



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:28 PM UTC

PDB ID : 2F9B / pdb_00002f9b
Title : Discovery of Novel Heterocyclic Factor VIIa Inhibitors
Authors : Rai, R.; Kolesnikov, A.; Sprengeler, P.A.; Torkelson, S.; Ton, T.; Katz, B.A.; Yu, C.; Hendrix, J.; Shrader, W.D.; Stephens, R.; Cabuslay, R.; Sanford, E.; Young, W.B.
Deposited on : 2005-12-05
Resolution : 2.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

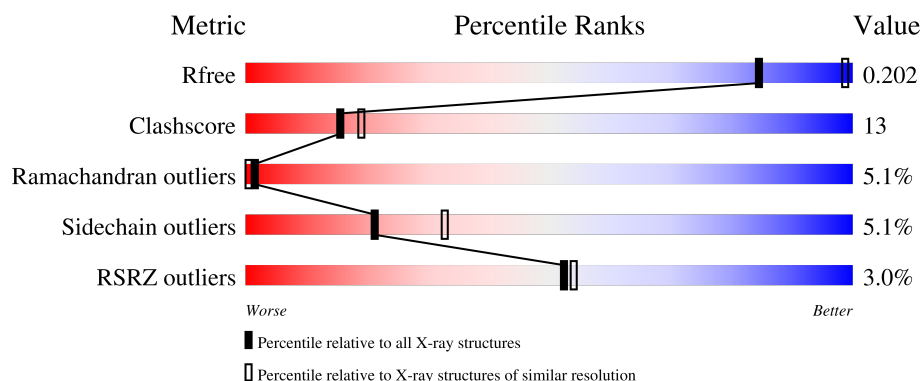
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	152	3% 36% 21% 5% 38%
2	H	254	2% 50% 37% 11%
3	T	218	2% 33% 25% 9% 32%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4059 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 Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	94	Total	C	N	O	S	0	0	0
			706	425	123	145	13			

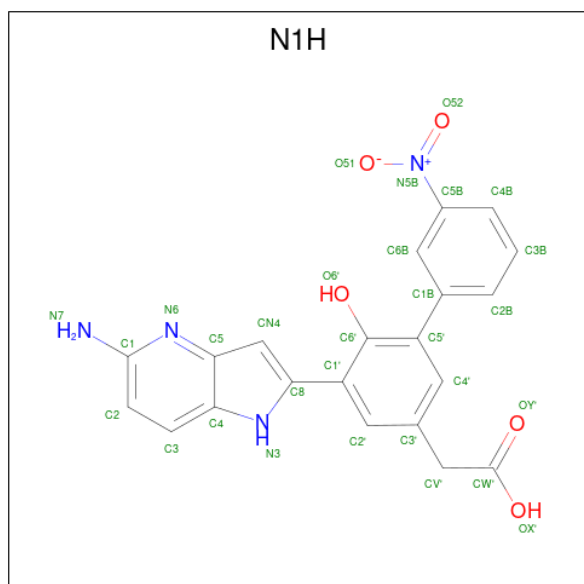
- Molecule 2 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	254	Total	C	N	O	S	0	0	0
			1974	1253	351	357	13			

- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	149	Total	C	N	O	S	0	0	0
			1194	756	196	240	2			

- Molecule 4 is {5-(5-AMINO-1H-PYRROLO[3,2-B]PYRIDIN-2-YL)-6-HYDROXY-3'-NITRO-BIPHENYL-3-YL]-ACETIC ACID (CCD ID: N1H) (formula: C₂₁H₁₆N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			30	21	4	5		

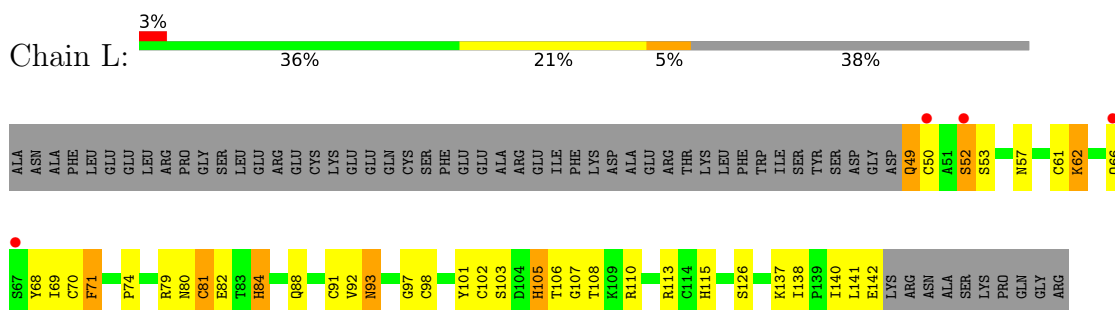
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	25	Total	O	0	0
			25	25		
5	H	85	Total	O	0	1
			86	86		
5	T	43	Total	O	0	1
			44	44		

