



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 PM UTC

PDB ID : 2FLB / pdb_00002flb
Title : Discovery of a Novel Hydroxy Pyrazole Based Factor IXa Inhibitor
Authors : Katz, B.A.
Deposited on : 2006-01-05
Resolution : 1.95 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

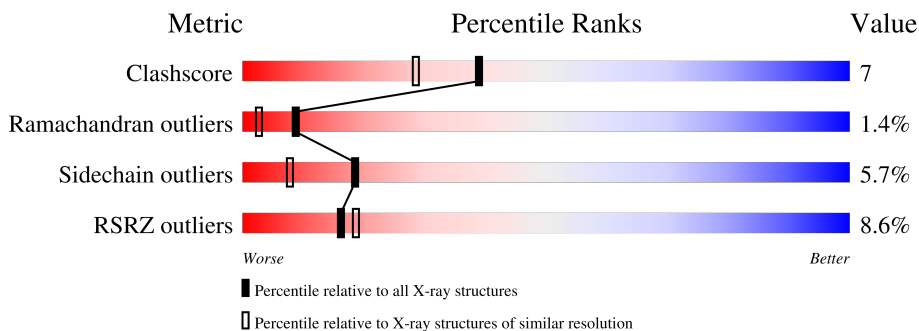
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	 5% 44% 15% 37%
2	H	254	 4% 74% 22%
3	T	218	 11% 46% 20% 31%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4278 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
			Total	C	N	O	S			
1	L	96	727	439	126	149	13	0	2	0

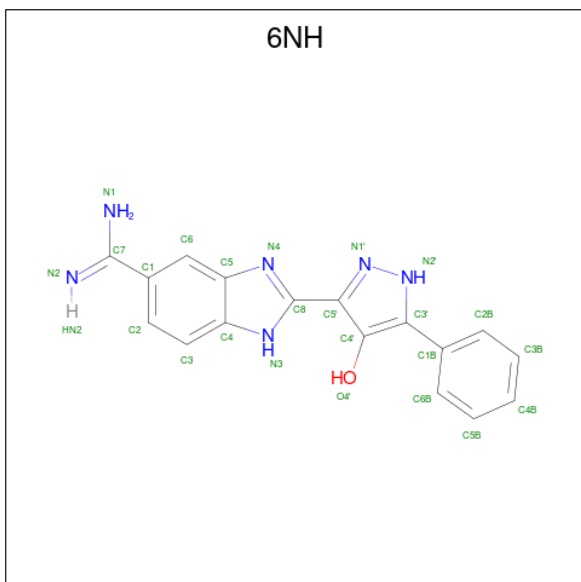
- Molecule 2 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	254	1988	1263	353	359	13	0	3	0

- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	T	151	1218	774	198	244	2	0	0	0

- Molecule 4 is 2-(4-HYDROXY-5-PHENYL-1H-PYRAZOL-3-YL)-1H-BENZOIMIDAZOLE-5-CARBOXAMIDINE (CCD ID: 6NH) (formula: C₁₇H₁₄N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			24	17	6	1		

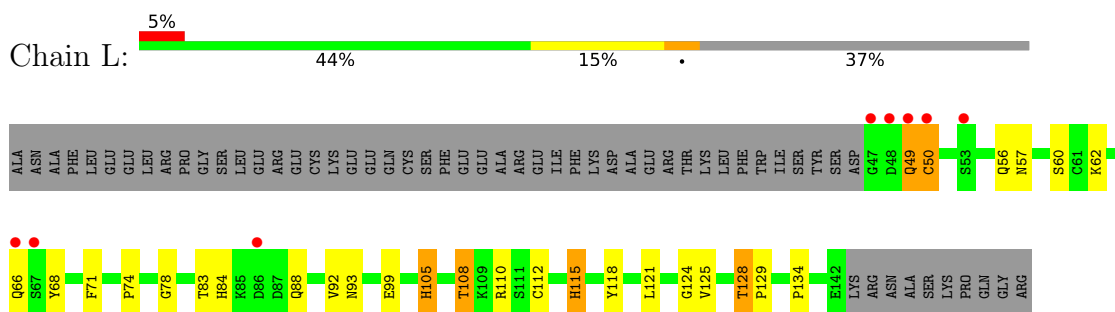
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	65	Total	O	0	0
			65	65		
5	H	161	Total	O	0	0
			161	161		
5	T	95	Total	O	0	0
			95	95		

