Molecule 1: INFLUENZA A SUBTYPE N9 NEURAMINIDASE

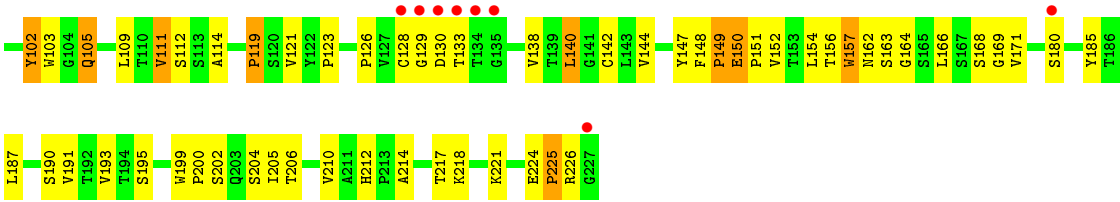


• Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)



• 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, 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) 33.0 (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}	0.165 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 19343 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6594	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	1.04	2/3158 (0.1%)	1.84	82/4301 (1.9%)
2	L	0.90	0/1708	1.83	47/2323 (2.0%)
3	H	0.86	0/1707	1.73	30/2326 (1.3%)
All	All	0.96	2/6573 (0.0%)	1.81	159/8950 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	5
2	L	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	297	GLY	C-O	5.42	1.32	1.23
1	N	403	TRP	CD1-NE1	-5.09	1.29	1.38

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	54	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	N	284	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	N	218	TRP	CD1-CG-CD2	10.33	114.56	106.30
2	L	148	TRP	CD1-CG-CD2	10.13	114.40	106.30
3	H	36	TRP	CD1-CG-CD2	9.37	113.79	106.30
3	H	103	TRP	CD1-CG-CD2	9.37	113.79	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	50	TRP	CD1-CG-CD2	9.31	113.75	106.30
2	L	140	TYR	CB-CG-CD1	-9.21	115.48	121.00
2	L	96	TRP	CD1-CG-CD2	9.13	113.60	106.30
1	N	361	TRP	CD1-CG-CD2	8.63	113.21	106.30
1	N	297	GLY	CA-C-N	-8.39	98.74	117.20
2	L	96	TRP	CE2-CD2-CG	-8.27	100.69	107.30
1	N	218	TRP	CE2-CD2-CG	-8.22	100.72	107.30
3	H	157	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	N	437	TRP	CD1-CG-CD2	7.84	112.57	106.30
2	L	50	TRP	CE2-CD2-CG	-7.84	101.03	107.30
2	L	148	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	N	178	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	N	243	ASP	CB-CG-OD1	7.74	125.27	118.30
2	L	79	GLN	CA-CB-CG	7.69	130.32	113.40
3	H	50	TRP	CD1-CG-CD2	7.66	112.42	106.30
1	N	293	ASP	CA-C-N	-7.60	100.48	117.20
1	N	438	TRP	CG-CD2-CE3	7.52	140.66	133.90
3	H	36	TRP	CE2-CD2-CG	-7.52	101.29	107.30
2	L	155	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	L	163	TRP	CD1-CG-CD2	7.39	112.21	106.30
3	H	185	TYR	CB-CG-CD2	-7.37	116.58	121.00
3	H	157	TRP	CE2-CD2-CG	-7.34	101.43	107.30
3	H	94	ARG	CB-CG-CD	-7.31	92.59	111.60
1	N	265	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	N	412(B)	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	N	218	TRP	CG-CD1-NE1	-7.20	102.90	110.10
1	N	403	TRP	CE2-CD2-CG	-7.20	101.54	107.30
3	H	103	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	N	161	TRP	CD1-CG-CD2	7.18	112.04	106.30
1	N	456	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	N	265	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	N	178	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	N	161	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	N	456	TRP	CD1-CG-CD2	7.11	111.98	106.30