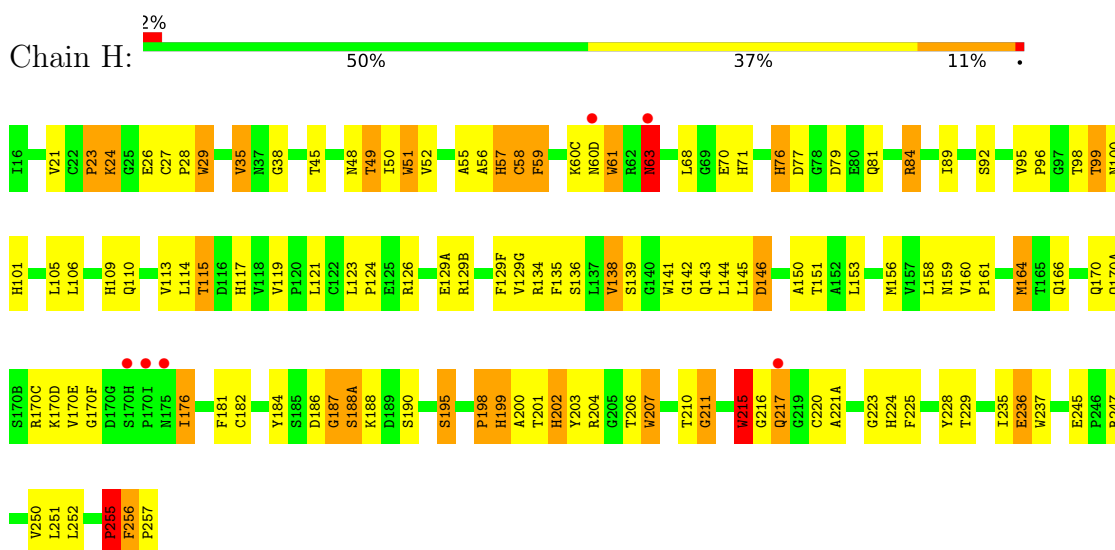
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

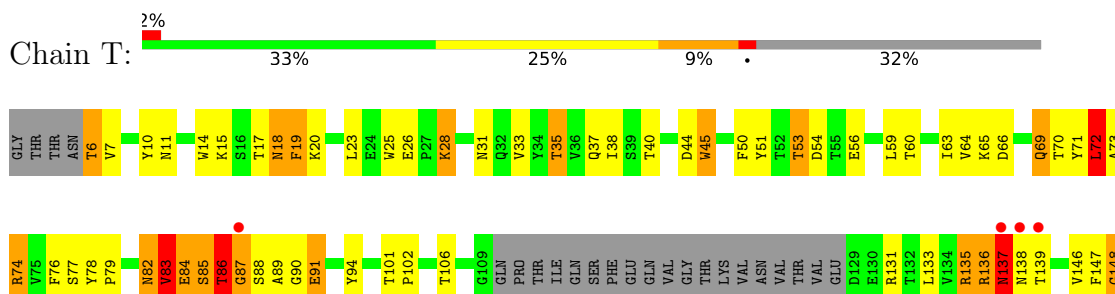
• Molecule 1: Coagulation factor VII

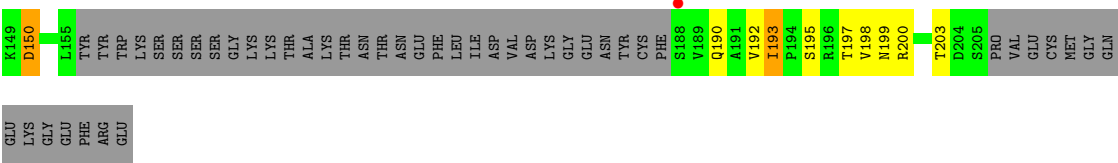


• Molecule 2: Coagulation factor VII



• Molecule 3: Tissue factor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.07Å 68.94Å 78.73Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.54 20.00 – 2.54	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.54) 95.0 (20.00-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.51Å)	Xtriage
Refinement program	XTALVIEW, X-PLOR 3.851	Depositor
R, R_{free}	0.226 , 0.286 (Not available) , 0.202	Depositor DCC
R_{free} test set	2742 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 153.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.033 for h,-k,-l 0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4059	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: N1H

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	L	1.82	5/719 (0.7%)	1.83	12/971 (1.2%)
2	H	1.94	29/2024 (1.4%)	2.05	82/2755 (3.0%)
3	T	1.72	4/1218 (0.3%)	1.97	41/1657 (2.5%)
All	All	1.85	38/3961 (1.0%)	1.99	135/5383 (2.5%)

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
3	T	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	117	HIS	CG-ND1	-8.18	1.29	1.38
2	H	101	HIS	CG-ND1	-8.12	1.29	1.38
2	H	76	HIS	CG-ND1	-7.97	1.29	1.38
2	H	202	HIS	CG-ND1	-7.96	1.29	1.38
1	L	115	HIS	CG-ND1	-7.91	1.29	1.38
2	H	224	HIS	CG-ND1	-7.89	1.29	1.38
2	H	109	HIS	CG-ND1	-7.70	1.29	1.38
2	H	57	HIS	CG-ND1	-7.67	1.29	1.38
2	H	71	HIS	CD2-NE2	-7.64	1.29	1.37
1	L	105	HIS	CG-ND1	-7.30	1.30	1.38
2	H	142	GLY	N-CA	7.02	1.50	1.44
2	H	199	HIS	CG-ND1	-6.97	1.30	1.38
2	H	211	GLY	N-CA	6.91	1.52	1.45
1	L	84	HIS	CG-ND1	-6.73	1.30	1.38
2	H	58	CYS	CA-CB	-6.69	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	161	PRO	CA-CB	-6.20	1.47	1.54
3	T	91	GLU	N-CA	6.02	1.50	1.46
2	H	71	HIS	CG-ND1	-5.87	1.31	1.38
2	H	215	TRP	CG-CD2	-5.86	1.33	1.43
2	H	51	TRP	NE1-CE2	-5.72	1.31	1.37
3	T	78	TYR	N-CA	5.63	1.52	1.45
2	H	109	HIS	CD2-NE2	-5.48	1.31	1.37
3	T	87	GLY	N-CA	5.41	1.50	1.44
2	H	224	HIS	CD2-NE2	-5.40	1.31	1.37
2	H	215	TRP	NE1-CE2	-5.37	1.31	1.37
1	L	105	HIS	CD2-NE2	-5.23	1.32	1.37
2	H	76	HIS	CD2-NE2	-5.22	1.32	1.37
2	H	57	HIS	CD2-NE2	-5.21	1.32	1.37
3	T	45	TRP	CG-CD2	-5.21	1.34	1.43
2	H	117	HIS	CD2-NE2	-5.14	1.32	1.37
1	L	84	HIS	CD2-NE2	-5.10	1.32	1.37
2	H	126	ARG	C-N	-5.10	1.27	1.33
2	H	129(A)	GLU	CA-CB	-5.08	1.45	1.53
2	H	188(A)	SER	CA-C	5.08	1.57	1.52
2	H	51	TRP	CG-CD2	-5.05	1.34	1.43
2	H	237	TRP	CG-CD2	-5.04	1.34	1.43
2	H	207	TRP	CG-CD2	-5.02	1.34	1.43
2	H	101	HIS	CD2-NE2	-5.01	1.32	1.37