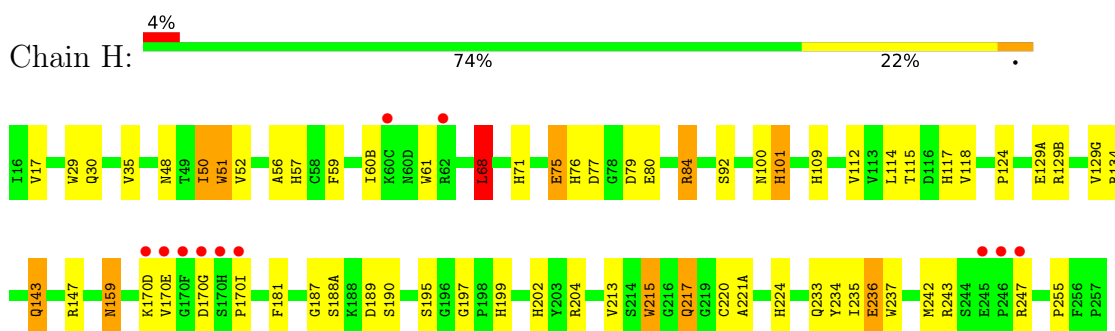
3 Residue-property plots [i](#)

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.

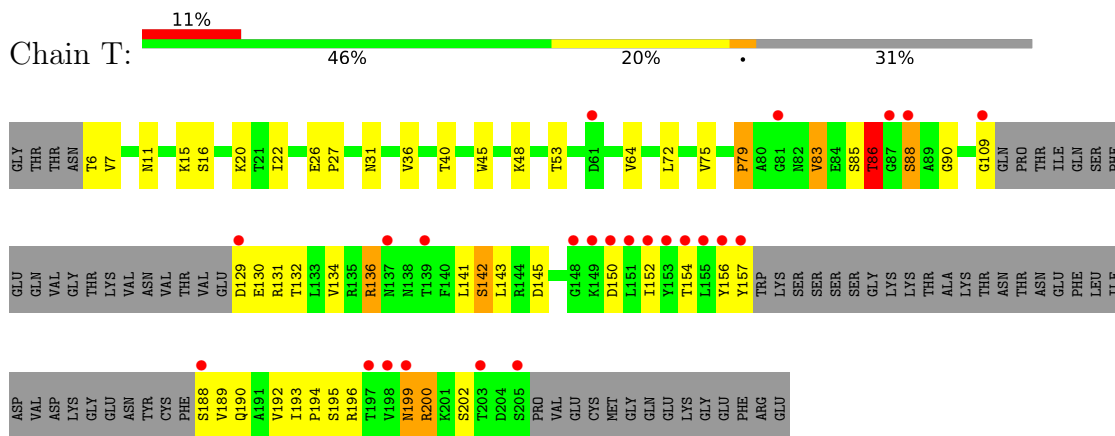
- Molecule 1: Coagulation factor VII



- Molecule 2: Coagulation factor VII



- Molecule 3: Tissue factor



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.45Å 69.03Å 78.76Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	7.00 – 1.95 7.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.95) 91.2 (7.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.247 , 0.280 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.962	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 97.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.024 for h,-k,-l 0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4278	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: 6NH