2	L	54	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	N	430	ARG	NE-CZ-NH1	7.03	123.82	120.30
2	L	163	TRP	CE2-CD2-CG	-7.03	101.67	107.30
2	L	61	ARG	NE-CZ-NH2	-7.02	116.79	120.30
3	H	152	VAL	CG1-CB-CG2	-7.02	99.67	110.90
1	N	437	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	L	87	TYR	CB-CG-CD1	-7.00	116.80	121.00
1	N	297	GLY	O-C-N	7.00	133.90	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	361	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	N	295	TRP	CD1-CG-CD2	6.91	111.83	106.30
1	N	403	TRP	CD1-CG-CD2	6.86	111.79	106.30
1	N	218	TRP	CG-CD2-CE3	6.82	140.04	133.90
1	N	347	ASN	CA-C-N	-6.79	102.62	116.20
1	N	412(B)	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	N	438	TRP	CB-CG-CD1	-6.72	118.27	127.00
1	N	190	MET	CA-CB-CG	-6.71	101.89	113.30
3	H	27	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	N	132	TYR	CB-CG-CD2	-6.65	117.01	121.00
3	H	47	TRP	CE2-CD2-CG	-6.64	101.99	107.30
2	L	33	VAL	CA-CB-CG2	-6.52	101.12	110.90
3	H	50	TRP	CE2-CD2-CG	-6.50	102.10	107.30
2	L	201	SER	CA-C-N	-6.49	102.92	117.20
1	N	121	TYR	CA-CB-CG	6.48	125.71	113.40
1	N	156	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	L	107	LYS	CA-C-N	-6.44	103.03	117.20
2	L	78	VAL	CG1-CB-CG2	-6.37	100.70	110.90
3	H	103	TRP	CG-CD1-NE1	-6.36	103.74	110.10
1	N	127	ASP	N-CA-CB	-6.33	99.21	110.60
1	N	210	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	L	3	VAL	CA-CB-CG2	-6.28	101.48	110.90
1	N	292	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	N	295	TRP	CE2-CD2-CG	-6.22	102.33	107.30
1	N	97	TRP	CE2-CD2-CG	-6.21	102.33	107.30
2	L	11	MET	CG-SD-CE	-6.12	90.41	100.20
3	H	57	PRO	CA-C-N	-6.11	103.75	117.20
3	H	36	TRP	CG-CD1-NE1	-6.10	104.00	110.10
2	L	35	TRP	CE2-CD2-CG	-6.09	102.43	107.30
1	N	239	VAL	CG1-CB-CG2	-6.07	101.18	110.90
3	H	47	TRP	CD1-CG-CD2	6.05	111.14	106.30
2	L	36	TYR	CB-CG-CD2	-6.04	117.37	121.00
2	L	148	TRP	CG-CD1-NE1	-6.04	104.06	110.10
1	N	438	TRP	CD1-CG-CD2	6.03	111.12	106.30
1	N	412(B)	TRP	CB-CG-CD1	-6.01	119.19	127.00
1	N	428	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	N	391	THR	CA-CB-CG2	-5.98	104.03	112.40
3	H	102	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	N	206	TRP	CE2-CD2-CG	-5.96	102.53	107.30
2	L	50	TRP	CG-CD1-NE1	-5.94	104.16	110.10
1	N	438	TRP	CE2-CD2-CG	-5.93	102.55	107.30
1	N	264	LYS	CA-CB-CG	5.91	126.40	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	364	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	N	293	ASP	CA-C-O	5.88	132.44	120.10
2	L	163	TRP	CG-CD2-CE3	5.86	139.17	133.90
1	N	107	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	H	199	TRP	CE2-CD2-CG	-5.85	102.62	107.30