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	129(G)	VAL	N-CA-C	-13.47	88.33	107.99
2	H	119	VAL	N-CA-C	-11.17	100.03	109.19
2	H	170(C)	ARG	N-CA-C	-11.04	96.83	110.41
2	H	190	SER	N-CA-C	-9.67	97.00	110.35
2	H	199	HIS	N-CA-C	-9.63	91.14	107.80
3	T	84	GLU	N-CA-C	-9.59	102.08	113.88
2	H	170(D)	LYS	N-CA-C	9.54	121.62	111.03
3	T	19	PHE	CA-CB-CG	-9.24	104.56	113.80
2	H	170(E)	VAL	N-CA-C	8.85	119.61	108.82
2	H	170(F)	GLY	N-CA-C	-8.82	97.88	110.75
3	T	7	VAL	N-CA-C	-8.46	95.79	108.99
2	H	181	PHE	CA-CB-CG	8.30	122.10	113.80
3	T	28	LYS	N-CA-C	-8.13	97.83	109.62
2	H	134	ARG	N-CA-C	8.02	119.81	111.14
3	T	20	LYS	N-CA-C	-8.01	97.61	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	151	THR	N-CA-C	-7.98	100.24	110.53
3	T	150	ASP	N-CA-C	-7.49	103.74	113.17
2	H	115	THR	OG1-CB-CG2	-7.48	94.35	109.30
2	H	256	PHE	CA-CB-CG	-7.38	106.42	113.80
3	T	23	LEU	N-CA-C	-7.37	98.24	109.95
2	H	101	HIS	CA-CB-CG	-7.28	106.52	113.80
2	H	114	LEU	N-CA-C	-7.14	100.42	110.50
2	H	59	PHE	CA-CB-CG	-7.08	106.72	113.80
1	L	115	HIS	CA-CB-CG	-7.02	106.78	113.80
2	H	84	ARG	N-CA-C	-7.00	101.29	110.53
3	T	15	LYS	N-CA-C	-6.94	96.96	108.34
2	H	224	HIS	CA-CB-CG	-6.84	106.96	113.80
2	H	237	TRP	NE1-CE2-CZ2	6.83	140.35	130.10
1	L	62	LYS	N-CA-C	-6.81	97.87	109.24
2	H	100	ASN	OD1-CG-ND2	-6.79	115.81	122.60
2	H	160	VAL	N-CA-CB	-6.79	107.15	111.83
2	H	123	LEU	N-CA-C	-6.77	96.35	108.47
2	H	153	LEU	N-CA-C	-6.73	104.11	112.72
1	L	71	PHE	N-CA-C	-6.70	97.60	108.52
3	T	40	THR	N-CA-C	-6.69	99.38	109.96
3	T	86	THR	N-CA-CB	-6.69	100.05	111.69
1	L	93	ASN	CA-CB-CG	-6.68	105.92	112.60
3	T	72	LEU	N-CA-C	-6.60	98.99	109.23
3	T	53	THR	N-CA-C	-6.54	103.80	113.61
3	T	136	ARG	N-CA-C	-6.43	98.50	109.24
2	H	29	TRP	CG-CD1-NE1	-6.42	101.85	110.20
2	H	129(A)	GLU	N-CA-C	6.39	119.06	111.33
3	T	82	ASN	CA-CB-CG	-6.39	106.21	112.60
2	H	164	MET	N-CA-C	-6.38	99.90	110.17
3	T	190	GLN	N-CA-C	-6.37	99.62	109.24
2	H	141	TRP	NE1-CE2-CZ2	6.29	139.53	130.10
2	H	109	HIS	N-CA-C	-6.27	105.29	113.12
2	H	251	LEU	N-CA-C	-6.26	99.44	109.96
2	H	216	GLY	N-CA-C	-6.26	98.35	113.18
3	T	45	TRP	NE1-CE2-CZ2	6.24	139.45	130.10
3	T	45	TRP	CG-CD1-NE1	-6.20	102.14	110.20
2	H	99	THR	CA-CB-OG1	-6.18	100.33	109.60
2	H	110	GLN	N-CA-C	-6.17	99.52	109.58
3	T	137	ASN	CA-CB-CG	-6.16	106.44	112.60
3	T	35	THR	N-CA-C	-6.12	98.66	109.06
2	H	61	TRP	CG-CD1-NE1	-6.10	102.27	110.20
2	H	170(A)	GLN	N-CA-C	6.06	120.68	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	44	ASP	N-CA-C	-6.04	101.58	110.52
2	H	229	THR	N-CA-C	-6.02	99.84	109.96
2	H	63	ASN	N-CA-C	-6.02	106.59	112.97
3	T	83	VAL	N-CA-CB	-6.01	101.32	111.23
2	H	105	LEU	N-CA-C	-5.94	99.50	109.07
2	H	170	GLN	OE1-CD-NE2	-5.92	116.68	122.60
2	H	29	TRP	NE1-CE2-CZ2	5.92	138.98	130.10
3	T	25	TRP	NE1-CE2-CZ2	5.90	138.96	130.10
3	T	65	LYS	N-CA-C	-5.90	104.77	111.14
2	H	237	TRP	CG-CD1-NE1	-5.88	102.56	110.20
2	H	207	TRP	NE1-CE2-CZ2	5.86	138.89	130.10
3	T	70	THR	N-CA-C	-5.82	99.41	108.90
2	H	60(D)	ASN	OD1-CG-ND2	-5.81	116.79	122.60
2	H	176	ILE	N-CA-C	-5.80	98.27	107.15
2	H	134	ARG	CA-CB-CG	-5.76	102.58	114.10
