



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

PDB ID : 2F9B  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

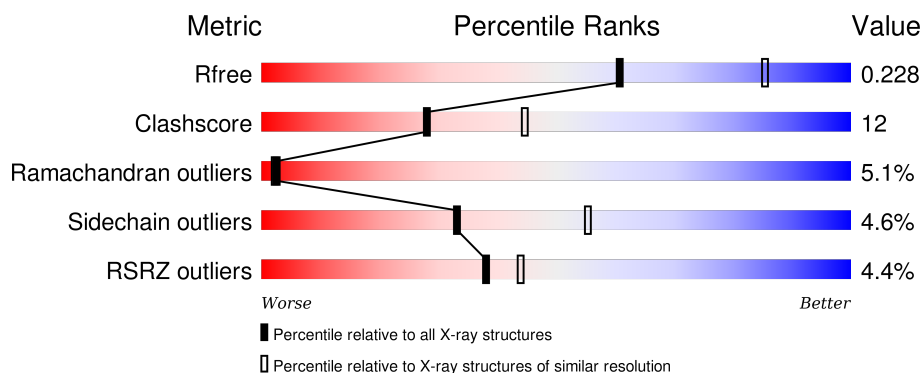
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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  $\geq 3$ , 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	L	152	<div> <div>3%</div> <div>40%18%•38%</div> </div>
2	H	254	<div> <div>4%</div> <div>64%28%7%•</div> </div>
3	T	218	<div> <div>3%</div> <div>42%21%5%32%</div> </div>

## 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			

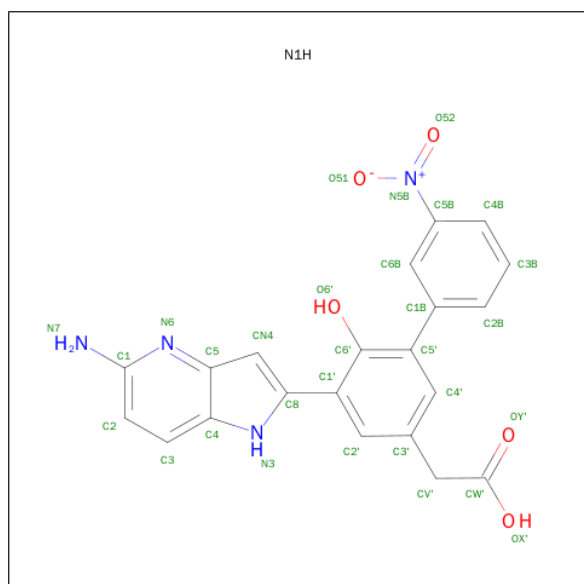
- Molecule 2 is a protein called Coagulation factor VII.

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 (three-letter code: N1H) (formula: C<sub>21</sub>H<sub>16</sub>N<sub>4</sub>O<sub>5</sub>).



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

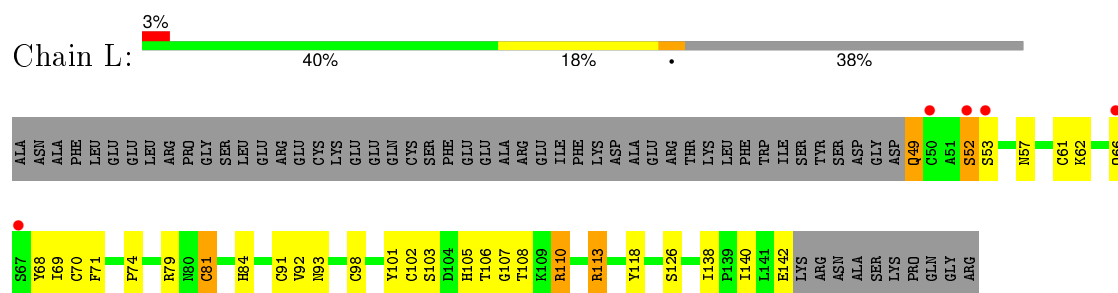
- Molecule 5 is water.