1	N	268	LEU	CA-CB-CG	5.83	128.71	115.30
1	N	361	TRP	CG-CD2-CE3	5.77	139.10	133.90
1	N	361	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	N	468	LEU	CA-C-O	-5.75	108.01	120.10
2	L	91	HIS	CA-CB-CG	5.73	123.35	113.60
1	N	99	ILE	CB-CA-C	-5.72	100.16	111.60
1	N	292	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	N	412	ASP	CB-CG-OD1	5.70	123.43	118.30
1	N	363	GLY	O-C-N	5.69	131.80	122.70
3	H	105	GLN	CG-CD-NE2	5.67	130.32	116.70
2	L	49	TYR	CB-CG-CD1	-5.66	117.60	121.00
1	N	218	TRP	CB-CG-CD1	-5.65	119.65	127.00
2	L	15	VAL	CA-CB-CG2	-5.62	102.47	110.90
3	H	12	LYS	CA-CB-CG	5.62	125.77	113.40
3	H	57	PRO	O-C-N	5.55	131.58	122.70
3	H	3	GLN	CA-CB-CG	5.52	125.54	113.40
2	L	171	SER	N-CA-CB	-5.51	102.23	110.50
1	N	243	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	N	161	TRP	CB-CG-CD1	-5.50	119.85	127.00
2	L	205	ILE	N-CA-C	-5.49	96.19	111.00
3	H	50	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	N	107	ARG	NE-CZ-NH2	-5.47	117.56	120.30
3	H	34	MET	CG-SD-CE	-5.46	91.46	100.20
1	N	189	ARG	CA-C-N	-5.45	105.21	117.20
1	N	81	ILE	N-CA-C	-5.45	96.29	111.00
3	H	128	CYS	CA-CB-SG	5.44	123.79	114.00
2	L	61	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	N	226	GLN	CA-CB-CG	5.42	125.32	113.40
1	N	169	VAL	CG1-CB-CG2	-5.41	102.24	110.90
3	H	111	VAL	CA-CB-CG2	-5.40	102.80	110.90
2	L	35	TRP	CD1-CG-CD2	5.38	110.61	106.30
2	L	148	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	N	127	ASP	N-CA-C	5.37	125.51	111.00
1	N	97	TRP	CD1-CG-CD2	5.35	110.58	106.30
2	L	92	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	N	132	TYR	CG-CD2-CE2	-5.34	117.03	121.30
2	L	29	VAL	N-CA-CB	-5.33	99.77	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	86	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	N	466	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	N	169(A)	TYR	CB-CG-CD1	-5.28	117.83	121.00
3	H	199	TRP	CD1-CG-CD2	5.27	110.52	106.30
1	N	412(B)	TRP	CG-CD2-CE3	5.26	138.64	133.90
2	L	151	ASP	CB-CG-OD1	5.26	123.03	118.30
2	L	186	TYR	CB-CG-CD1	-5.24	117.85	121.00
1	N	168	THR	N-CA-CB	-5.21	100.39	110.30
2	L	61	ARG	CB-CG-CD	-5.20	98.08	111.60
2	L	96	TRP	CB-CG-CD1	-5.18	120.27	127.00
2	L	163	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	N	236	VAL	CG1-CB-CG2	-5.15	102.66	110.90
3	H	128	CYS	CA-C-N	5.12	126.44	116.20
1	N	82	ARG	N-CA-C	-5.11	97.20	111.00
2	L	96	TRP	CG-CD1-NE1	-5.09	105.01	110.10
3	H	86	ASP	CB-CG-OD1	5.08	122.88	118.30
1	N	213	THR	CA-CB-CG2	5.08	119.51	112.40
1	N	344	ASN	CA-C-N	-5.08	106.03	117.20
1	N	327	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	N	361	TRP	CB-CG-CD1	-5.06	120.42	127.00
2	L	140	TYR	CA-CB-CG	-5.05	103.81	113.40
1	N	172	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	N	226	GLN	N-CA-C	5.03	124.57	111.00
2	L	58	VAL	N-CA-C	-5.02	97.44	111.00