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	1.01	4/748 (0.5%)	1.75	15/1009 (1.5%)
2	H	1.22	12/2046 (0.6%)	1.83	45/2784 (1.6%)
3	T	0.92	1/1244 (0.1%)	1.71	18/1693 (1.1%)
All	All	1.10	17/4038 (0.4%)	1.78	78/5486 (1.4%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	52	VAL	CA-CB	8.03	1.64	1.54
2	H	101	HIS	CD2-NE2	-7.00	1.30	1.37
2	H	71	HIS	CD2-NE2	-6.97	1.30	1.37
1	L	84	HIS	CD2-NE2	-6.79	1.30	1.37
2	H	202	HIS	CA-CB	-6.55	1.44	1.53
2	H	109	HIS	CD2-NE2	-6.51	1.30	1.37
1	L	115	HIS	CD2-NE2	-6.48	1.30	1.37
2	H	199	HIS	CD2-NE2	-6.46	1.30	1.37
2	H	76	HIS	CD2-NE2	-6.44	1.30	1.37
2	H	224	HIS	CD2-NE2	-6.04	1.31	1.37
2	H	57	HIS	CG-ND1	-6.03	1.31	1.38
2	H	202	HIS	CD2-NE2	-6.00	1.31	1.37
2	H	57	HIS	CD2-NE2	-5.66	1.31	1.37
2	H	117	HIS	CD2-NE2	-5.62	1.31	1.37
3	T	22	ILE	CA-CB	5.50	1.61	1.54
1	L	105	HIS	CD2-NE2	-5.45	1.31	1.37
1	L	115	HIS	CG-ND1	-5.28	1.32	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	79	ASP	N-CA-C	9.83	125.08	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	134	ARG	CA-CB-CG	-9.25	95.60	114.10
2	H	189	ASP	CA-CB-CG	8.18	120.78	112.60
3	T	199	ASN	CA-CB-CG	-8.13	104.47	112.60
1	L	84	HIS	CB-CG-CD2	-8.12	120.65	131.20
2	H	188(A)	SER	N-CA-C	7.91	123.44	112.45
2	H	233	GLN	OE1-CD-NE2	-7.60	115.00	122.60
2	H	51	TRP	CG-CD2-CE3	7.45	141.35	133.90
3	T	26	GLU	O-C-N	-7.40	116.97	121.71
2	H	68	LEU	CD1-CG-CD2	7.32	126.91	110.80
2	H	170(G)	ASP	CA-CB-CG	7.20	119.80	112.60
3	T	157	TYR	N-CA-C	-7.00	91.39	111.00
2	H	77	ASP	O-C-N	-6.94	113.25	122.14
2	H	129(G)	VAL	N-CA-C	-6.94	98.59	108.58
1	L	105	HIS	CB-CG-CD2	-6.77	122.40	131.20
3	T	7	VAL	N-CA-C	-6.73	97.89	108.86
3	T	83	VAL	N-CA-CB	-6.68	100.21	111.23
2	H	101	HIS	CB-CG-CD2	-6.60	122.62	131.20
2	H	30	GLN	OE1-CD-NE2	-6.59	116.01	122.60
2	H	197	GLY	CA-C-N	6.55	127.07	119.99
2	H	197	GLY	C-N-CA	6.55	127.07	119.99
1	L	49	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	L	84	HIS	CB-CG-ND1	6.54	132.50	122.70
1	L	50	CYS	N-CA-C	6.30	124.21	110.80
2	H	50	ILE	CB-CA-C	-6.28	104.03	110.93
2	H	109	HIS	CB-CG-CD2	-6.23	123.10	131.20
2	H	80	GLU	CA-C-O	-6.11	114.44	121.47
2	H	181	PHE	CA-CB-CG	6.11	119.91	113.80
2	H	159	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	L	108	THR	CA-CB-CG2	6.03	120.75	110.50
3	T	53	THR	N-CA-C	-6.00	105.92	113.72