2	H	215	TRP	CG-CD2-CE3	-5.75	128.15	133.90
2	H	55	ALA	N-CA-C	5.74	118.02	108.20
2	H	225	PHE	CA-C-N	-5.73	116.01	121.57
2	H	225	PHE	C-N-CA	-5.73	116.01	121.57
2	H	76	HIS	N-CA-C	-5.72	100.39	109.76
3	T	25	TRP	CG-CD1-NE1	-5.70	102.79	110.20
2	H	138	VAL	N-CA-C	-5.67	100.12	108.85
3	T	37	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	L	106	THR	OG1-CB-CG2	-5.63	98.03	109.30
3	T	69	GLN	N-CA-C	-5.62	101.64	110.36
3	T	54	ASP	N-CA-C	-5.62	103.29	110.53
3	T	78	TYR	N-CA-C	-5.61	100.44	109.58
2	H	129(F)	PHE	CA-CB-CG	-5.59	108.21	113.80
2	H	250	VAL	N-CA-C	-5.59	97.72	109.34
2	H	81	GLN	N-CA-C	-5.58	99.91	109.24
3	T	11	ASN	OD1-CG-ND2	-5.56	117.04	122.60
3	T	31	ASN	OD1-CG-ND2	-5.55	117.05	122.60
3	T	14	TRP	CG-CD1-NE1	-5.55	102.99	110.20
3	T	197	THR	N-CA-C	-5.54	105.56	112.93
2	H	61	TRP	NE1-CE2-CZ2	5.53	138.40	130.10
2	H	141	TRP	CG-CD1-NE1	-5.53	103.01	110.20
3	T	193	ILE	N-CA-C	-5.52	96.96	108.88
2	H	223	GLY	N-CA-C	-5.50	106.61	115.08
2	H	207	TRP	CG-CD1-NE1	-5.50	103.06	110.20
3	T	14	TRP	N-CA-C	-5.49	100.75	109.76
2	H	99	THR	OG1-CB-CG2	-5.49	98.33	109.30
2	H	71	HIS	CA-CB-CG	-5.47	108.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	217	GLN	OE1-CD-NE2	-5.45	117.15	122.60
3	T	14	TRP	NE1-CE2-CZ2	5.43	138.24	130.10
2	H	60(C)	LYS	N-CA-C	-5.39	104.97	112.30
2	H	237	TRP	NE1-CE2-CD2	-5.38	100.41	107.40
2	H	117	HIS	CE1-NE2-CD2	-5.37	103.64	109.00
2	H	207	TRP	CG-CD2-CE3	-5.36	128.54	133.90
2	H	224	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
2	H	60(D)	ASN	N-CA-C	-5.30	104.08	110.44
2	H	29	TRP	CD1-NE1-CE2	5.28	118.41	108.90
2	H	206	THR	CA-CB-OG1	-5.25	101.72	109.60
2	H	237	TRP	CG-CD2-CE3	-5.25	128.65	133.90
3	T	17	THR	N-CA-C	-5.23	100.50	109.24
3	T	203	THR	N-CA-C	-5.20	100.96	109.80
1	L	82	GLU	CA-C-N	-5.18	114.01	121.42
1	L	82	GLU	C-N-CA	-5.18	114.01	121.42
2	H	135	PHE	N-CA-C	5.18	118.25	109.76
2	H	215	TRP	NE1-CE2-CZ2	5.18	137.87	130.10
3	T	106	THR	N-CA-C	-5.18	103.85	110.53
2	H	29	TRP	NE1-CE2-CD2	-5.18	100.67	107.40
2	H	71	HIS	ND1-CG-CD2	5.16	111.26	106.10
2	H	35	VAL	N-CA-C	-5.14	100.71	108.12
2	H	51	TRP	CG-CD1-NE1	-5.14	103.52	110.20
2	H	61	TRP	CD1-NE1-CE2	5.13	118.13	108.90
2	H	181	PHE	N-CA-C	-5.12	101.46	108.38
1	L	141	LEU	N-CA-C	-5.12	104.65	111.87
1	L	88	GLN	OE1-CD-NE2	-5.12	117.48	122.60
2	H	170(E)	VAL	N-CA-CB	-5.10	106.74	112.45
2	H	76	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
3	T	135	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	L	97	GLY	N-CA-C	-5.08	108.10	115.27
2	H	170(E)	VAL	CA-C-N	-5.08	106.04	116.20
2	H	200	ALA	N-CA-C	5.08	117.18	108.90
1	L	137	LYS	N-CA-C	-5.08	101.59	109.72
1	L	93	ASN	OD1-CG-ND2	-5.07	117.53	122.60
3	T	138	ASN	OD1-CG-ND2	-5.07	117.53	122.60
2	H	195	SER	CA-C-O	-5.05	115.61	121.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	28	LYS	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	L	706	0	640	22	0
2	H	1974	0	1950	51	0
3	T	1194	0	1163	38	0
4	H	30	0	15	2	0
5	H	86	0	0	1	0
5	L	25	0	0	0	0
5	T	44	0	0	0	0
All	All	4059	0	3768	102	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 13.