1	N	116	VAL	N-CA-C	-5.02	97.45	111.00
2	L	163	TRP	CG-CD1-NE1	-5.02	105.08	110.10
2	L	148	TRP	CB-CG-CD1	-5.00	120.50	127.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	140	TYR	Sidechain
2	L	209	PHE	Peptide
1	N	107	ARG	Sidechain
1	N	118	ARG	Sidechain
1	N	210	ARG	Sidechain
1	N	224	ARG	Sidechain
1	N	406	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	3075	0	2902	59	0
2	L	1667	0	1598	31	0
3	H	1665	0	1612	35	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	66	0	0	3	0
All	All	6594	0	6211	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:TRP:H	1:N:395:GLN:HE22	1.32	0.76
1:N:442:SER:HB2	1:N:460:ASP:OD1	1.94	0.66
1:N:192:ILE:HG12	1:N:205:ILE:HG13	1.78	0.66
1:N:272:ALA:HA	1:N:316:TYR:CE1	2.30	0.66
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.80	0.63
2:L:38:GLN:HE22	3:H:39:GLN:HE22	1.46	0.62
1:N:152:ARG:HD2	1:N:198:ASN:HD21	1.65	0.61
2:L:195:GLU:HB2	2:L:206:VAL:HG13	1.81	0.60
2:L:46:LEU:HD22	2:L:55:HIS:HB2	1.84	0.60
3:H:140:LEU:HD11	3:H:205:ILE:HD12	1.84	0.59
1:N:97:TRP:N	1:N:395:GLN:HE22	2.01	0.59
1:N:364:ARG:HH11	1:N:377:LEU:HD11	1.68	0.59
3:H:154:LEU:HG	3:H:210:VAL:HG22	1.86	0.58
3:H:123:PRO:HD3	3:H:221:LYS:HG3	1.85	0.57
1:N:430:ARG:HG2	1:N:434:ASP:HA	1.86	0.57
3:H:16:GLU:O	3:H:82(C):LEU:HG	2.05	0.57
1:N:94:ILE:HG23	1:N:448:SER:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:THR:H	1:N:170:ASN:HD21	1.52	0.56
1:N:226:GLN:HE22	1:N:240:VAL:H	1.53	0.56
2:L:159:VAL:HA	2:L:178:THR:O	2.06	0.56
2:L:54:ARG:NE	2:L:60:ASP:HA	2.21	0.56
2:L:115:VAL:O	2:L:207:LYS:HE3	2.06	0.55
1:N:121:TYR:CG	1:N:228:SER:HA	2.42	0.55
1:N:89:LYS:HG2	1:N:417:CYS:HA	1.89	0.54
1:N:114:VAL:O	1:N:139:THR:HA	2.07	0.54
1:N:272:ALA:HA	1:N:316:TYR:HE1	1.70	0.53
3:H:200:PRO:HB3	3:H:225:PRO:HG3	1.91	0.53
2:L:30:SER:O	2:L:31:THR:HB	2.08	0.53
1:N:168:THR:HB	1:N:170:ASN:ND2	2.24	0.52
1:N:426:LEU:HB2	1:N:442:SER:HB3	1.91	0.52
1:N:411:MET:SD	1:N:418:TYR:HB3	2.50	0.51
1:N:199:ASN:HA	1:N:220:ARG:O	2.11	0.51
1:N:276:GLU:HB2	1:N:292:ARG:HD3	1.91	0.51
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.93	0.51
1:N:152:ARG:HD2	1:N:198:ASN:ND2	2.26	0.51
1:N:94:ILE:HG12	1:N:359:ASN:ND2	2.26	0.51
2:L:38:GLN:HE22	3:H:39:GLN:NE2	2.09	0.51
3:H:121:VAL:HG22	3:H:144:VAL:HG13	1.94	0.50
3:H:84:ASN:HA	3:H:111:VAL:HG11	1.94	0.49
1:N:115:LEU:HD12	1:N:159:ILE:HD13	1.94	0.49
1:N:276:GLU:HB2	1:N:292:ARG:HB3	1.95	0.49
3:H:87:LYS:HA	3:H:109:LEU:O	2.13	0.49
1:N:392:GLN:HE22	1:N:452:PHE:HE1	1.60	0.49
3:H:30:THR:HG22	3:H:53:ASN:HD22	1.78	0.48
3:H:166:LEU:HD23	3:H:191:VAL:HG21	1.96	0.48
3:H:12:LYS:O	3:H:111:VAL:HA	2.14	0.48
2:L:17:ASP:O	2:L:78:VAL:HG23	2.14	0.47
2:L:13:THR:HG21	2:L:78:VAL:HG21	1.95	0.47
1:N:144:HIS:HD2	8:N:39:HOH:O	1.98	0.47
1:N:110:GLU:HB2	1:N:467:PHE:CZ	2.50	0.47