2	H	75	GLU	N-CA-C	5.98	118.27	108.52
1	L	108	THR	CA-CB-OG1	-5.98	100.63	109.60
2	H	220	CYS	N-CA-C	-5.97	97.74	108.48
3	T	86	THR	N-CA-CB	-5.95	100.36	111.13
1	L	125	VAL	N-CA-C	5.93	117.10	112.12
3	T	40	THR	N-CA-C	-5.92	102.01	110.59
2	H	30	GLN	CG-CD-NE2	5.91	125.27	116.40
2	H	143	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	L	93	ASN	OD1-CG-ND2	-5.86	116.74	122.60
2	H	51	TRP	CB-CG-CD1	-5.84	118.14	126.90
3	T	145	ASP	CA-CB-CG	5.84	118.44	112.60
2	H	71	HIS	CB-CG-CD2	-5.83	123.62	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	108	THR	N-CA-CB	-5.76	101.67	111.69
2	H	117	HIS	CB-CG-CD2	-5.75	123.73	131.20
2	H	56	ALA	N-CA-C	5.74	119.09	111.75
2	H	217	GLN	N-CA-C	-5.65	99.31	108.41
2	H	129(B)	ARG	CA-C-O	5.58	125.51	119.15
3	T	190	GLN	OE1-CD-NE2	-5.56	117.04	122.60
3	T	199	ASN	OD1-CG-ND2	-5.50	117.10	122.60
2	H	129(A)	GLU	N-CA-C	5.46	117.23	111.28
1	L	105	HIS	CB-CG-ND1	5.45	130.87	122.70
3	T	136	ARG	N-CA-C	-5.44	99.56	108.76
1	L	78	GLY	N-CA-C	-5.44	106.78	111.95
2	H	224	HIS	CB-CG-CD2	-5.43	124.14	131.20
2	H	61	TRP	CG-CD2-CE3	5.40	139.30	133.90
2	H	199	HIS	N-CA-C	-5.37	98.61	108.02
3	T	15	LYS	N-CA-C	-5.33	99.83	108.52
3	T	31	ASN	CA-CB-CG	5.33	117.93	112.60
2	H	115	THR	N-CA-C	-5.29	101.44	108.74
3	T	86	THR	CA-CB-OG1	-5.28	101.68	109.60
3	T	31	ASN	OD1-CG-ND2	-5.27	117.33	122.60
2	H	215	TRP	CG-CD2-CE3	5.27	139.17	133.90
2	H	100	ASN	OD1-CG-ND2	-5.27	117.33	122.60
2	H	51	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	L	57	ASN	OD1-CG-ND2	-5.21	117.39	122.60
2	H	57	HIS	CA-CB-CG	5.21	119.01	113.80
2	H	114	LEU	N-CA-C	-5.15	102.13	110.32
3	T	88	SER	N-CA-C	5.15	121.77	110.80
1	L	49	GLN	CG-CD-NE2	5.13	124.10	116.40
2	H	170(E)	VAL	N-CA-C	5.09	119.93	109.34
1	L	56	GLN	OE1-CD-NE2	-5.06	117.54	122.60
2	H	61	TRP	CE2-CD2-CG	-5.06	101.13	107.20
2	H	243	ARG	CB-CG-CD	-5.04	99.70	111.30
2	H	29	TRP	CE2-CD2-CG	-5.04	101.16	107.20
2	H	134	ARG	N-CA-C	5.04	116.58	111.14
3	T	142	SER	CA-CB-OG	5.02	121.14	111.10
2	H	237	TRP	CE2-CD2-CG	-5.02	101.18	107.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	727	0	663	10	0
2	H	1988	0	1968	22	0
3	T	1218	0	1181	20	0
4	H	24	0	14	6	0
5	H	161	0	0	3	0
5	L	65	0	0	0	0
5	T	95	0	0	0	0
All	All	4278	0	3826	52	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 7.

