



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:18 am BST

PDB ID : 1X7A
Title : Porcine Factor IXa Complexed to 1-{3-[amino(imino)methyl]phenyl}-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide
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Deposited on : 2004-08-13
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

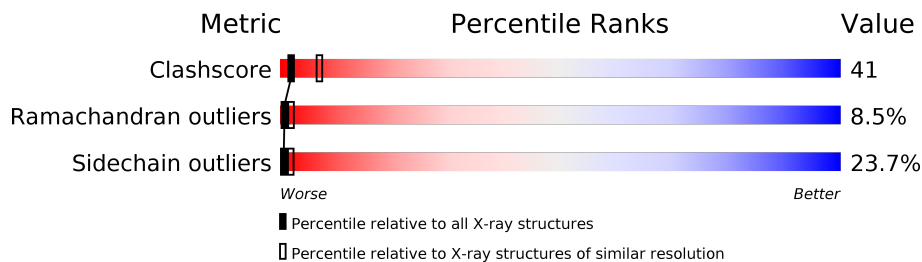
1 Overall quality at a glance

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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	235	
2	L	146	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2595 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 IXa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	235	1833	1170	312	343	8	28	0	0

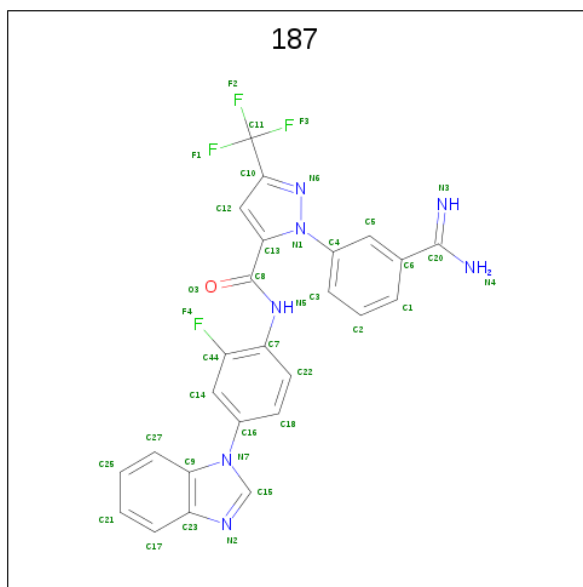
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	174	PHE	VAL	SEE REMARK 999	UNP P16293
C	192	GLN	LEU	SEE REMARK 999	UNP P16293
C	238	ILE	-	SEE REMARK 999	UNP P16293
C	239	LYS	-	SEE REMARK 999	UNP P16293
C	240	GLU	-	SEE REMARK 999	UNP P16293
C	241	LYS	-	SEE REMARK 999	UNP P16293
C	242	THR	-	SEE REMARK 999	UNP P16293
C	243	LYS	-	SEE REMARK 999	UNP P16293
C	244	LEU	-	SEE REMARK 999	UNP P16293
C	245	THR	-	SEE REMARK 999	UNP P16293

- Molecule 2 is a protein called Coagulation Factor IX, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	97	725	442	130	140	13	82	0	0

- Molecule 3 is 1-{3-[AMINO(IMINO)METHYL]PHENYL}-N-[4-(1H-BENZIMIDAZOL-1-YL)-2-FLUOROPHENYL]-3-(TRIFLUOROMETHYL)-1H-PYRAZOLE-5-CARBOXAMID E (three-letter code: 187) (formula: C₂₅H₁₇F₄N₇O).



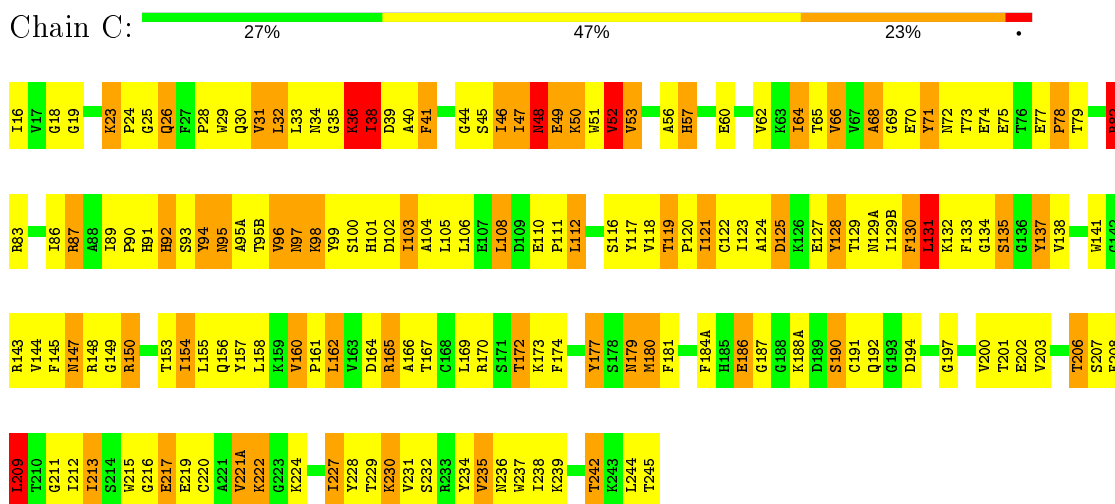
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	C	1	37	25	4	7	1	0	0