1:N:81:ILE:HG23	1:N:83:ASP:O	2.15	0.47
1:N:426:LEU:O	1:N:441:ASN:HA	2.15	0.47
1:N:281:TYR:CE1	1:N:288:THR:HB	2.51	0.46
3:H:150:GLU:OE1	3:H:151:PRO:HA	2.16	0.46
3:H:156:THR:HB	3:H:164:GLY:H	1.81	0.46
2:L:48:ILE:HA	2:L:53:THR:O	2.14	0.46
2:L:115:VAL:HG22	2:L:136:LEU:HG	1.97	0.46
3:H:169:GLY:O	3:H:191:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:GLN:NE2	3:H:39:GLN:HE22	2.11	0.46
2:L:136:LEU:HD23	2:L:144:ILE:HD13	1.98	0.46
2:L:66:GLY:HA3	2:L:71:TYR:CD1	2.51	0.46
1:N:463:LYS:C	1:N:465:GLU:H	2.19	0.45
2:L:32:ALA:HA	2:L:91:HIS:CE1	2.52	0.45
1:N:149:ILE:HD11	1:N:431:PRO:HD3	1.98	0.45
1:N:81:ILE:HG13	1:N:82:ARG:H	1.83	0.44
3:H:212:HIS:HB3	3:H:217:THR:HB	1.99	0.44
1:N:436:VAL:CG1	1:N:464:ILE:HD12	2.47	0.44
2:L:108:ARG:HG2	2:L:109:ALA:N	2.33	0.44
1:N:97:TRP:HB3	1:N:446:MET:HG2	1.99	0.44
1:N:100:TYR:CE2	1:N:163:LEU:HD11	2.53	0.43
2:L:16:GLY:HA2	2:L:77:SER:HA	1.99	0.43
2:L:89:GLN:HG2	2:L:90:GLN:N	2.33	0.43
1:N:99:ILE:HG13	1:N:99:ILE:H	1.52	0.43
1:N:281:TYR:HA	8:N:57:HOH:O	2.18	0.43
1:N:89:LYS:HG2	1:N:416:GLU:O	2.18	0.43
3:H:11:LEU:HD11	3:H:148:PHE:HE2	1.83	0.43
3:H:11:LEU:HD13	3:H:149:PRO:HB3	2.01	0.43
1:N:277:GLU:HG3	8:N:32:HOH:O	2.18	0.43
3:H:212:HIS:CE1	3:H:214:ALA:HB3	2.53	0.43
2:L:18:ARG:HG3	2:L:18:ARG:HH11	1.84	0.43
1:N:436:VAL:HG11	1:N:464:ILE:HD12	2.00	0.43
1:N:464:ILE:O	1:N:464:ILE:CG2	2.66	0.43
3:H:27:TYR:CE1	3:H:29:PHE:HA	2.53	0.43
3:H:34:MET:HB2	3:H:51:ILE:HG22	2.00	0.43
2:L:19:VAL:O	2:L:74:THR:HA	2.19	0.43
3:H:1:GLN:HA	3:H:1:GLN:OE1	2.18	0.43
2:L:55:HIS:CE1	2:L:56:ILE:HG22	2.53	0.43
1:N:323:THR:HA	1:N:364:ARG:HB3	2.00	0.43
1:N:463:LYS:C	1:N:465:GLU:N	2.72	0.43
3:H:138:VAL:HG13	3:H:193:VAL:HG23	2.00	0.43
1:N:89:LYS:HB2	1:N:418:TYR:CE2	2.54	0.43
1:N:235:GLY:O	1:N:258:LYS:HA	2.19	0.43
1:N:135:SER:O	1:N:156:ARG:HA	2.19	0.42
3:H:162:ASN:ND2	3:H:206:THR:H	2.17	0.42
1:N:81:ILE:N	1:N:126:PRO:HG2	2.34	0.42
1:N:321:VAL:HG21	1:N:390:PRO:HD3	2.00	0.42
1:N:188:THR:HG22	1:N:207:TYR:CZ	2.54	0.42
1:N:226:GLN:HG3	1:N:278:CYS:O	2.19	0.42
1:N:161:TRP:CH2	1:N:167:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:152:ARG:HH11	1:N:198:ASN:HD21	1.66	0.42
1:N:458:TRP:HA	1:N:459:PRO:HD2	1.80	0.42
3:H:114:ALA:HB3	3:H:148:PHE:CE2	2.55	0.41
3:H:43:LYS:HD2	3:H:43:LYS:HA	1.96	0.41
2:L:195:GLU:HG3	2:L:204:PRO:HB3	2.01	0.41
2:L:29:VAL:HG21	2:L:90:GLN:HG2	2.03	0.41
1:N:102:LYS:O	1:N:164:SER:HB3	2.20	0.41
2:L:32:ALA:HB1	2:L:91:HIS:ND1	2.36	0.41
1:N:94:ILE:HG12	1:N:359:ASN:HD21	1.86	0.41
3:H:140:LEU:HD23	3:H:140:LEU:N	2.36	0.41
3:H:171:VAL:HG22	3:H:191:VAL:HG23	2.03	0.41
2:L:108:ARG:HG2	2:L:109:ALA:H	1.86	0.41
1:N:277:GLU:HB3	1:N:350:LYS:HD2	2.03	0.41
3:H:142:CYS:HB2	3:H:157:TRP:CH2	2.56	0.41
3:H:66:ARG:HD2	3:H:66:ARG:HH11	1.70	0.41
3:H:140:LEU:HD21	3:H:193:VAL:HG22	2.03	0.40
1:N:168:THR:H	1:N:170:ASN:ND2	2.18	0.40