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

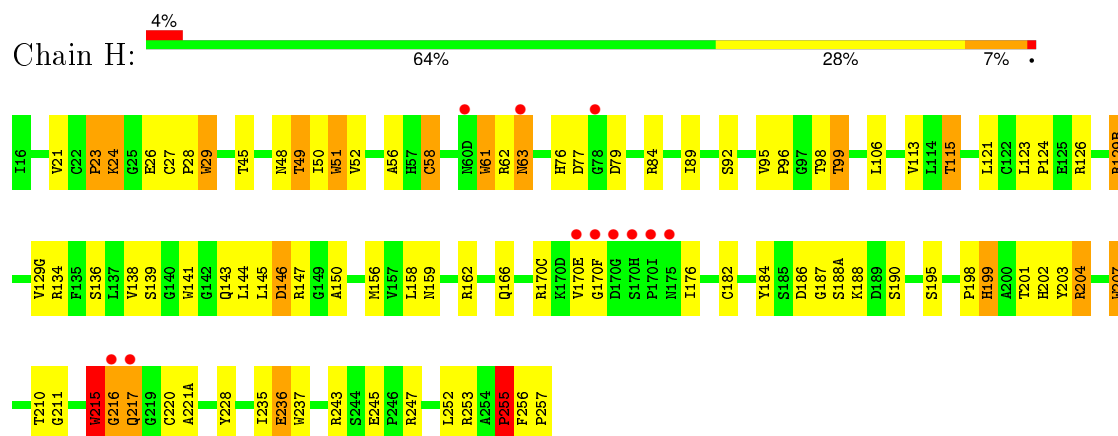
### 3 Residue-property plots

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.

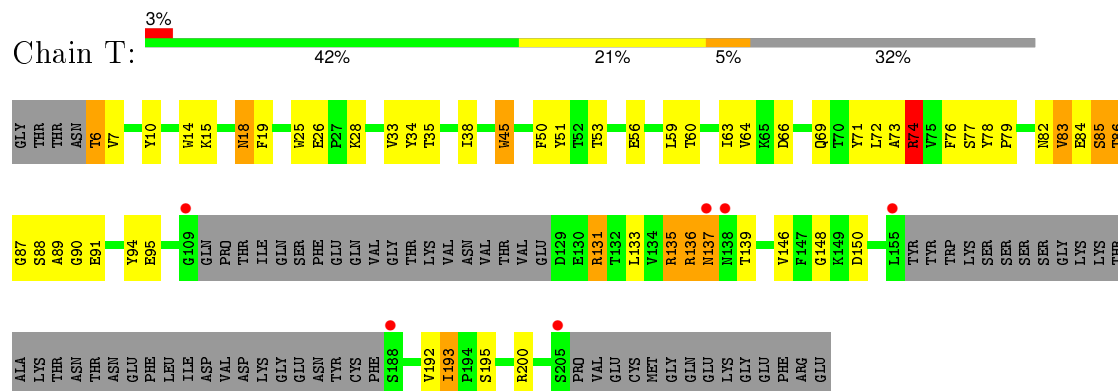
#### • Molecule 1: Coagulation factor VII



#### • 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, $\alpha$ , $\beta$ , $\gamma$	78.07Å 68.94Å 78.73Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.54 7.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.54) 99.2 (7.00-2.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.226 , 0.286 0.225 , 0.228	Depositor DCC
$R_{free}$ test set	2673 reflections (10.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 146.4	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.033 for h,-k,-l 0.013 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27036 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	1.33	0/719	1.43	4/971 (0.4%)
2	H	1.40	5/2024 (0.2%)	1.74	52/2755 (1.9%)
3	T	1.30	1/1218 (0.1%)	1.67	24/1657 (1.4%)
All	All	1.36	6/3961 (0.2%)	1.67	80/5383 (1.5%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	215	TRP	CG-CD2	-6.15	1.33	1.43
3	T	45	TRP	CG-CD2	-5.46	1.34	1.43
2	H	58	CYS	CA-CB	-5.36	1.42	1.53
2	H	51	TRP	CG-CD2	-5.29	1.34	1.43
2	H	237	TRP	CG-CD2	-5.28	1.34	1.43
2	H	207	TRP	CG-CD2	-5.25	1.34	1.43