All (102) 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:H:195:SER:OG	5:H:332:HOH:O	1.98	0.80
2:H:21:VAL:HG22	2:H:156:MET:SD	2.31	0.71
1:L:49:GLN:N	1:L:52:SER:HG	1.95	0.65
3:T:72:LEU:HD13	3:T:73:ALA:N	2.14	0.62
1:L:71:PHE:CE2	3:T:131:ARG:HD3	2.36	0.61
2:H:195:SER:OG	4:H:258:N1H:O6'	2.20	0.60
1:L:61:CYS:SG	1:L:68:TYR:HB2	2.42	0.59
3:T:66:ASP:CG	3:T:69:GLN:HG2	2.28	0.58
2:H:136:SER:CB	2:H:199:HIS:CE1	2.86	0.58
2:H:136:SER:HB2	2:H:199:HIS:CE1	2.39	0.57
1:L:140:ILE:HD11	2:H:26:GLU:HG3	1.87	0.56
1:L:140:ILE:HD11	2:H:26:GLU:CG	2.37	0.55
3:T:63:ILE:HD12	3:T:63:ILE:C	2.32	0.55
3:T:45:TRP:CE2	3:T:74:ARG:NH2	2.75	0.55
3:T:51:TYR:CD1	3:T:83:VAL:CG2	2.91	0.54
3:T:51:TYR:CE1	3:T:83:VAL:HG22	2.42	0.54
3:T:86:THR:OG1	3:T:90:GLY:C	2.53	0.52
3:T:150:ASP:O	3:T:193:ILE:HA	2.10	0.52
1:L:105:HIS:HB2	1:L:108:THR:HG23	1.91	0.51
2:H:21:VAL:CG2	2:H:156:MET:SD	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:245:GLU:H	2:H:247:ARG:NH1	2.09	0.51
2:H:48:ASN:ND2	2:H:51:TRP:HB2	2.26	0.50
2:H:23:PRO:O	2:H:24:LYS:C	2.55	0.50
2:H:50:ILE:HG13	2:H:51:TRP:CD1	2.46	0.50
1:L:103:SER:O	1:L:110:ARG:HB2	2.12	0.49
3:T:59:LEU:O	3:T:60:THR:C	2.55	0.49
2:H:27:CYS:N	2:H:28:PRO:CD	2.75	0.48
1:L:49:GLN:OE1	1:L:49:GLN:C	2.57	0.48
2:H:48:ASN:HD21	2:H:51:TRP:CD1	2.31	0.48
2:H:184:TYR:CD1	2:H:188:LYS:HB2	2.48	0.48
3:T:82:ASN:C	3:T:84:GLU:H	2.21	0.48
2:H:99:THR:HG22	2:H:215:TRP:CD1	2.49	0.47
2:H:144:LEU:HD12	2:H:150:ALA:O	2.14	0.47
3:T:87:GLY:O	3:T:90:GLY:N	2.47	0.47
1:L:79:ARG:HH21	3:T:56:GLU:CD	2.21	0.47
2:H:176:ILE:HD12	2:H:182:CYS:SG	2.54	0.47
2:H:186:ASP:O	2:H:188(A):SER:N	2.47	0.47
1:L:101:TYR:HB2	1:L:113:ARG:HB2	1.97	0.47
3:T:35:THR:HG23	3:T:50:PHE:HA	1.97	0.47
3:T:136:ARG:O	3:T:137:ASN:C	2.57	0.47
2:H:202:HIS:HB2	2:H:207:TRP:CH2	2.50	0.47
2:H:145:LEU:O	2:H:146:ASP:C	2.58	0.46
3:T:89:ALA:O	3:T:91:GLU:HG3	2.15	0.46
2:H:201:THR:OG1	2:H:210:THR:HG21	2.16	0.46
3:T:19:PHE:CE2	3:T:146:VAL:HG11	2.50	0.46
2:H:124:PRO:O	2:H:235:ILE:HD13	2.15	0.46
2:H:236:GLU:H	2:H:236:GLU:CD	2.23	0.46
3:T:51:TYR:CD1	3:T:83:VAL:HG21	2.51	0.46
2:H:23:PRO:HB2	2:H:26:GLU:CD	2.41	0.46
2:H:45:THR:HG21	2:H:121:LEU:HD23	1.98	0.46
2:H:113:VAL:O	2:H:115:THR:HG23	2.16	0.45
3:T:87:GLY:O	3:T:89:ALA:N	2.49	0.45
1:L:110:ARG:HD2	1:L:110:ARG:C	2.42	0.45
2:H:45:THR:O	2:H:52:VAL:HA	2.16	0.45
2:H:186:ASP:O	2:H:187:GLY:C	2.60	0.44
3:T:101:THR:O	3:T:102:PRO:C	2.60	0.44
1:L:69:ILE:CG2	3:T:133:LEU:HD21	2.48	0.44
2:H:164:MET:HE3	3:T:91:GLU:HB3	1.99	0.44
2:H:202:HIS:HD1	2:H:207:TRP:NE1	2.15	0.44
1:L:91:CYS:O	2:H:129(B):ARG:HD3	2.17	0.44
1:L:93:ASN:HB2	3:T:50:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:HIS:CB	1:L:108:THR:HG23	2.48	0.44
2:H:203:TYR:CZ	2:H:204:ARG:NE	2.85	0.44
3:T:147:PHE:O	3:T:148:GLY:C	2.61	0.43
2:H:92:SER:OG	2:H:255:PRO:HA	2.19	0.43
3:T:18:ASN:O	3:T:19:PHE:HB2	2.18	0.43
3:T:63:ILE:HA	3:T:71:TYR:CZ	2.53	0.43
3:T:135:ARG:HA	3:T:139:THR:O	2.18	0.43
3:T:192:VAL:HA	3:T:200:ARG:O	2.18	0.43
2:H:35:VAL:C	2:H:38:GLY:N	2.76	0.43
2:H:256:PHE:CD1	2:H:257:PRO:HA	2.53	0.43
1:L:138:ILE:O	1:L:142:GLU:HG2	2.19	0.43
1:L:80:ASN:O	1:L:81:CYS:C	2.61	0.42
2:H:58:CYS:HA	4:H:258:N1H:C4B	2.49	0.42
2:H:215:TRP:CD1	2:H:215:TRP:H	2.37	0.42
1:L:61:CYS:SG	1:L:68:TYR:CB	3.08	0.42
3:T:79:PRO:HD2	3:T:85:SER:CB	2.49	0.42
2:H:143:GLN:NE2	2:H:146:ASP:O	2.53	0.42
3:T:6:THR:HG22	3:T:77:SER:CB	2.50	0.42
2:H:68:LEU:C	2:H:70:GLU:H	2.28	0.42
2:H:228:TYR:CD1	2:H:228:TYR:N	2.88	0.41
3:T:10:TYR:CE1	3:T:26:GLU:HB2	2.55	0.41
3:T:60:THR:O	3:T:64:VAL:HG22	2.20	0.41
1:L:49:GLN:O	1:L:50:CYS:C	2.62	0.41
1:L:70:CYS:HB3	1:L:81:CYS:SG	2.61	0.41
2:H:28:PRO:HG2	2:H:29:TRP:CZ3	2.55	0.41
2:H:95:VAL:HB	2:H:98:THR:CG2	2.51	0.41
3:T:198:VAL:O	3:T:199:ASN:C	2.63	0.41
2:H:199:HIS:HB3	2:H:211:GLY:CA	2.50	0.41
1:L:62:LYS:O	1:L:68:TYR:HA	2.21	0.41
2:H:63:ASN:OD1	2:H:63:ASN:N	2.54	0.41
3:T:38:ILE:HD12	3:T:59:LEU:HD13	2.03	0.41
3:T:76:PHE:CD1	3:T:94:TYR:HB3	2.56	0.41
2:H:89:ILE:HA	2:H:252:LEU:O	2.21	0.41
3:T:79:PRO:HD2	3:T:85:SER:HB2	2.03	0.41
2:H:158:LEU:HD11	2:H:188:LYS:HB3	2.03	0.40
2:H:57:HIS:C	2:H:59:PHE:N	2.78	0.40
2:H:166:GLN:HB2	3:T:94:TYR:CE1	2.57	0.40
1:L:98:CYS:SG	1:L:102:CYS:HB2	2.61	0.40
3:T:133:LEU:N	3:T:133:LEU:HD22	2.36	0.40
2:H:76:HIS:CE1	2:H:77:ASP:O	2.75	0.40
2:H:138:VAL:HA	2:H:198:PRO:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	92/152 (60%)	77 (84%)	9 (10%)	6 (6%)	1	0
2	H	252/254 (99%)	211 (84%)	28 (11%)	13 (5%)	1	0
3	T	143/218 (66%)	118 (82%)	19 (13%)	6 (4%)	2	1
All	All	487/624 (78%)	406 (83%)	56 (12%)	25 (5%)	1	0