3 Residue-property plots

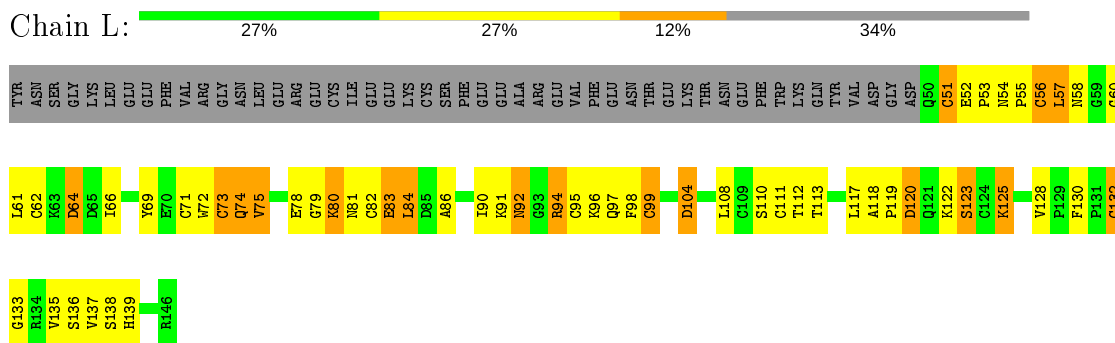
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: Coagulation Factor IXa



- Molecule 2: Coagulation Factor IX, light chain



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.00Å 129.00Å 71.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2595	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: 187

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	C	0.67	1/1877 (0.1%)	0.94	9/2547 (0.4%)
2	L	0.88	5/739 (0.7%)	1.09	9/999 (0.9%)
All	All	0.74	6/2616 (0.2%)	0.99	18/3546 (0.5%)

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
1	C	0	7
2	L	0	3
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	56	CYS	CB-SG	-6.57	1.71	1.82
2	L	95	CYS	CB-SG	-6.27	1.71	1.82
2	L	128	VAL	C-N	-5.59	1.23	1.34
2	L	62	CYS	CB-SG	5.54	1.91	1.82
1	C	119	THR	C-N	-5.19	1.24	1.34
2	L	71	CYS	CB-SG	-5.11	1.73	1.81

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	71	CYS	CA-CB-SG	-11.43	93.42	114.00
2	L	75	VAL	CG1-CB-CG2	-9.14	96.27	110.90
1	C	147	ASN	CA-CB-CG	-8.32	95.10	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	VAL	CG1-CB-CG2	-8.29	97.63	110.90
2	L	51	CYS	CA-CB-SG	-7.65	100.22	114.00
1	C	52	VAL	CG1-CB-CG2	6.78	121.74	110.90
1	C	131	LEU	CB-CG-CD1	-6.64	99.72	111.00
1	C	160	VAL	CG1-CB-CG2	6.45	121.22	110.90
1	C	112	LEU	CB-CG-CD1	-6.39	100.14	111.00
2	L	120	ASP	CB-CG-OD2	-6.32	112.61	118.30
2	L	99	CYS	CA-CB-SG	-6.27	102.72	114.00
1	C	138	VAL	CG1-CB-CG2	6.23	120.87	110.90
2	L	120	ASP	CB-CG-OD1	6.13	123.81	118.30
1	C	144	VAL	CG1-CB-CG2	-6.11	101.13	110.90
2	L	61	LEU	CB-CG-CD1	-6.08	100.67	111.00
2	L	135	VAL	CG1-CB-CG2	-5.94	101.40	110.90
2	L	64	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	C	209	LEU	CB-CG-CD2	5.73	120.74	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	128	TYR	Sidechain
1	C	130	PHE	Sidechain
1	C	137	TYR	Sidechain
1	C	172	THR	Peptide
1	C	36	LYS	Mainchain
1	C	71	TYR	Sidechain
1	C	82	ARG	Mainchain
2	L	52	GLU	Peptide
2	L	72	TRP	Peptide
2	L	98	PHE	Sidechain