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	29	TRP	CD1-NE1-CE2	10.45	118.41	109.00
2	H	61	TRP	CD1-NE1-CE2	10.15	118.13	109.00
2	H	237	TRP	CD1-NE1-CE2	9.87	117.88	109.00
3	T	45	TRP	CD1-NE1-CE2	9.78	117.81	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	74	ARG	NE-CZ-NH2	-9.59	115.50	120.30
2	H	129(B)	ARG	NE-CZ-NH2	-9.48	115.56	120.30
3	T	25	TRP	CD1-NE1-CE2	9.35	117.42	109.00
2	H	141	TRP	CD1-NE1-CE2	9.34	117.41	109.00
3	T	14	TRP	CD1-NE1-CE2	9.13	117.22	109.00
2	H	237	TRP	NE1-CE2-CZ2	9.05	140.35	130.40
2	H	51	TRP	CD1-NE1-CE2	8.94	117.05	109.00
2	H	253	ARG	NE-CZ-NH2	-8.63	115.98	120.30
2	H	129(G)	VAL	N-CA-C	-8.40	88.33	111.00
2	H	141	TRP	NE1-CE2-CZ2	8.30	139.53	130.40
2	H	29	TRP	CG-CD1-NE1	-8.25	101.85	110.10
3	T	45	TRP	NE1-CE2-CZ2	8.23	139.45	130.40
1	L	113	ARG	NE-CZ-NH2	-8.14	116.23	120.30
2	H	207	TRP	CD1-NE1-CE2	8.05	116.24	109.00
3	T	45	TRP	CG-CD1-NE1	-7.96	102.14	110.10
2	H	215	TRP	CD1-NE1-CE2	7.95	116.15	109.00
1	L	118	TYR	CB-CG-CD2	-7.84	116.30	121.00
2	H	61	TRP	CG-CD1-NE1	-7.83	102.27	110.10
2	H	29	TRP	NE1-CE2-CZ2	7.80	138.98	130.40
3	T	25	TRP	NE1-CE2-CZ2	7.78	138.96	130.40
3	T	135	ARG	NE-CZ-NH1	-7.77	116.41	120.30
2	H	207	TRP	NE1-CE2-CZ2	7.72	138.89	130.40
1	L	118	TYR	CB-CG-CD1	7.71	125.62	121.00
2	H	243	ARG	NE-CZ-NH2	-7.67	116.47	120.30
2	H	237	TRP	CG-CD1-NE1	-7.54	102.56	110.10
2	H	199	HIS	N-CA-C	-7.36	91.14	111.00
3	T	25	TRP	CG-CD1-NE1	-7.31	102.79	110.10
2	H	61	TRP	NE1-CE2-CZ2	7.27	138.40	130.40
3	T	14	TRP	NE1-CE2-CZ2	7.13	138.24	130.40
3	T	14	TRP	CG-CD1-NE1	-7.11	102.99	110.10
2	H	141	TRP	CG-CD1-NE1	-7.09	103.01	110.10
2	H	207	TRP	CG-CD1-NE1	-7.04	103.06	110.10
2	H	147	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	H	237	TRP	NE1-CE2-CD2	-6.89	100.41	107.30
2	H	115	THR	OG1-CB-CG2	-6.81	94.35	110.00
2	H	215	TRP	NE1-CE2-CZ2	6.79	137.87	130.40