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	57	ASN
3	T	85	SER
3	T	88	SER
1	L	66	GLN
1	L	107	GLY
2	H	61	TRP
2	H	146	ASP
2	H	187	GLY
2	H	220	CYS
2	H	221(A)	ALA
2	H	49	THR
2	H	56	ALA
3	T	137	ASN
1	L	81	CYS
2	H	24	LYS
2	H	217	GLN
3	T	18	ASN
1	L	53	SER
2	H	23	PRO
2	H	96	PRO
3	T	148	GLY

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Mol	Chain	Res	Type
2	H	79	ASP
2	H	255	PRO
3	T	83	VAL
1	L	74	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	L	82/132 (62%)	77 (94%)	5 (6%)	17	25
2	H	216/216 (100%)	206 (95%)	10 (5%)	24	36
3	T	137/199 (69%)	130 (95%)	7 (5%)	21	33
All	All	435/547 (80%)	413 (95%)	22 (5%)	21	33

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	49	GLN
1	L	52	SER
1	L	84	HIS
1	L	92	VAL
1	L	126	SER
2	H	49	THR
2	H	63	ASN
2	H	84	ARG
2	H	106	LEU
2	H	139	SER
2	H	159	ASN
2	H	198	PRO
2	H	215	TRP
2	H	236	GLU
2	H	255	PRO
3	T	6	THR
3	T	33	VAL
3	T	53	THR