2:L:159:VAL:HG22	2:L:179:LEU:HD12	2.03	0.40
3:H:36:TRP:CZ3	3:H:92:CYS:HB3	2.55	0.40
2:L:39:LYS:HG3	2:L:40:PRO:HD2	2.02	0.40
2:L:86:TYR:O	2:L:101:GLY:HA2	2.21	0.40
1:N:152:ARG:HB2	1:N:178:TRP:CG	2.56	0.40
2:L:125:LEU:O	2:L:183:LYS:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	387/389 (100%)	343 (89%)	40 (10%)	4 (1%)	19	34
2	L	212/214 (99%)	190 (90%)	14 (7%)	8 (4%)	4	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	219/221 (99%)	191 (87%)	16 (7%)	12 (6%)	2	2
All	All	818/824 (99%)	724 (88%)	70 (9%)	24 (3%)	6	8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	222	ILE
2	L	157	ASN
2	L	171	SER
3	H	163	SER
3	H	226	ARG
2	L	60	ASP
3	H	62	GLU
3	H	102	TYR
1	N	226	GLN
2	L	204	PRO
3	H	14	PRO
3	H	41	PRO
3	H	43	LYS
3	H	180	SER
1	N	359	ASN
3	H	82(C)	LEU
3	H	130	ASP
3	H	225	PRO
2	L	40	PRO
2	L	119	PRO
2	L	187	GLU
3	H	129	GLY
2	L	68	GLY
1	N	349	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	342/342 (100%)	311 (91%)	31 (9%)	12	22
2	L	190/190 (100%)	162 (85%)	28 (15%)	4	7
3	H	187/187 (100%)	160 (86%)	27 (14%)	4	7
All	All	719/719 (100%)	633 (88%)	86 (12%)	6	12

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	81	ILE
1	N	87	LEU
1	N	89	LYS
1	N	99	ILE
1	N	118	ARG
1	N	120	PRO
1	N	127	ASP
1	N	134	LEU
1	N	136	GLN
1	N	141	ARG
1	N	154	GLN
1	N	168	THR
1	N	170	ASN
1	N	204	VAL
1	N	214	GLU
1	N	224	ARG
1	N	226	GLN
1	N	227	GLU
1	N	253	ARG
1	N	264	LYS
1	N	268	LEU
1	N	271	THR
1	N	283	GLU
1	N	329	ASP
1	N	330	ASP
1	N	345	ASN
1	N	364	ARG
1	N	399	LEU
1	N	441	ASN
1	N	445	SER
1	N	446	MET
2	L	5	THR
2	L	11	MET
2	L	15	VAL

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Mol	Chain	Res	Type
2	L	17	ASP
2	L	20	THR
2	L	46	LEU
2	L	65	SER
2	L	76	SER
2	L	77	SER
2	L	79	GLN
2	L	90	GLN
2	L	91	HIS
2	L	116	SER
2	L	123	GLU
2	L	138	ASN
2	L	151	ASP
2	L	160	LEU
2	L	163	TRP
2	L	164	THR
2	L	175	MET
2	L	181	LEU
2	L	182	THR
2	L	190	ASN
2	L	191	SER
2	L	195	GLU
2	L	197	THR
2	L	200	THR
2	L	204	PRO
3	H	10	GLU
3	H	14	PRO
3	H	28	THR
3	H	37	VAL
3	H	56	GLU
3	H	61	GLU
3	H	70	SER
3	H	71	LEU
3	H	79	ASN
3	H	87	LYS
3	H	100(B)	LEU
3	H	105	GLN
3	H	112	SER
3	H	119	PRO
3	H	126	PRO
3	H	133	THR
3	H	140	LEU

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Mol	Chain	Res	Type
3	H	149	PRO
3	H	150	GLU
3	H	168	SER
3	H	187	LEU
3	H	190	SER
3	H	195	SER
3	H	202	SER
3	H	204	SER
3	H	218	LYS
3	H	224	GLU

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

Mol	Chain	Res	Type
1	N	144	HIS
1	N	154	GLN
1	N	170	ASN
1	N	198	ASN
1	N	226	GLN
1	N	325	ASN
1	N	345	ASN
1	N	381	ASN
1	N	392	GLN
1	N	395	GLN
1	N	441	ASN
1	N	455	GLN
2	L	55	HIS
3	H	6	GLN
3	H	39	GLN
3	H	53	ASN
3	H	79	ASN
3	H	81	GLN
3	H	82(A)	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 ⓘ

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	14,14,15	0.70	0	15,19,21	0.87	0