All (52) 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)
3:T:152:ILE:HG13	3:T:192:VAL:HG23	1.68	0.73
2:H:195:SER:OG	4:H:1246:6NH:O4'	2.08	0.66
3:T:86:THR:HG23	3:T:90:GLY:HA2	1.79	0.65
2:H:187:GLY:HA2	2:H:221(A):ALA:O	1.98	0.64
4:H:1246:6NH:N3	5:H:1321:HOH:O	2.29	0.60
1:L:121[A]:LEU:HD21	1:L:128:THR:HB	1.85	0.58
2:H:59:PHE:HA	2:H:60(B):ILE:HG12	1.87	0.56
2:H:236:GLU:H	2:H:236:GLU:CD	2.14	0.56
4:H:1246:6NH:H2B	5:H:1354:HOH:O	2.07	0.54
1:L:99:GLU:HA	2:H:204:ARG:HD3	1.89	0.54
3:T:154:THR:O	3:T:189:VAL:HA	2.08	0.53
2:H:101:HIS:HA	2:H:234:TYR:OH	2.11	0.50
2:H:195:SER:HG	4:H:1246:6NH:HN3	1.56	0.49
2:H:84:ARG:H	2:H:84:ARG:HD2	1.77	0.49
1:L:115:HIS:O	1:L:118:TYR:HB2	2.13	0.49
2:H:68:LEU:HD13	2:H:112:VAL:HG11	1.93	0.49
2:H:236:GLU:HG3	5:H:1383:HOH:O	2.13	0.48
2:H:50:ILE:HG13	2:H:51:TRP:CD1	2.48	0.48
3:T:16:SER:HA	3:T:20:LYS:O	2.14	0.47
2:H:143:GLN:NE2	2:H:147:ARG:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:HIS:HB3	1:L:108:THR:HG22	1.96	0.47
2:H:35:VAL:HG21	2:H:60(B):ILE:HD12	1.97	0.47
3:T:192:VAL:HA	3:T:200:ARG:O	2.15	0.46
2:H:68:LEU:HD22	2:H:118:VAL:HG13	1.96	0.46
2:H:92:SER:OG	2:H:255:PRO:HA	2.16	0.46
3:T:109:GLY:O	3:T:202:SER:HB2	2.15	0.46
3:T:193:ILE:HB	3:T:196:ARG:HD2	1.97	0.46
1:L:112:CYS:HB2	1:L:124:GLY:O	2.16	0.46
3:T:132:THR:HG22	3:T:143:LEU:HD12	1.99	0.45
2:H:195:SER:OG	4:H:1246:6NH:N3	2.40	0.45
3:T:86:THR:CG2	3:T:90:GLY:HA2	2.44	0.45
2:H:213:VAL:HG12	4:H:1246:6NH:H3	2.00	0.44
2:H:170(I):PRO:HD2	2:H:215:TRP:CZ3	2.52	0.44
3:T:45:TRP:HH2	3:T:72:LEU:HD12	1.81	0.44
1:L:71:PHE:CE2	3:T:131:ARG:HD3	2.53	0.44
2:H:48:ASN:HD21	2:H:242:MET:CE	2.31	0.44
3:T:136:ARG:HB3	3:T:141:LEU:HD21	1.99	0.44
3:T:79:PRO:HD2	3:T:85:SER:HB2	2.00	0.43
3:T:152:ILE:HD11	3:T:194:PRO:HG3	1.99	0.43
1:L:62:LYS:O	1:L:68:TYR:HA	2.19	0.43
3:T:36:VAL:HG22	3:T:75:VAL:HG22	2.00	0.42
3:T:48:LYS:HE3	3:T:48:LYS:HB3	1.94	0.42
3:T:130:GLU:O	3:T:142:SER:HB2	2.20	0.42
3:T:79:PRO:HD2	3:T:85:SER:CB	2.50	0.41
2:H:124:PRO:O	2:H:235:ILE:HD13	2.20	0.41
1:L:129:PRO:HB3	1:L:134:PRO:HG3	2.03	0.41
2:H:48:ASN:ND2	2:H:242:MET:HE1	2.36	0.41
3:T:131:ARG:HA	3:T:142:SER:HA	2.02	0.41
1:L:110:ARG:HD2	1:L:110:ARG:C	2.46	0.40
3:T:64:VAL:HB	3:T:134:VAL:HA	2.02	0.40
1:L:105:HIS:HB3	1:L:108:THR:CG2	2.52	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	96/152 (63%)	85 (88%)	10 (10%)	1 (1%)	12	5
2	H	255/254 (100%)	239 (94%)	15 (6%)	1 (0%)	30	21
3	T	145/218 (66%)	133 (92%)	7 (5%)	5 (3%)	3	0
All	All	496/624 (80%)	457 (92%)	32 (6%)	7 (1%)	9	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	50	CYS
3	T	156	TYR
3	T	88	SER
3	T	200	ARG
2	H	170(D)	LYS
3	T	150	ASP
3	T	199	ASN