2	H	29	TRP	NE1-CE2-CD2	-6.63	100.67	107.30
2	H	51	TRP	CG-CD1-NE1	-6.58	103.52	110.10
3	T	78	TYR	CB-CG-CD1	6.39	124.84	121.00
2	H	215	TRP	CG-CD2-CE3	-6.39	128.15	133.90
2	H	141	TRP	NE1-CE2-CD2	-6.29	101.01	107.30
3	T	78	TYR	CB-CG-CD2	-6.29	117.23	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	45	TRP	NE1-CE2-CD2	-6.28	101.03	107.30
2	H	215	TRP	CG-CD1-NE1	-6.16	103.94	110.10
2	H	61	TRP	NE1-CE2-CD2	-6.15	101.15	107.30
2	H	170(F)	GLY	N-CA-C	-6.09	97.88	113.10
2	H	51	TRP	NE1-CE2-CD2	-5.99	101.31	107.30
2	H	207	TRP	CG-CD2-CE3	-5.95	128.54	133.90
2	H	216	GLY	N-CA-C	-5.90	98.35	113.10
2	H	162	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	H	237	TRP	CG-CD2-CE3	-5.84	128.65	133.90
2	H	126	ARG	NE-CZ-NH2	-5.83	117.38	120.30
3	T	25	TRP	NE1-CE2-CD2	-5.79	101.51	107.30
2	H	51	TRP	NE1-CE2-CZ2	5.78	136.76	130.40
2	H	215	TRP	NE1-CE2-CD2	-5.78	101.52	107.30
2	H	134	ARG	NE-CZ-NH2	-5.78	117.41	120.30
3	T	7	VAL	N-CA-C	-5.63	95.79	111.00
2	H	123	LEU	N-CA-C	-5.43	96.35	111.00
3	T	86	THR	N-CA-CB	-5.39	100.05	110.30
3	T	14	TRP	NE1-CE2-CD2	-5.35	101.95	107.30
2	H	204	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	H	62	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	T	136	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	H	170(C)	ARG	N-CA-C	-5.25	96.83	111.00
1	L	106	THR	OG1-CB-CG2	-5.20	98.03	110.00
3	T	193	ILE	N-CA-C	-5.20	96.96	111.00
3	T	15	LYS	N-CA-C	-5.20	96.96	111.00
2	H	190	SER	N-CA-C	-5.18	97.00	111.00
2	H	170(C)	ARG	NE-CZ-NH2	-5.17	117.71	120.30
3	T	131	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	H	207	TRP	NE1-CE2-CD2	-5.09	102.21	107.30
2	H	170(E)	VAL	CA-C-N	-5.08	106.04	116.20
2	H	129(B)	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	H	99	THR	OG1-CB-CG2	-5.08	98.33	110.00
3	T	34	TYR	CB-CG-CD1	-5.05	117.97	121.00
3	T	95	GLU	OE1-CD-OE2	5.03	129.34	123.30