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	C	1833	0	1802	172	0
2	L	725	0	692	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	37	0	16	3	0
All	All	2595	0	2510	200	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 41.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:CYS:SG	2:L:132:CYS:HB2	1.89	1.11
1:C:33:LEU:HD21	1:C:106:LEU:HD11	1.40	1.00
2:L:51:CYS:SG	2:L:64:ASP:HB3	2.02	0.99
1:C:19:GLY:HA2	1:C:158:LEU:HD13	1.56	0.88
1:C:187:GLY:HA3	1:C:222:LYS:HA	1.57	0.86
1:C:190:SER:OG	3:C:298:187:N4	2.08	0.84
1:C:47:ILE:HD12	1:C:53:VAL:HB	1.60	0.84
1:C:229:THR:HG22	1:C:234:TYR:HE2	1.45	0.81
2:L:92:ASN:O	2:L:99:CYS:HB2	1.81	0.80
1:C:231:VAL:HG12	1:C:235:VAL:HG23	1.65	0.79
2:L:118:ALA:HB2	2:L:125:LYS:HD3	1.65	0.77
1:C:124:ALA:HB2	1:C:208:PHE:CD2	2.19	0.77
1:C:28:PRO:HB2	1:C:119:THR:HB	1.66	0.76
1:C:97:ASN:HD21	1:C:100:SER:HB3	1.52	0.75
1:C:49:GLU:O	1:C:112:LEU:HD12	1.86	0.74
1:C:147:ASN:OD1	1:C:220:CYS:HB2	1.88	0.74
2:L:73:CYS:O	2:L:74:GLN:HB2	1.88	0.73
1:C:124:ALA:HB2	1:C:208:PHE:HD2	1.53	0.73
1:C:60:GLU:HB2	1:C:62:VAL:HG22	1.70	0.72
1:C:34:ASN:O	1:C:64:ILE:HG22	1.90	0.70
1:C:93:SER:HB2	1:C:101:HIS:HD2	1.56	0.70
1:C:200:VAL:HG12	1:C:209:LEU:HA	1.74	0.70
1:C:32:LEU:HB2	1:C:141:TRP:CZ3	2.28	0.69
1:C:87:ARG:HH11	1:C:89:ILE:HD11	1.59	0.67
1:C:53:VAL:HG22	1:C:104:ALA:O	1.94	0.66
2:L:80:LYS:HB2	2:L:83:GLU:OE2	1.96	0.66
1:C:38:ILE:O	1:C:39:ASP:HB2	1.94	0.66
1:C:129(A):ASN:O	1:C:132:LYS:HG3	1.96	0.65
1:C:242:THR:O	1:C:244:LEU:HD12	1.97	0.65
1:C:52:VAL:HG13	1:C:108:LEU:HD21	1.79	0.65
1:C:47:ILE:HD12	1:C:53:VAL:CB	2.27	0.64
1:C:47:ILE:O	1:C:48:ASN:HB3	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLY:HA2	1:C:162:LEU:HB2	1.80	0.63
1:C:56:ALA:HB2	1:C:103:ILE:O	1.98	0.63
1:C:29:TRP:CD2	1:C:121:ILE:HG23	2.35	0.62
1:C:66:VAL:HG11	1:C:108:LEU:HD11	1.82	0.61
2:L:78:GLU:HG3	2:L:86:ALA:HA	1.82	0.61
1:C:229:THR:HG22	1:C:234:TYR:CE2	2.32	0.61
2:L:78:GLU:HG2	2:L:86:ALA:HB2	1.81	0.61
1:C:31:VAL:HG21	1:C:52:VAL:HG11	1.82	0.61
1:C:143:ARG:NH2	1:C:148:ARG:HA	2.16	0.60
2:L:75:VAL:HG23	2:L:122:LYS:HE2	1.83	0.60
1:C:203:VAL:O	1:C:203:VAL:HG13	2.02	0.60
1:C:23:LYS:HG2	1:C:26:GLN:HB3	1.83	0.59
2:L:54:ASN:OD1	2:L:55:PRO:HD2	2.02	0.59
1:C:45:SER:HB3	1:C:121:ILE:HD11	1.85	0.59
