



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:54 am BST

PDB ID : 2G20  
Title : Ketopiperazine-Based Renin Inhibitors: Optimization of the C Ring  
Authors : Holsworth, D.D.; Jalaiea, M.; Zhanga, E.; Mcconnella, P.  
Deposited on : 2006-02-15  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

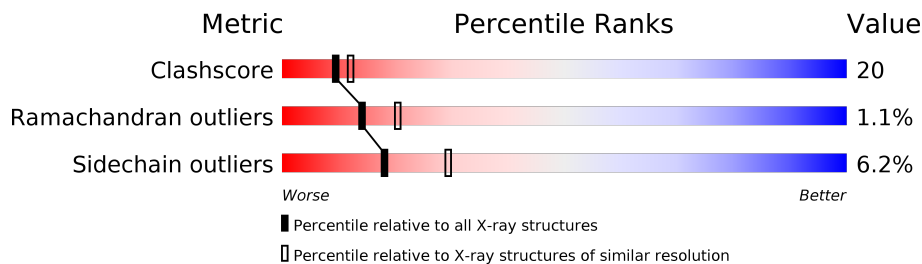
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	

## 2 Entry composition i

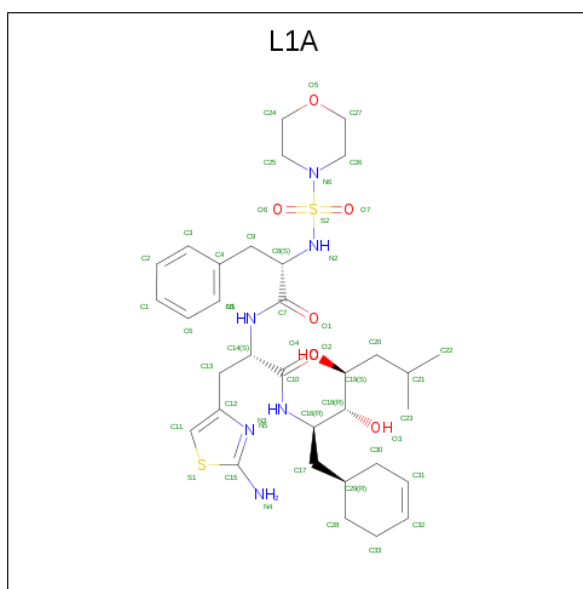
There are 3 unique types of molecules in this entry. The entry contains 5343 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Renin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	Total 2572	1642	416	500	14	0	0	0
1	B	333	Total 2572	1642	416	500	14	0	0	0

- Molecule 2 is N-(MORPHOLIN-4-YLSULFONYL)-L-PHENYLALANYL-3-(2-AMINO-1,3-THIAZOL-4-YL)-N-[(1R,2R,3S)-1-[(1R)-CYCLOHEX-3-EN-1-YLMETHYL]-2,3-DIHYDROXY-5-METHYLHEXYL]-L-ALANINAMIDE (three-letter code: L1A) (formula: C<sub>33</sub>H<sub>50</sub>N<sub>6</sub>O<sub>7</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 48	33	6	7	2	0	0
2	B	1	Total 48	33	6	7	2	0	0

- Molecule 3 is water.

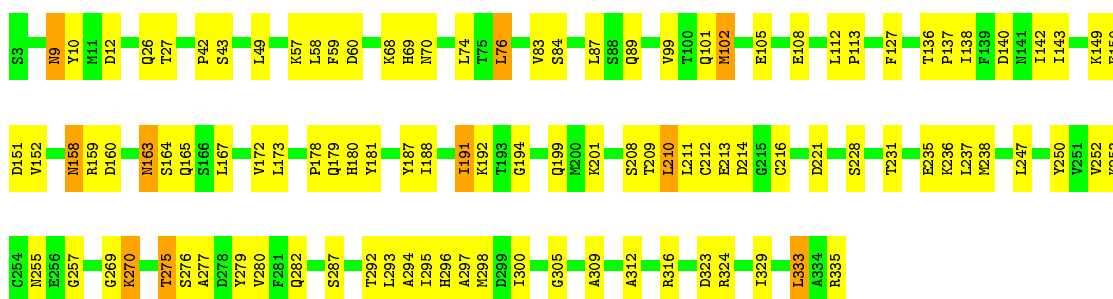
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	61	Total 61	O 61	0	0
3	B	42	Total 42	O 42	0	0

### 3 Residue-property plots [i](#)

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.

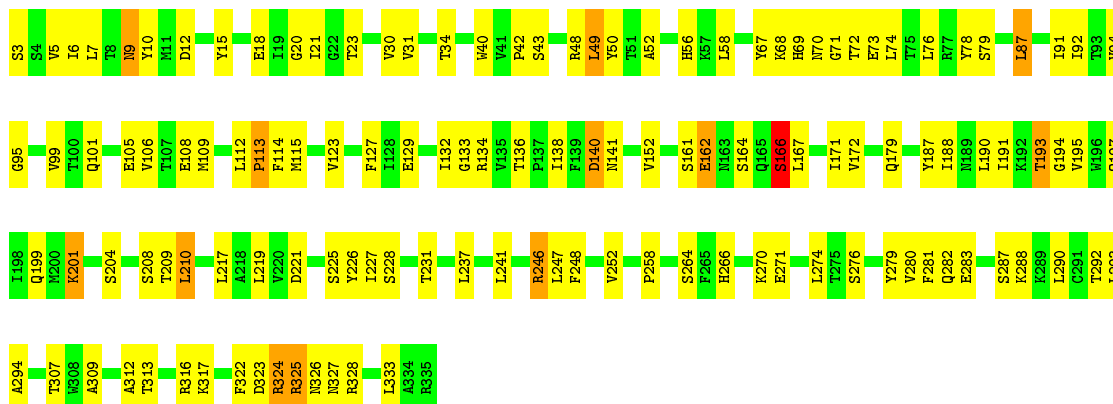
- Molecule 1: Renin

Chain A: 



- Molecule 1: Renin

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.33Å 141.33Å 141.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 33.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 81.4 (33.31-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 2.39Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.260 0.252 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	5343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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, 0.333 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: L1A

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	A	0.36	0/2632	0.67	0/3568
1	B	0.35	0/2632	0.67	0/3568
All	All	0.35	0/5264	0.67	0/7136

There are no bond length outliers.