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	19	0
2	H	1974	0	1950	44	0
3	T	1194	0	1163	34	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	89	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 12.

All (89) 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
1:L:61:CYS:SG	1:L:68:TYR:HB2	2.42	0.59
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: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:66:ASP:CG	3:T:69:GLN:HG2	2.28	0.54
3:T:51:TYR:CE1	3:T:83:VAL:HG22	2.42	0.54
2:H:195:SER:OG	4:H:258:N1H:O6'	2.20	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:63:ILE:C	3:T:63:ILE:HD12	2.32	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
2:H:27:CYS:N	2:H:28:PRO:CD	2.75	0.48
2:H:184:TYR:CD1	2:H:188:LYS:HB2	2.48	0.48
2:H:99:THR:HG22	2:H:215:TRP:CD1	2.49	0.47
3:T:87:GLY:O	3:T:90:GLY:N	2.47	0.47
2:H:144:LEU:HD12	2:H:150:ALA:O	2.14	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
3:T:86:THR:OG1	3:T:90:GLY:C	2.53	0.47
3:T:35:THR:HG23	3:T:50:PHE:HA	1.97	0.47
1:L:101:TYR:HB2	1:L:113:ARG:HB2	1.97	0.47
2:H:202:HIS:HB2	2:H:207:TRP:CH2	2.50	0.47
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
3:T:51:TYR:CD1	3:T:83:VAL:HG21	2.51	0.46
2:H:45:THR:HG21	2:H:121:LEU:HD23	1.98	0.46
2:H:23:PRO:O	2:H:24:LYS:C	2.55	0.45
3:T:87:GLY:O	3:T:89:ALA:N	2.49	0.45
2:H:113:VAL:O	2:H:115:THR:HG23	2.16	0.45
2:H:45:THR:O	2:H:52:VAL:HA	2.16	0.45
3:T:59:LEU:O	3:T:60:THR:C	2.55	0.44
1:L:69:ILE:CG2	3:T:133:LEU:HD21	2.48	0.44
1:L:79:ARG:HH21	3:T:56:GLU:CD	2.21	0.44
1:L:49:GLN:OE1	1:L:49:GLN:C	2.57	0.44
1:L:105:HIS:CB	1:L:108:THR:HG23	2.48	0.44
1:L:93:ASN:HB2	3:T:50:PHE:CZ	2.53	0.44
1:L:91:CYS:O	2:H:129(B):ARG:HD3	2.17	0.44
2:H:203:TYR:CZ	2:H:204:ARG:NE	2.85	0.44
3:T:82:ASN:C	3:T:84:GLU:H	2.21	0.43
2:H:92:SER:OG	2:H:255:PRO:HA	2.19	0.43
3:T:63:ILE:HA	3:T:71:TYR:CZ	2.53	0.43
3:T:18:ASN:O	3:T:19:PHE:HB2	2.18	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: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
2:H:58:CYS:HA	4:H:258:N1H:C4B	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:216:GLY:O	2:H:217:GLN:CB	2.67	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
3:T:136:ARG:O	3:T:137:ASN:C	2.57	0.42
2:H:143:GLN:NE2	2:H:146:ASP:O	2.53	0.42
2:H:145:LEU:O	2:H:146:ASP:C	2.58	0.42
3:T:6:THR:HG22	3:T:77:SER:CB	2.50	0.42
3:T:60:THR:O	3:T:64:VAL:HG22	2.20	0.41
3:T:10:TYR:CE1	3:T:26:GLU:HB2	2.55	0.41
2:H:228:TYR:N	2:H:228:TYR:CD1	2.88	0.41
2:H:28:PRO:HG2	2:H:29:TRP:CZ3	2.55	0.41
1:L:70:CYS:HB3	1:L:81:CYS:SG	2.61	0.41
2:H:236:GLU:CD	2:H:236:GLU:H	2.23	0.41
2:H:95:VAL:HB	2:H:98:THR:CG2	2.51	0.41
2:H:199:HIS:HB3	2:H:211:GLY:CA	2.50	0.41
2:H:23:PRO:HB2	2:H:26:GLU:CD	2.41	0.41
1:L:62:LYS:O	1:L:68:TYR:HA	2.21	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:63:ASN:N	2:H:63:ASN:OD1	2.54	0.41
3:T:79:PRO:HD2	3:T:85:SER:HB2	2.03	0.41
2:H:89:ILE:HA	2:H:252:LEU:O	2.21	0.41
2:H:158:LEU:HD11	2:H:188:LYS:HB3	2.03	0.40
2:H:166:GLN:HB2	3:T:94:TYR:CE1	2.57	0.40
3:T:133:LEU:HD22	3:T:133:LEU:N	2.36	0.40
1:L:98:CYS:SG	1:L:102:CYS:HB2	2.61	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	1
2	H	252/254 (99%)	211 (84%)	28 (11%)	13 (5%)	2	2
3	T	143/218 (66%)	118 (82%)	19 (13%)	6 (4%)	3	3
All	All	487/624 (78%)	406 (83%)	56 (12%)	25 (5%)	2	2