1:C:187:GLY:HA3	1:C:222:LYS:CA	2.31	0.58
1:C:41:PHE:HE1	1:C:64:ILE:HG21	1.69	0.58
1:C:129(A):ASN:HD22	1:C:132:LYS:HD2	1.68	0.58
1:C:72:ASN:HB2	1:C:154:ILE:HG23	1.86	0.58
1:C:213:ILE:HA	1:C:228:TYR:CD2	2.39	0.58
2:L:118:ALA:HB1	2:L:119:PRO:CD	2.33	0.58
2:L:78:GLU:CG	2:L:86:ALA:HA	2.33	0.58
1:C:23:LYS:O	1:C:26:GLN:HG2	2.04	0.57
1:C:147:ASN:HD21	1:C:219:GLU:HG2	1.70	0.57
1:C:215:TRP:HE3	1:C:216:GLY:N	2.02	0.57
1:C:103:ILE:HD12	1:C:212:ILE:HG13	1.86	0.57
2:L:118:ALA:CB	2:L:125:LYS:HD3	2.33	0.57
1:C:93:SER:HB2	1:C:101:HIS:CD2	2.38	0.57
1:C:97:ASN:ND2	1:C:100:SER:HB3	2.19	0.57
1:C:121:ILE:HG21	1:C:200:VAL:HG11	1.87	0.56
1:C:100:SER:OG	1:C:101:HIS:N	2.39	0.56
1:C:179:ASN:HB2	1:C:234:TYR:OH	2.04	0.56
1:C:79:THR:HG21	1:C:117:TYR:CG	2.40	0.56
1:C:34:ASN:HB3	1:C:65:THR:OG1	2.06	0.56
1:C:213:ILE:CD1	3:C:298:187:H1	2.36	0.56
1:C:177:TYR:N	1:C:177:TYR:CD1	2.75	0.55
2:L:64:ASP:HA	2:L:69:TYR:HB2	1.88	0.55
2:L:91:LYS:HG3	2:L:94:ARG:NH1	2.21	0.55
1:C:33:LEU:HD21	1:C:106:LEU:CD1	2.26	0.55
1:C:83:ARG:HD2	1:C:110:GLU:O	2.05	0.55
1:C:197:GLY:O	1:C:213:ILE:HG23	2.06	0.55
1:C:132:LYS:O	1:C:133:PHE:HD1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:MET:HB2	1:C:227:ILE:HD12	1.89	0.54
1:C:25:GLY:HA3	2:L:137:VAL:HG21	1.89	0.54
1:C:16:ILE:HB	1:C:156:GLN:HB3	1.88	0.54
2:L:78:GLU:HG2	2:L:86:ALA:CB	2.38	0.54
1:C:66:VAL:O	1:C:82:ARG:HA	2.08	0.53
1:C:31:VAL:HG11	1:C:52:VAL:HG21	1.89	0.53
1:C:36:LYS:O	1:C:38:ILE:HB	2.07	0.53
1:C:235:VAL:HG12	1:C:236:ASN:N	2.24	0.53
2:L:57:LEU:O	2:L:58:ASN:HB2	2.09	0.53
1:C:83:ARG:NH2	1:C:111:PRO:O	2.41	0.53
1:C:57:HIS:O	1:C:57:HIS:CG	2.61	0.53
1:C:160:VAL:HG23	1:C:160:VAL:O	2.09	0.53
1:C:129(B):ILE:HG22	1:C:133:PHE:CE1	2.44	0.53
1:C:93:SER:O	1:C:101:HIS:CD2	2.62	0.53
1:C:95(A):ALA:O	1:C:95(B):THR:HB	2.09	0.53
1:C:68:ALA:O	1:C:70:GLU:N	2.41	0.52
1:C:177:TYR:H	1:C:177:TYR:HD1	1.58	0.52
1:C:202:GLU:HA	1:C:207:SER:HA	1.90	0.52
1:C:47:ILE:HD11	1:C:238:ILE:HD13	1.91	0.52
1:C:19:GLY:CA	1:C:158:LEU:HD13	2.33	0.52
2:L:96:LYS:HB2	2:L:123:SER:HA	1.92	0.52
1:C:122:CYS:SG	2:L:132:CYS:O	2.68	0.52
1:C:135:SER:HA	1:C:160:VAL:O	2.10	0.52
1:C:121:ILE:HD13	1:C:209:LEU:HG	1.91	0.52
1:C:216:GLY:O	1:C:219:GLU:N	2.43	0.52
1:C:234:TYR:O	1:C:237:TRP:HB3	2.10	0.52