5.3.2 Protein sidechains [i](#)

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	85/132 (64%)	77 (91%)	8 (9%)	8	2
2	H	219/216 (101%)	210 (96%)	9 (4%)	27	17
3	T	139/199 (70%)	130 (94%)	9 (6%)	15	6
All	All	443/547 (81%)	417 (94%)	26 (6%)	18	7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	49	GLN
1	L	60	SER
1	L	66	GLN

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Mol	Chain	Res	Type
1	L	74	PRO
1	L	83	THR
1	L	88	GLN
1	L	92	VAL
1	L	128	THR
2	H	68	LEU
2	H	75	GLU
2	H	84	ARG
2	H	159	ASN
2	H	190[A]	SER
2	H	190[B]	SER
2	H	217	GLN
2	H	236	GLU
2	H	247	ARG
3	T	6	THR
3	T	11	ASN
3	T	27	PRO
3	T	79	PRO
3	T	83	VAL
3	T	86	THR
3	T	129	ASP
3	T	188	SER
3	T	195	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	100	ASN
2	H	143	GLN
2	H	159	ASN
2	H	217	GLN
2	H	233	GLN
3	T	199	ASN

5.3.3 RNA

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	6NH	H	1246	-	27,27,27	1.94	6 (22%)	31,39,39	2.56	13 (41%)

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	6NH	H	1246	-	-	3/12/12/12	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1246	6NH	N2'-N1'	4.15	1.45	1.36
4	H	1246	6NH	C4-N3	-3.94	1.31	1.38
4	H	1246	6NH	C1B-C3'	-3.91	1.41	1.47
4	H	1246	6NH	C1-C7	-3.58	1.40	1.47
4	H	1246	6NH	C5'-C8	-2.89	1.42	1.46
4	H	1246	6NH	C5-N4	-2.70	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1246	6NH	C4-N3-C8	-5.06	100.92	106.85
4	H	1246	6NH	C5-N4-C8	-5.00	99.61	104.68
4	H	1246	6NH	C3'-N2'-N1'	-4.84	104.68	112.88
4	H	1246	6NH	N3-C8-N4	4.58	118.13	113.22
4	H	1246	6NH	C5-C4-N3	4.12	110.66	105.71
4	H	1246	6NH	C2-C1-C6	3.57	123.38	119.25
4	H	1246	6NH	C1B-C3'-N2'	3.42	125.57	121.23
4	H	1246	6NH	O4'-C4'-C3'	3.33	132.04	125.54
4	H	1246	6NH	C8-C5'-N1'	3.03	126.86	119.86
4	H	1246	6NH	C3-C4-N3	-2.88	125.01	130.83
4	H	1246	6NH	C6B-C1B-C2B	2.33	121.54	118.57
4	H	1246	6NH	C5B-C6B-C1B	-2.16	118.25	120.36
4	H	1246	6NH	C3-C4-C5	2.03	124.33	122.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