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
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%)	76 (93%)	6 (7%)	17	31
2	H	216/216 (100%)	207 (96%)	9 (4%)	36	60
3	T	137/199 (69%)	132 (96%)	5 (4%)	42	67
All	All	435/547 (80%)	415 (95%)	20 (5%)	33	55

All (20) 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	110	ARG
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	215	TRP
2	H	236	GLU
2	H	255	PRO
3	T	6	THR
3	T	33	VAL
3	T	53	THR
3	T	74	ARG
3	T	195	SER

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

Mol	Chain	Res	Type
1	L	80	ASN
2	H	100	ASN
2	H	110	GLN
2	H	143	GLN
2	H	159	ASN
3	T	11	ASN
3	T	31	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	28,33,33	3.40	8 (28%)	36,48,48	2.64	10 (27%)

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	-	-	0/13/16/16	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	258	N1H	C5'-C1B	-5.68	1.40	1.49
4	H	258	N1H	C3-C4	-3.13	1.36	1.41
4	H	258	N1H	C5-C4	-2.82	1.32	1.42
4	H	258	N1H	C5-N6	-2.70	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	258	N1H	C1'-C8	-2.17	1.41	1.48
4	H	258	N1H	CN4-C5	-2.06	1.34	1.42
4	H	258	N1H	C6B-C1B	2.03	1.43	1.39
4	H	258	N1H	O52-N5B	15.59	1.53	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	258	N1H	C2-C3-C4	-5.64	114.76	120.88
4	H	258	N1H	C2-C1-N6	-5.31	116.39	122.20
4	H	258	N1H	O52-N5B-C5B	2.04	122.55	118.89
4	H	258	N1H	C3-C2-C1	2.34	121.84	119.55
4	H	258	N1H	C8-N3-C4	3.91	112.54	104.47
4	H	258	N1H	CN4-C8-C1'	4.05	135.03	129.40
4	H	258	N1H	C6B-C5B-N5B	4.19	122.48	118.80
4	H	258	N1H	C1-N6-C5	4.87	123.60	117.78
4	H	258	N1H	CN4-C5-C4	6.26	111.69	106.24
4	H	258	N1H	N7-C1-N6	7.00	122.59	118.03

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

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	L	94/152 (61%)	-0.14	5 (5%)	30	35	20, 45, 89, 96	8 (8%)
2	H	254/254 (100%)	-0.36	11 (4%)	39	45	12, 36, 88, 100	23 (9%)
3	T	149/218 (68%)	-0.18	6 (4%)	42	48	15, 49, 90, 99	20 (13%)
All	All	497/624 (79%)	-0.26	22 (4%)	38	44	12, 41, 90, 100	51 (10%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	137	ASN	6.8
1	L	66	GLN	6.4
3	T	138	ASN	5.9
2	H	170(I)	PRO	5.5
2	H	170(E)	VAL	5.1
2	H	170(F)	GLY	5.1
3	T	188	SER	4.5
1	L	52	SER	4.4
2	H	216	GLY	4.0
2	H	60(D)	ASN	3.8
2	H	63	ASN	3.8
1	L	50	CYS	3.7
2	H	170(G)	ASP	3.5
2	H	170(H)	SER	3.3
2	H	175	ASN	3.2
3	T	205	SER	2.8
1	L	67	SER	2.8
3	T	155	LEU	2.6
1	L	53	SER	2.4
3	T	109	GLY	2.3
2	H	217	GLN	2.2
2	H	78	GLY	2.2

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	N1H	H	258	30/30	0.97	0.12	-0.35	18,40,50,55	4

## 6.5 Other polymers [i](#)

There are no such residues in this entry.