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Mol	Chain	Res	Type
3	T	72	LEU
3	T	74	ARG
3	T	86	THR
3	T	195	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	71	HIS
2	H	100	ASN
2	H	110	GLN
2	H	143	GLN
2	H	159	ASN
3	T	31	ASN
3	T	137	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	N1H	H	258	-	33,33,33	3.91	11 (33%)	44,48,48	2.33	15 (34%)

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	N1H	H	258	-	-	0/14/16/16	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	258	N1H	O52-N5B	17.93	1.53	1.22
4	H	258	N1H	C5-CN4	-5.62	1.34	1.42
4	H	258	N1H	C4-C5	-5.19	1.32	1.40
4	H	258	N1H	C5'-C1B	-5.14	1.40	1.49
4	H	258	N1H	C5B-N5B	-5.12	1.33	1.45
4	H	258	N1H	C8-N3	-4.01	1.33	1.38
4	H	258	N1H	C1'-C8	-3.80	1.41	1.47
4	H	258	N1H	C4-N3	-3.06	1.33	1.38
4	H	258	N1H	OX'-CW'	-2.50	1.22	1.30
4	H	258	N1H	C3-C4	-2.22	1.36	1.39
4	H	258	N1H	C6B-C1B	2.14	1.43	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	258	N1H	C4-C5-CN4	6.79	111.69	107.35
4	H	258	N1H	C4-C5-N6	-6.59	118.48	123.34
4	H	258	N1H	C2-C1-N6	-4.52	116.39	121.83
4	H	258	N1H	C6B-C5B-N5B	4.34	122.48	118.74
4	H	258	N1H	N7-C1-N6	3.73	122.59	116.59
4	H	258	N1H	C3-C2-C1	3.14	121.84	119.13
4	H	258	N1H	CN4-C8-N3	-3.09	104.65	108.65
4	H	258	N1H	O52-N5B-C5B	2.71	122.55	118.82
4	H	258	N1H	C1'-C6'-C5'	2.61	123.21	119.79
4	H	258	N1H	C3-C4-C5	2.58	124.94	122.10
4	H	258	N1H	O6'-C6'-C1'	-2.54	116.58	121.11
4	H	258	N1H	C2-C3-C4	-2.50	114.76	119.57
4	H	258	N1H	C2'-C1'-C6'	-2.41	116.58	119.39
4	H	258	N1H	C4-N3-C8	2.37	112.54	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	258	N1H	OY'-CW'-CV'	-2.34	115.89	122.94

There are no chirality outliers.

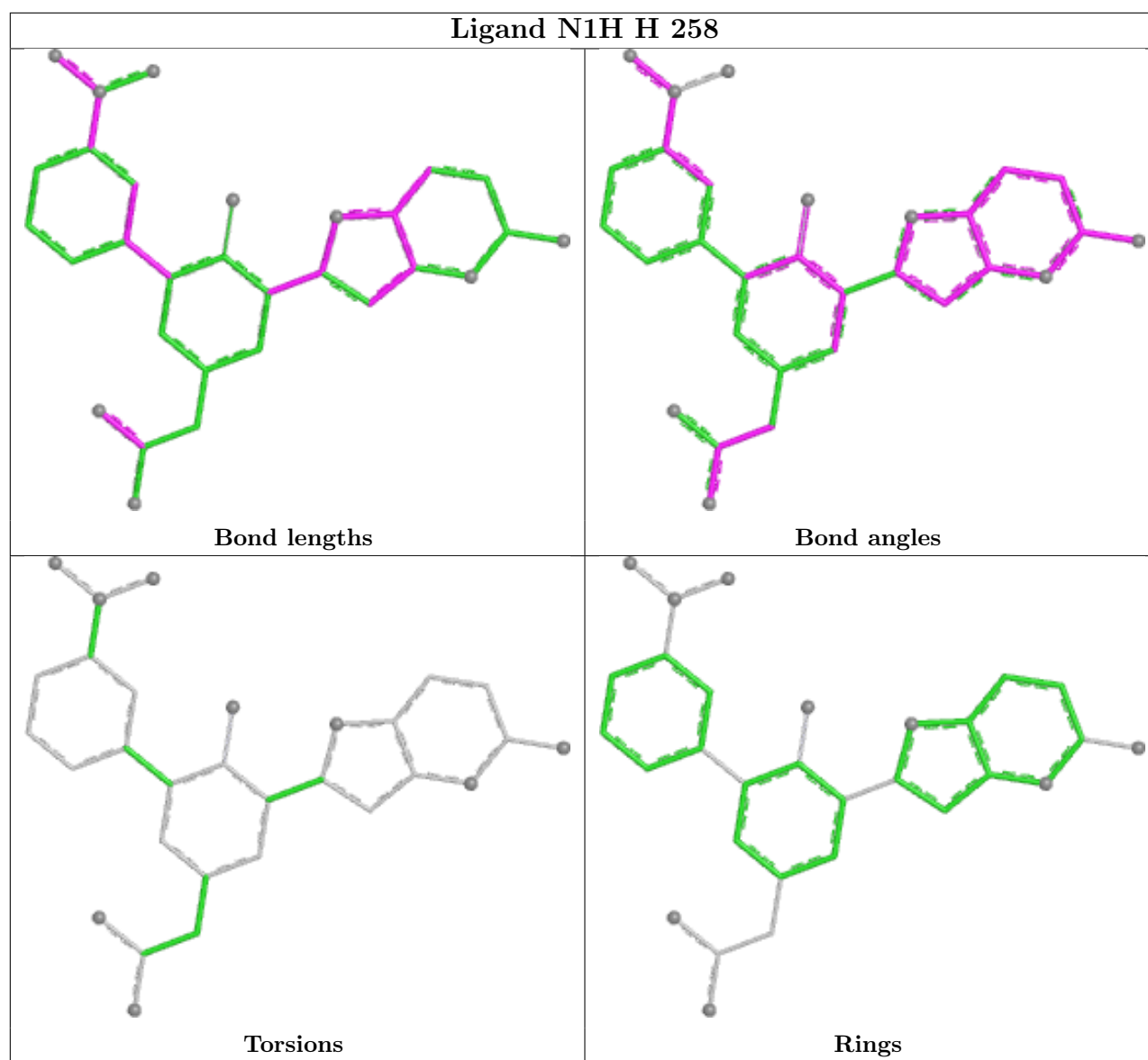
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	258	N1H	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	L	94/152 (61%)	-0.28	4 (4%)	40 40	1, 43, 89, 96	8 (8%)
2	H	254/254 (100%)	-0.47	6 (2%)	59 61	10, 35, 69, 100	23 (9%)
3	T	149/218 (68%)	-0.27	5 (3%)	48 49	15, 47, 87, 99	20 (13%)
All	All	497/624 (79%)	-0.38	15 (3%)	52 54	1, 39, 86, 100	51 (10%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	137	ASN	4.6
3	T	188	SER	3.9
2	H	170(H)	SER	3.8
3	T	87	GLY	3.5
1	L	52	SER	3.2
1	L	66	GLN	3.1
2	H	217	GLN	3.0
2	H	63	ASN	2.8
3	T	138	ASN	2.7
1	L	50	CYS	2.5
2	H	170(I)	PRO	2.3
2	H	175	ASN	2.1
1	L	67	SER	2.1
3	T	139	THR	2.1
2	H	60(D)	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