4	NAG	N	470(B)	4	14,14,15	1.05	0	15,19,21	1.90	2 (13%)
4	BMA	N	471(C)	4	11,11,12	0.91	0	14,15,17	0.99	1 (7%)
4	MAN	N	472(D)	4	11,11,12	0.56	0	14,15,17	1.19	1 (7%)
4	MAN	N	473(E)	4	11,11,12	1.15	1 (9%)	14,15,17	1.35	3 (21%)
4	MAN	N	474(F)	4	11,11,12	1.13	0	14,15,17	1.53	3 (21%)
6	NAG	N	476(A)	1,6	14,14,15	0.52	0	15,19,21	1.52	2 (13%)
6	NAG	N	477(B)	6	14,14,15	0.94	1 (7%)	15,19,21	1.20	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	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	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	473(E)	MAN	C2-C3	2.24	1.55	1.52
6	N	477(B)	NAG	C1-C2	2.24	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	477(B)	NAG	C4-C3-C2	-3.33	106.05	111.23
4	N	472(D)	MAN	O2-C2-C1	-3.10	102.98	109.21
4	N	470(B)	NAG	C4-C3-C2	-2.44	107.43	111.23
4	N	473(E)	MAN	C6-C5-C4	-2.44	107.01	113.02
4	N	473(E)	MAN	O3-C3-C4	-2.12	105.55	110.34
4	N	474(F)	MAN	O4-C4-C3	-2.01	105.82	110.34
4	N	471(C)	BMA	C1-O5-C5	2.30	115.16	112.25
4	N	473(E)	MAN	C3-C4-C5	2.40	114.38	110.20
4	N	474(F)	MAN	O5-C5-C6	2.58	112.94	107.35
6	N	476(A)	NAG	C6-C5-C4	2.80	119.92	113.02
4	N	474(F)	MAN	C1-O5-C5	2.90	115.93	112.25
6	N	476(A)	NAG	C2-N2-C7	4.15	128.38	123.04
4	N	470(B)	NAG	C1-O5-C5	6.15	120.05	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	14,14,15	0.82	0	15,19,21	1.68	2 (13%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(A)	NAG	C4-C3-C2	-2.77	106.93	111.23
5	N	475(A)	NAG	C1-O5-C5	4.66	118.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	N	389/389 (100%)	-1.44	0 100 100	2, 8, 24, 48	0
2	L	214/214 (100%)	-0.99	4 (1%) 70 73	5, 26, 42, 47	0
3	H	221/221 (100%)	-0.84	10 (4%) 37 42	4, 26, 41, 46	0
All	All	824/824 (100%)	-1.16	14 (1%) 73 76	2, 18, 39, 48	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	128	CYS	7.5
2	L	214	CYS	5.3
3	H	133	THR	4.7
3	H	227	GLY	4.5
2	L	212	ASN	4.0
3	H	134	THR	4.0
3	H	42	GLY	4.0
2	L	211	ARG	3.7
3	H	130	ASP	3.5
3	H	180	SER	3.3
3	H	129	GLY	3.2
2	L	213	GLU	2.4
3	H	135	GLY	2.3
3	H	43	LYS	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	BMA	N	471(C)	11/12	0.98	0.07	1.49	8,12,14,15	0
4	NAG	N	470(B)	14/15	0.99	0.06	0.28	12,14,17,18	0
4	NAG	N	469(A)	14/15	0.99	0.06	-0.01	6,11,22,24	0
4	MAN	N	474(F)	11/12	0.99	0.05	-1.41	11,13,15,16	0
6	NAG	N	476(A)	14/15	0.91	0.15	-	42,47,53,56	0
4	MAN	N	472(D)	11/12	0.97	0.08	-	8,11,14,18	0
6	NAG	N	477(B)	14/15	0.86	0.18	-	55,57,60,61	0
4	MAN	N	473(E)	11/12	0.99	0.07	-	15,17,19,20	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, 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	LLDF	B-factors(Å ²)	Q<0.9
7	CA	N	0	1/1	0.99	0.07	0.96	27,27,27,27	0
5	NAG	N	475(A)	14/15	0.91	0.14	0.25	37,40,45,45	0

6.5 Other polymers

There are no such residues in this entry.