



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:05 PM 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 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

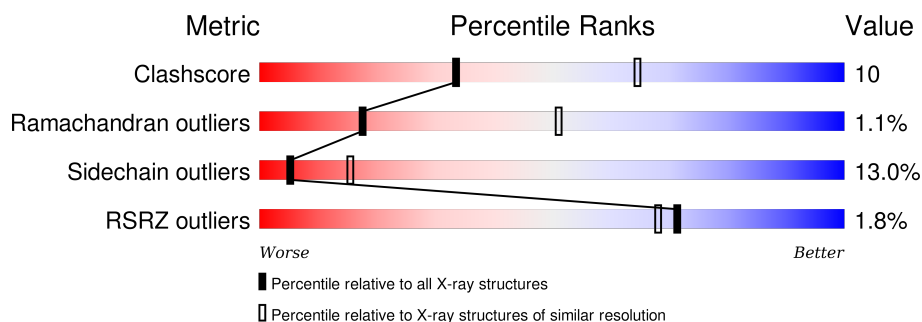
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 ≥ 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	
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 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
			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

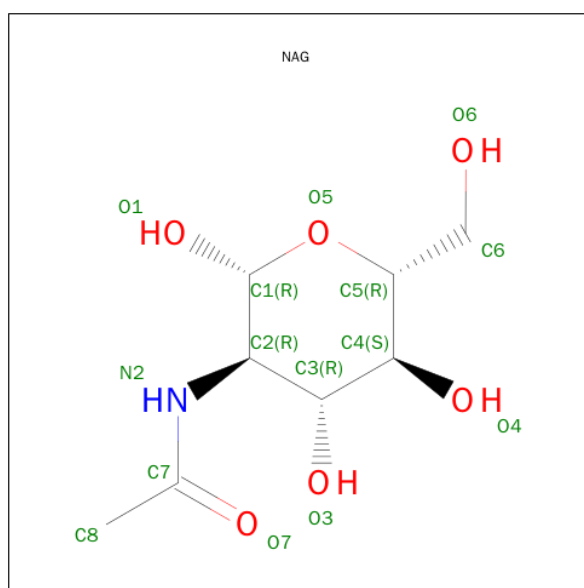
- Molecule 3 is a protein called IGG2A-KAPPA NC41 FAB (HEAVY CHAIN).

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: $C_8H_{15}NO_6$).



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 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.00 Å 167.00 Å 124.00 Å 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) 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.6	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 31846 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	6585	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 3.69% 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	1.02	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 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	3069	0	2886	62	0
2	L	1667	0	1598	38	0
3	H	1665	0	1612	34	0
4	N	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (129) 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)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:THR:HG22	2:L:50:TRP:HE3	1.82	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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%)	352 (91%)	33 (8%)	2 (0%)	34 71
2	L	212/214 (99%)	197 (93%)	14 (7%)	1 (0%)	34 71
3	H	219/221 (99%)	192 (88%)	21 (10%)	6 (3%)	6 25
All	All	818/824 (99%)	741 (91%)	68 (8%)	9 (1%)	17 51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	295	TRP
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%)	8	22
2	L	190/190 (100%)	160 (84%)	30 (16%)	3	9
3	H	187/187 (100%)	162 (87%)	25 (13%)	5	13
All	All	718/718 (100%)	625 (87%)	93 (13%)	5	15

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

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Mol	Chain	Res	Type
1	N	189	ARG
1	N	204	VAL
1	N	224	ARG
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