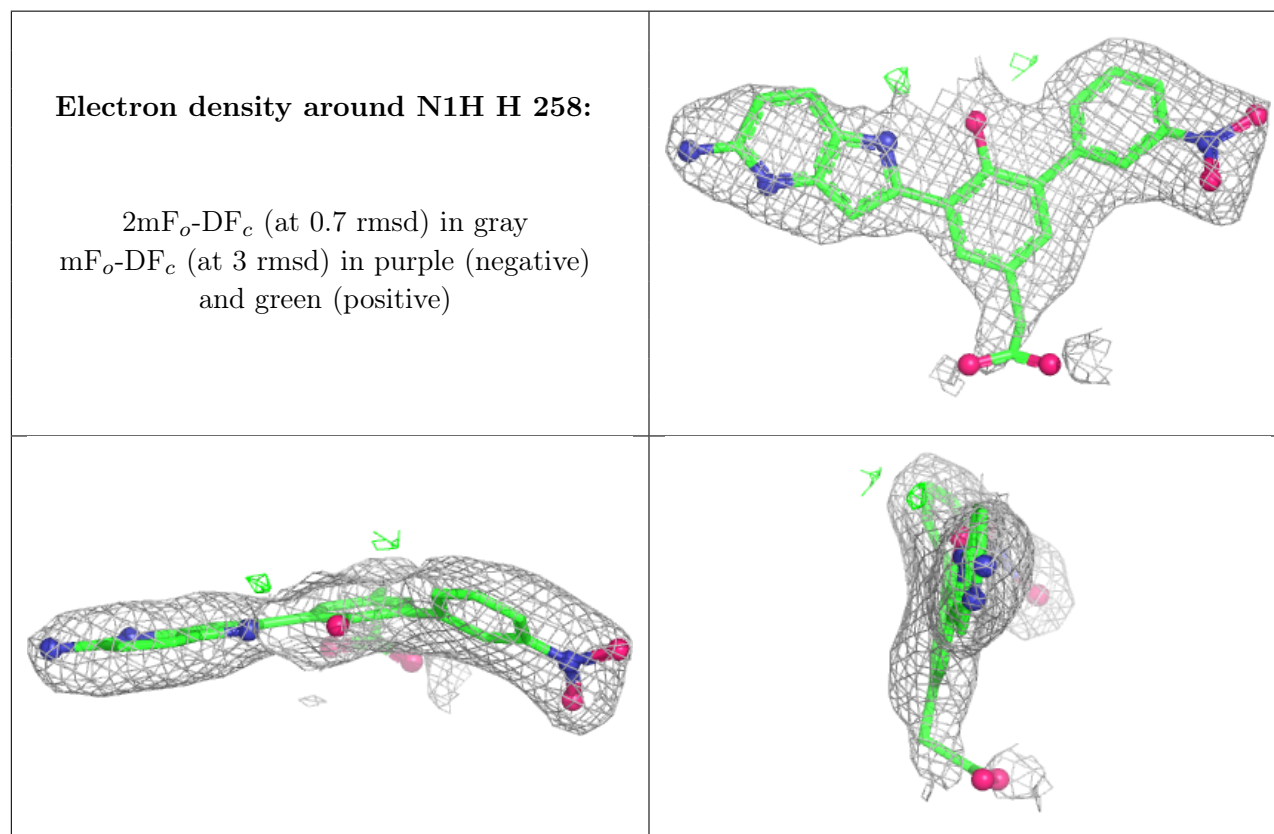
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	N1H	H	258	30/30	0.96	0.06	18,40,50,55	4

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.