1:C:41:PHE:CE1	1:C:64:ILE:HG21	2.45	0.52
1:C:130:PHE:HB3	1:C:201:THR:OG1	2.09	0.51
1:C:103:ILE:HD13	1:C:234:TYR:CD2	2.46	0.51
1:C:29:TRP:CZ3	2:L:133:GLY:HA2	2.46	0.51
1:C:95:ASN:OD1	1:C:95(B):THR:N	2.42	0.51
1:C:33:LEU:HD11	1:C:106:LEU:HD12	1.93	0.51
1:C:215:TRP:CE3	1:C:216:GLY:N	2.79	0.51
2:L:118:ALA:HB1	2:L:119:PRO:HD3	1.92	0.51
1:C:91:HIS:CD2	1:C:92:HIS:N	2.79	0.50
1:C:229:THR:CG2	1:C:234:TYR:HE2	2.22	0.50
2:L:55:PRO:O	2:L:81:ASN:HB3	2.11	0.50
1:C:95:ASN:HB2	1:C:96:VAL:O	2.11	0.50
1:C:143:ARG:HD2	1:C:149:GLY:H	1.75	0.50
1:C:172:THR:HA	1:C:217:GLU:OE2	2.12	0.50
1:C:180:MET:HE3	1:C:215:TRP:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLN:HB2	3:C:298:187:N6	2.27	0.49
1:C:72:ASN:HA	1:C:154:ILE:HG23	1.93	0.49
1:C:167:THR:O	1:C:170:ARG:HB2	2.12	0.49
1:C:215:TRP:HE3	1:C:216:GLY:CA	2.25	0.49
1:C:48:ASN:HA	1:C:120:PRO:HB3	1.94	0.49
1:C:48:ASN:HD21	1:C:244:LEU:HD11	1.78	0.49
2:L:83:GLU:HB2	2:L:84:LEU:HD23	1.93	0.49
1:C:187:GLY:CA	1:C:222:LYS:HA	2.37	0.49
1:C:73:THR:HG23	1:C:153:THR:O	2.13	0.49
1:C:173:LYS:HZ1	1:C:224:LYS:HZ1	1.61	0.48
2:L:110:SER:HA	2:L:117:LEU:HD22	1.95	0.48
1:C:98:LYS:HG3	1:C:99:TYR:CD1	2.49	0.48
1:C:71:TYR:O	1:C:154:ILE:HA	2.14	0.48
1:C:219:GLU:HB3	1:C:221(A):VAL:HG11	1.96	0.48
1:C:184(A):PHE:HB3	1:C:186:GLU:O	2.13	0.47
1:C:211:GLY:HA2	1:C:229:THR:O	2.13	0.47
2:L:55:PRO:CG	2:L:69:TYR:CE2	2.97	0.47
1:C:106:LEU:HD23	1:C:106:LEU:N	2.29	0.47
1:C:134:GLY:O	1:C:161:PRO:HA	2.15	0.47
1:C:72:ASN:CB	1:C:154:ILE:HG23	2.44	0.46
1:C:30:GLN:HG2	1:C:155:LEU:HD11	1.97	0.46
1:C:68:ALA:HB1	1:C:118:VAL:HG22	1.97	0.46
1:C:101:HIS:HA	1:C:234:TYR:OH	2.15	0.46
2:L:118:ALA:HA	2:L:125:LYS:NZ	2.30	0.46
1:C:127:GLU:OE2	1:C:129(B):ILE:HD11	2.15	0.46
1:C:82:ARG:HG2	1:C:82:ARG:H	1.60	0.46
1:C:145:PHE:HE2	1:C:150:ARG:NH2	2.13	0.46
1:C:72:ASN:CA	1:C:154:ILE:HG23	2.46	0.46
1:C:47:ILE:HD12	1:C:53:VAL:CG1	2.46	0.46
1:C:181:PHE:CE2	1:C:229:THR:O	2.69	0.46
1:C:215:TRP:CE2	1:C:227:ILE:HG12	2.51	0.46
1:C:57:HIS:O	1:C:57:HIS:CD2	2.69	0.46
1:C:100:SER:HG	1:C:101:HIS:CE1	2.34	0.45
2:L:57:LEU:O	2:L:82:CYS:HB2	2.16	0.45
2:L:79:GLY:O	2:L:81:ASN:N	2.49	0.45
1:C:16:ILE:HD13	1:C:194:ASP:OD2	2.17	0.45
1:C:206:THR:HB	1:C:208:PHE:HE1	1.82	0.45
1:C:73:THR:C	1:C:75:GLU:H	2.20	0.45