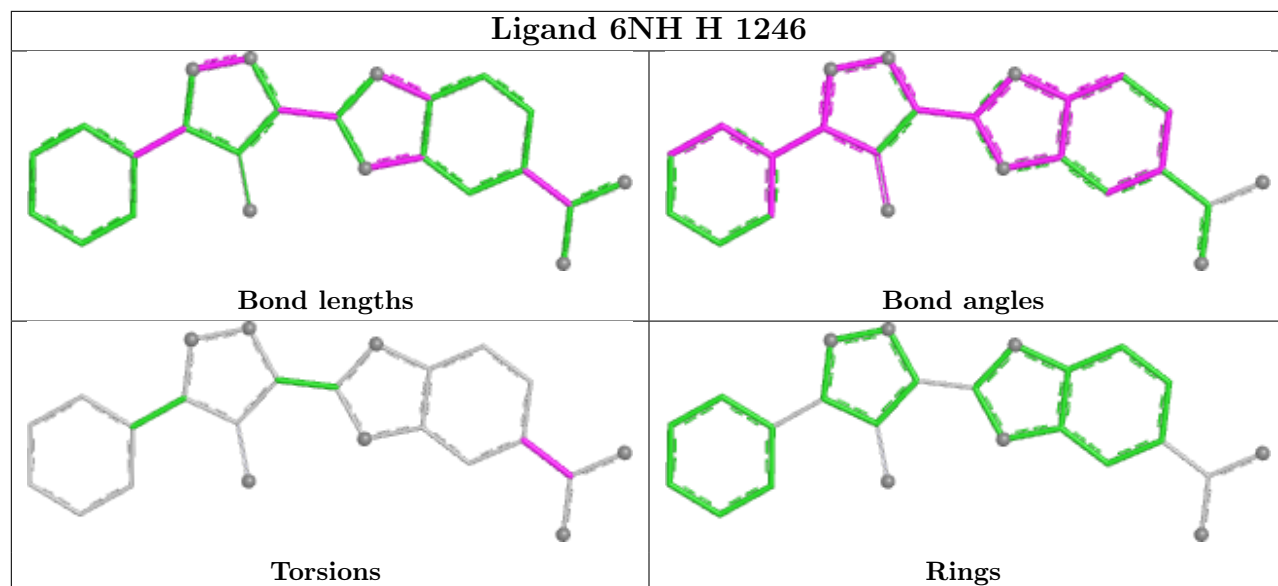
Mol	Chain	Res	Type	Atoms
4	H	1246	6NH	C2-C1-C7-N1
4	H	1246	6NH	C6-C1-C7-N1
4	H	1246	6NH	C2-C1-C7-N2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1246	6NH	6	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	96/152 (63%)	0.22	8 (8%) 17 20	0, 24, 44, 53	19 (19%)
2	H	254/254 (100%)	-0.11	11 (4%) 40 46	1, 18, 41, 70	25 (9%)
3	T	151/218 (69%)	0.71	24 (15%) 5 5	3, 27, 60, 87	24 (15%)
All	All	501/624 (80%)	0.20	43 (8%) 16 19	0, 22, 53, 87	68 (13%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	170(F)	GLY	14.6
3	T	188	SER	13.2
2	H	170(G)	ASP	12.5
3	T	205	SER	12.4
3	T	156	TYR	9.3
3	T	137	ASN	8.8
3	T	150	ASP	7.7
2	H	170(E)	VAL	7.2
3	T	81	GLY	6.3
1	L	53	SER	6.1
3	T	157	TYR	5.9
1	L	66	GLN	5.6
3	T	129	ASP	5.3
3	T	149	LYS	5.1
1	L	48	ASP	4.9
3	T	88	SER	4.4
3	T	87	GLY	4.4
2	H	60(C)	LYS	4.2
1	L	47	GLY	4.0
3	T	151	LEU	3.7
1	L	49	GLN	3.7
3	T	148	GLY	3.3
2	H	247	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
3	T	155	LEU	3.2
2	H	170(H)	SER	3.2
3	T	152	ILE	3.1
2	H	170(I)	PRO	3.1
2	H	246	PRO	2.9
3	T	153	TYR	2.8
3	T	198	VAL	2.8
1	L	67	SER	2.7
3	T	109	GLY	2.6
1	L	50	CYS	2.5
2	H	62	ARG	2.5
2	H	245	GLU	2.4
3	T	197	THR	2.3
2	H	170(D)	LYS	2.3
3	T	139	THR	2.3
3	T	61	ASP	2.2
3	T	199	ASN	2.2
3	T	203	THR	2.2
1	L	86	ASP	2.2
3	T	154	THR	2.1

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.