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Mol	Chain	Res	Type
2	L	122	SER
2	L	142	LYS
2	L	145	ASN
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
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 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	1.03	0	15,19,21	1.02	0
4	NAG	N	470(B)	4	14,14,15	0.82	0	15,19,21	1.40	2 (13%)
4	BMA	N	471(C)	4	11,11,12	1.23	1 (9%)	14,15,17	1.46	3 (21%)
4	MAN	N	472(D)	4	11,11,12	1.00	0	14,15,17	1.70	3 (21%)
4	MAN	N	473(E)	4	11,11,12	1.70	1 (9%)	14,15,17	1.08	0
4	MAN	N	474(F)	4	11,11,12	1.45	2 (18%)	14,15,17	2.19	1 (7%)
6	NAG	N	476(A)	1,6	14,14,15	0.79	0	15,19,21	1.59	2 (13%)
6	NAG	N	477(B)	6	14,14,15	1.21	1 (7%)	15,19,21	2.31	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	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	474(F)	MAN	C2-C3	-2.98	1.48	1.52
4	N	474(F)	MAN	O3-C3	-2.14	1.37	1.43
4	N	471(C)	BMA	C2-C3	2.98	1.56	1.52
6	N	477(B)	NAG	C1-C2	4.11	1.58	1.52
4	N	473(E)	MAN	C2-C3	4.72	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	476(A)	NAG	C4-C3-C2	-4.09	104.88	111.23
4	N	472(D)	MAN	O2-C2-C1	-3.59	102.00	109.21
6	N	477(B)	NAG	C3-C2-N2	-3.24	102.81	110.56
4	N	471(C)	BMA	O4-C4-C3	-2.65	104.38	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	472(D)	MAN	O3-C3-C4	-2.22	105.33	110.34
6	N	477(B)	NAG	C3-C4-C5	-2.21	106.34	110.20
4	N	471(C)	BMA	C6-C5-C4	2.04	118.04	113.02
4	N	471(C)	BMA	C1-O5-C5	2.08	114.89	112.25
4	N	470(B)	NAG	C1-O5-C5	2.42	115.32	112.25
6	N	476(A)	NAG	C6-C5-C4	2.77	119.85	113.02
4	N	470(B)	NAG	C8-C7-N2	2.88	121.62	116.11
4	N	472(D)	MAN	C1-O5-C5	3.38	116.53	112.25
6	N	477(B)	NAG	C2-N2-C7	4.74	129.13	123.04
6	N	477(B)	NAG	C1-O5-C5	4.90	118.47	112.25
4	N	474(F)	MAN	C1-O5-C5	7.31	121.53	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 [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	N	475(A)	1	14,14,15	0.76	0	15,19,21	1.76	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($^{\circ}$)	Ideal($^{\circ}$)
5	N	475(A)	NAG	C8-C7-N2	3.27	122.37	116.11
5	N	475(A)	NAG	C1-O5-C5	3.98	117.31	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%)	-0.97	0 100 100	2, 8, 24, 47	0
2	L	214/214 (100%)	-0.37	4 (1%) 70 66	4, 25, 42, 47	0
3	H	221/221 (100%)	-0.33	11 (4%) 32 26	4, 26, 40, 45	0
All	All	824/824 (100%)	-0.64	15 (1%) 71 68	2, 17, 38, 47	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	214	CYS	7.7
3	H	128	CYS	7.6
3	H	134	THR	5.7
3	H	129	GLY	5.3
3	H	130	ASP	5.2
3	H	135	GLY	5.0
2	L	213	GLU	4.7
3	H	133	THR	4.5
3	H	227	GLY	4.4
3	H	180	SER	4.1
2	L	211	ARG	3.9
2	L	212	ASN	3.4
3	H	136	SER	2.7
3	H	137	SER	2.4
3	H	183	ASP	2.3

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	MAN	N	473(E)	11/12	0.87	0.17	1.44	14,17,19,19	0
4	BMA	N	471(C)	11/12	0.94	0.12	0.98	8,11,13,13	0
4	MAN	N	474(F)	11/12	0.94	0.14	0.84	11,13,15,16	0
4	NAG	N	470(B)	14/15	0.94	0.12	0.64	12,14,16,20	0
4	NAG	N	469(A)	14/15	0.97	0.10	-0.60	5,11,23,24	0
6	NAG	N	476(A)	14/15	0.80	0.26	-	41,46,53,57	0
4	MAN	N	472(D)	11/12	0.92	0.14	-	9,11,14,19	0
6	NAG	N	477(B)	14/15	0.91	0.21	-	54,57,59,61	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	0.95	0.09	-1.82	20,20,20,20	0
5	NAG	N	475(A)	14/15	0.86	0.21	-	37,40,44,46	0

6.5 Other polymers

There are no such residues in this entry.