1:C:174:PHE:CD1	1:C:174:PHE:N	2.84	0.45
1:C:18:GLY:HA3	1:C:188(A):LYS:HB3	1.98	0.45
1:C:101:HIS:ND1	1:C:101:HIS:N	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:HG12	1:C:44:GLY:CA	2.47	0.44
1:C:123:ILE:HD11	1:C:209:LEU:HD12	2.00	0.44
1:C:191:CYS:O	1:C:194:ASP:HB2	2.17	0.44
1:C:108:LEU:N	1:C:108:LEU:HD13	2.33	0.44
2:L:54:ASN:HA	2:L:55:PRO:HD2	1.73	0.43
1:C:45:SER:CB	1:C:121:ILE:HD11	2.47	0.43
1:C:72:ASN:ND2	1:C:75:GLU:HB2	2.33	0.43
1:C:100:SER:HG	1:C:101:HIS:N	2.16	0.43
1:C:173:LYS:HZ1	1:C:224:LYS:NZ	2.15	0.43
1:C:77:GLU:HA	1:C:78:PRO:HD2	1.45	0.43
1:C:116:SER:N	2:L:130:PHE:CE1	2.86	0.43
1:C:52:VAL:CG1	1:C:108:LEU:HD21	2.46	0.43
1:C:46:ILE:HB	1:C:120:PRO:HA	1.99	0.43
1:C:35:GLY:O	1:C:38:ILE:N	2.51	0.43
1:C:73:THR:O	1:C:75:GLU:N	2.52	0.43
1:C:215:TRP:NE1	1:C:227:ILE:HD11	2.34	0.42
1:C:52:VAL:HG23	1:C:53:VAL:N	2.34	0.42
1:C:215:TRP:CE3	1:C:216:GLY:HA2	2.54	0.42
1:C:181:PHE:HD2	1:C:230:LYS:HG3	1.83	0.42
2:L:117:LEU:HD11	2:L:122:LYS:N	2.35	0.42
1:C:173:LYS:NZ	1:C:224:LYS:NZ	2.68	0.42
1:C:94:TYR:CD1	1:C:94:TYR:C	2.88	0.42
1:C:101:HIS:O	1:C:103:ILE:HG22	2.20	0.42
1:C:173:LYS:HB2	1:C:174:PHE:CD1	2.55	0.42
1:C:172:THR:OG1	1:C:174:PHE:N	2.52	0.42
1:C:190:SER:O	1:C:191:CYS:HB2	2.19	0.42
1:C:82:ARG:O	1:C:83:ARG:NE	2.50	0.41
1:C:165:ARG:HG3	1:C:166:ALA:N	2.36	0.41
1:C:211:GLY:H	1:C:231:VAL:HG21	1.85	0.41
1:C:91:HIS:C	1:C:93:SER:H	2.23	0.41
1:C:128:TYR:HB3	1:C:130:PHE:HE2	1.86	0.41
1:C:31:VAL:HG12	1:C:44:GLY:HA3	2.02	0.41
1:C:149:GLY:O	1:C:150:ARG:HB2	2.21	0.41
1:C:215:TRP:CE3	1:C:216:GLY:CA	3.04	0.41
1:C:145:PHE:HE2	1:C:150:ARG:HH21	1.69	0.41
1:C:158:LEU:HD21	1:C:188(A):LYS:HB2	2.03	0.41
1:C:24:PRO:HD3	1:C:71:TYR:CZ	2.55	0.41
1:C:28:PRO:O	1:C:119:THR:O	2.39	0.41
2:L:97:GLN:OE1	2:L:111:CYS:HA	2.20	0.41
1:C:50:LYS:HG2	1:C:111:PRO:HB3	2.03	0.40
1:C:100:SER:O	1:C:179:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:HD22	1:C:211:GLY:O	2.21	0.40
1:C:131:LEU:HD22	1:C:131:LEU:O	2.20	0.40
1:C:19:GLY:HA2	1:C:158:LEU:CD1	2.39	0.40
1:C:45:SER:HB3	1:C:121:ILE:CD1	2.49	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	C	233/235 (99%)	179 (77%)	35 (15%)	19 (8%)	1	2
2	L	95/146 (65%)	70 (74%)	16 (17%)	9 (10%)	0	1
All	All	328/381 (86%)	249 (76%)	51 (16%)	28 (8%)	1	2