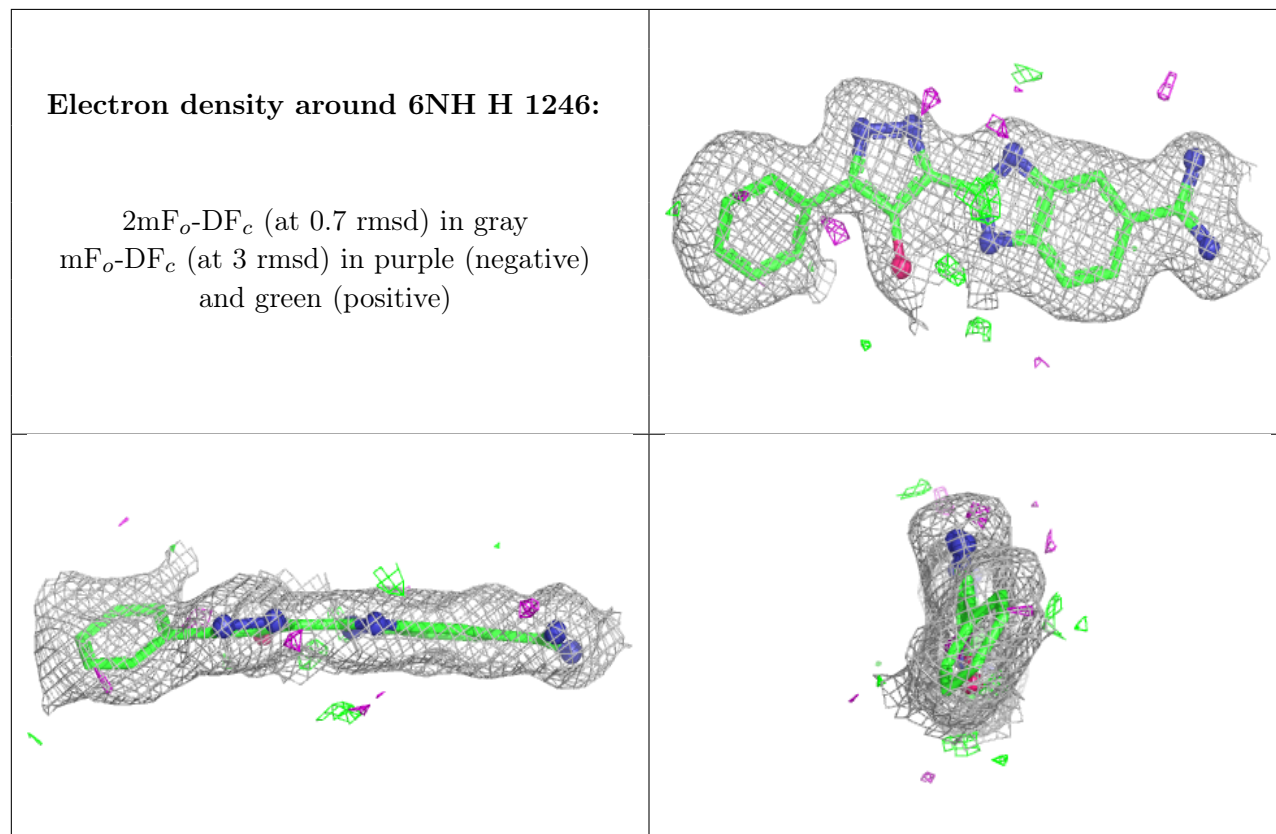
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	6NH	H	1246	24/24	0.90	0.07	16,21,27,31	0

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.