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	36	LYS
1	C	38	ILE
1	C	68	ALA
1	C	217	GLU
2	L	66	ILE
2	L	104	ASP
1	C	69	GLY
1	C	74	GLU
1	C	97	ASN
1	C	125	ASP
2	L	60	GLY
2	L	74	GLN
2	L	92	ASN
1	C	46	ILE

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Mol	Chain	Res	Type
1	C	48	ASN
1	C	92	HIS
1	C	102	ASP
1	C	190	SER
2	L	53	PRO
2	L	80	LYS
1	C	57	HIS
1	C	90	PRO
1	C	150	ARG
2	L	139	HIS
1	C	40	ALA
1	C	78	PRO
1	C	94	TYR
2	L	113	THR

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	C	198/198 (100%)	147 (74%)	51 (26%)	0 1
2	L	85/130 (65%)	69 (81%)	16 (19%)	1 4
All	All	283/328 (86%)	216 (76%)	67 (24%)	1 2

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LYS
1	C	26	GLN
1	C	31	VAL
1	C	32	LEU
1	C	38	ILE
1	C	41	PHE
1	C	47	ILE
1	C	48	ASN
1	C	49	GLU

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Mol	Chain	Res	Type
1	C	50	LYS
1	C	51	TRP
1	C	52	VAL
1	C	53	VAL
1	C	64	ILE
1	C	82	ARG
1	C	86	ILE
1	C	87	ARG
1	C	95	ASN
1	C	96	VAL
1	C	98	LYS
1	C	103	ILE
1	C	105	LEU
1	C	108	LEU
1	C	121	ILE
1	C	125	ASP
1	C	129	THR
1	C	131	LEU
1	C	135	SER
1	C	137	TYR
1	C	154	ILE
1	C	157	TYR
1	C	162	LEU
1	C	164	ASP
1	C	165	ARG
1	C	169	LEU
1	C	177	TYR
1	C	179	ASN
1	C	180	MET
1	C	186	GLU
1	C	206	THR
1	C	209	LEU
1	C	213	ILE
1	C	221(A)	VAL
1	C	222	LYS
1	C	227	ILE
1	C	230	LYS
1	C	232	SER
1	C	235	VAL
1	C	239	LYS
1	C	242	THR
1	C	245	THR

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Mol	Chain	Res	Type
2	L	56	CYS
2	L	57	LEU
2	L	73	CYS
2	L	83	GLU
2	L	84	LEU
2	L	90	ILE
2	L	94	ARG
2	L	104	ASP
2	L	108	LEU
2	L	112	THR
2	L	120	ASP
2	L	123	SER
2	L	125	LYS
2	L	132	CYS
2	L	136	SER
2	L	138	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	91	HIS
1	C	156	GLN
1	C	179	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 carbohydrates 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
3	187	C	298	-	40,41,41	2.37	15 (37%)	46,61,61	2.35	17 (36%)

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
3	187	C	298	-	-	9/23/26/26	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	298	187	C16-N7	-8.08	1.33	1.44
3	C	298	187	C9-C23	4.58	1.49	1.40
3	C	298	187	C5-C4	3.79	1.43	1.38
3	C	298	187	C12-C10	3.55	1.44	1.39
3	C	298	187	C14-C16	3.51	1.42	1.38
3	C	298	187	C14-C44	3.17	1.43	1.37
3	C	298	187	C12-C13	2.96	1.43	1.39
3	C	298	187	C25-C27	2.84	1.43	1.36
3	C	298	187	C8-N5	-2.69	1.28	1.35
3	C	298	187	C15-N7	-2.49	1.34	1.36
3	C	298	187	C3-C4	2.33	1.43	1.38
3	C	298	187	C13-C8	-2.33	1.36	1.50
3	C	298	187	C25-C21	2.26	1.44	1.38
3	C	298	187	N6-N1	-2.12	1.35	1.39
3	C	298	187	F2-C11	-2.08	1.25	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	298	187	C10-N6-N1	6.36	113.04	105.66
3	C	298	187	C3-C4-C5	-5.29	115.48	121.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	298	187	C14-C44-C7	-4.03	119.67	123.50
3	C	298	187	F2-C11-C10	-3.90	105.81	112.47
3	C	298	187	C2-C3-C4	3.87	123.65	118.63
3	C	298	187	C15-N7-C16	-3.65	119.04	125.23
3	C	298	187	C12-C10-N6	-3.49	106.35	111.41
3	C	298	187	C22-C7-C44	3.47	120.67	117.17
3	C	298	187	C7-N5-C8	-3.43	117.53	126.93
3	C	298	187	C5-C4-N1	3.29	123.27	119.07
3	C	298	187	C11-C10-N6	3.16	123.44	119.72
3	C	298	187	F4-C44-C14	3.08	124.74	118.61
3	C	298	187	F1-C11-C10	2.84	117.33	112.47
3	C	298	187	C21-C25-C27	2.76	124.31	120.44
3	C	298	187	C21-C17-C23	-2.20	116.91	120.08
3	C	298	187	C18-C16-N7	-2.20	116.76	119.41
3	C	298	187	C6-C20-N4	2.10	121.22	118.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	298	187	N6-C10-C11-F2
3	C	298	187	N6-C10-C11-F1
3	C	298	187	C12-C10-C11-F1
3	C	298	187	C14-C16-N7-C9
3	C	298	187	N6-C10-C11-F3
3	C	298	187	C12-C10-C11-F2
3	C	298	187	C44-C7-N5-C8
3	C	298	187	N4-C20-C6-C5
3	C	298	187	C12-C10-C11-F3

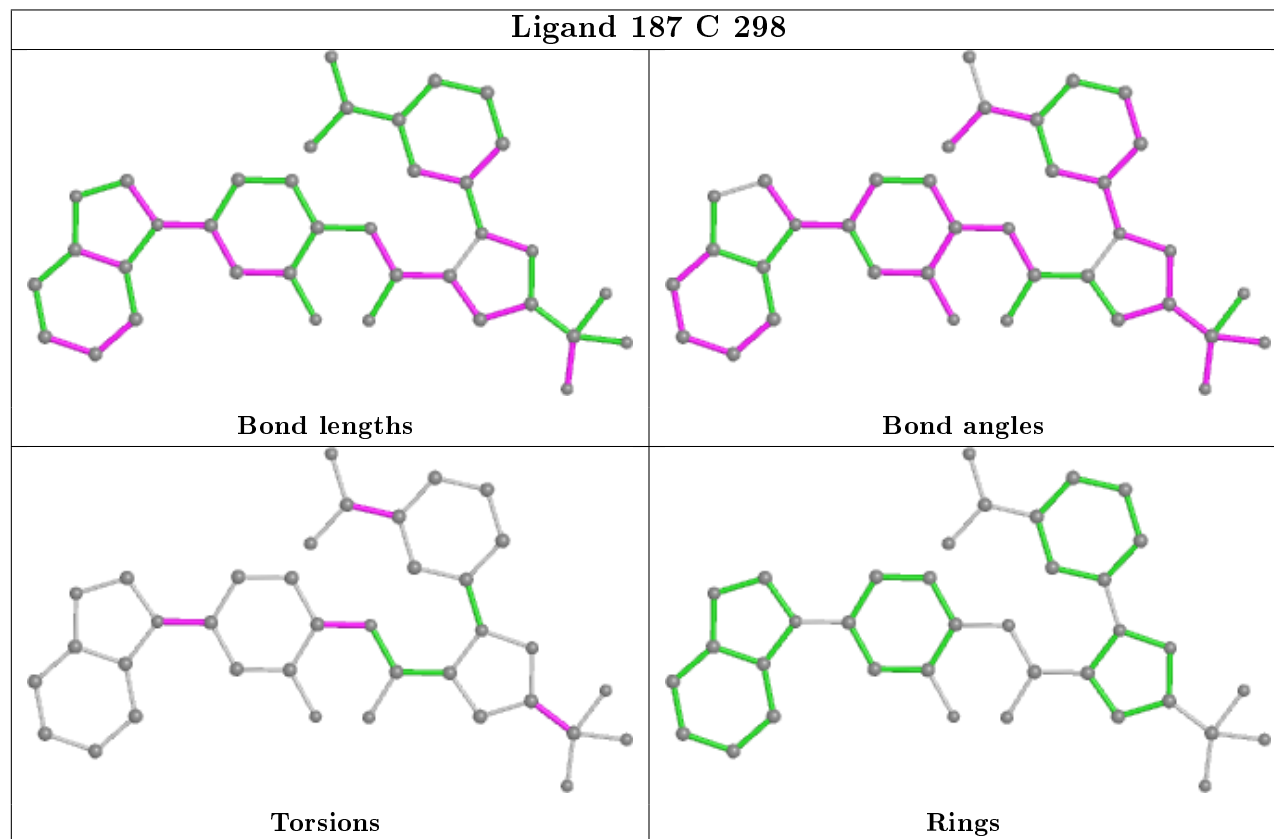
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	298	187	3	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.