There are no bond angle outliers.

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	A	2572	0	2501	94	0
1	B	2572	0	2501	109	0
2	A	48	0	50	3	0
2	B	48	0	50	5	0
3	A	61	0	0	8	0
3	B	42	0	0	7	0
All	All	5343	0	5102	203	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 20.

All (203) 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:B:52:ALA:HA	1:B:115:MET:HE3	1.40	1.02
1:B:217:LEU:HB2	1:B:307:THR:HG22	1.39	1.01
1:B:197:GLN:OE1	1:B:307:THR:HG21	1.70	0.90
1:A:276:SER:O	1:A:280:VAL:HG12	1.72	0.89
1:A:160:ASP:HB3	3:A:934:HOH:O	1.72	0.88
1:A:158:ASN:HD22	1:A:159:ARG:H	1.24	0.81
1:A:158:ASN:ND2	1:A:159:ARG:H	1.82	0.78
1:B:42:PRO:HG3	1:B:109:MET:HE1	1.65	0.77
1:A:275:THR:HG22	1:A:277:ALA:H	1.50	0.77
1:A:163:ASN:HD22	1:A:163:ASN:H	1.30	0.76
1:A:152:VAL:HG12	1:A:323:ASP:HA	1.68	0.76
1:B:201:LYS:HE3	1:B:266:HIS:CD2	2.20	0.76
1:B:193:THR:HG23	1:B:327:ASN:HD21	1.48	0.76
1:A:99:VAL:HG21	1:A:142:ILE:HG12	1.67	0.75
1:B:252:VAL:HG23	3:B:891:HOH:O	1.86	0.74
1:B:208:SER:O	1:B:210:LEU:HD22	1.87	0.74
1:B:193:THR:HG23	1:B:327:ASN:ND2	2.03	0.74
1:B:43:SER:HB2	1:B:105:GLU:HB3	1.69	0.73
1:B:247:LEU:HD23	1:B:248:PHE:HB2	1.70	0.73
1:B:201:LYS:HB2	1:B:266:HIS:HD2	1.55	0.72
1:B:9:ASN:C	1:B:9:ASN:HD22	1.94	0.71
1:B:161:SER:HB3	1:B:164:SER:HB3	1.71	0.70
1:A:26:GLN:HE22	1:A:60:ASP:H	1.39	0.70
1:B:52:ALA:HA	1:B:115:MET:CE	2.18	0.70
1:B:9:ASN:HD21	1:B:12:ASP:H	1.38	0.69
1:B:270:LYS:HG2	3:B:900:HOH:O	1.94	0.68
1:B:152:VAL:HG12	1:B:323:ASP:HA	1.76	0.67
1:A:158:ASN:HD22	1:A:159:ARG:N	1.93	0.67
1:A:275:THR:HG22	1:A:277:ALA:N	2.11	0.66
1:A:43:SER:HB2	1:A:105:GLU:HB3	1.78	0.66
1:A:151:ASP:O	1:A:324:ARG:HB2	1.96	0.66
1:B:74:LEU:HD22	1:B:87:LEU:HD13	1.78	0.66
1:B:9:ASN:HD22	1:B:10:TYR:N	1.94	0.65
1:B:276:SER:HA	1:B:279:TYR:CE2	2.31	0.65
1:A:9:ASN:HD21	1:A:12:ASP:H	1.43	0.65
1:A:210:LEU:HB2	1:A:236:LYS:NZ	2.12	0.64
1:A:158:ASN:ND2	1:A:159:ARG:N	2.46	0.64
1:B:161:SER:O	1:B:162:GLU:HB2	1.95	0.64
1:B:217:LEU:HB2	1:B:307:THR:CG2	2.23	0.63
1:B:201:LYS:HE3	1:B:266:HIS:HD2	1.63	0.62
1:A:163:ASN:ND2	1:A:163:ASN:H	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:HG12	1:B:92:ILE:HG12	1.82	0.62
1:B:226:TYR:HB3	1:B:294:ALA:O	2.00	0.60
1:B:6:ILE:HG23	1:B:167:LEU:CD1	2.31	0.60
1:A:68:LYS:HB2	1:A:89:GLN:HB3	1.83	0.60
1:A:210:LEU:HB2	1:A:236:LYS:HZ1	1.66	0.59
1:A:191:ILE:HG22	1:A:192:LYS:N	2.18	0.59
1:B:227:ILE:HG13	1:B:313:THR:HB	1.84	0.58
1:B:247:LEU:CD2	1:B:248:PHE:HB2	2.34	0.58
1:B:70:ASN:ND2	3:B:895:HOH:O	2.37	0.58
1:B:42:PRO:HB2	1:B:58:LEU:HD23	1.85	0.57
1:A:84:SER:HB3	1:A:108:GLU:OE1	2.04	0.57
1:B:49:LEU:O	1:B:49:LEU:HD12	2.03	0.57
1:B:101:GLN:NE2	1:B:138:ILE:HA	2.19	0.57
1:B:99:VAL:HA	3:B:909:HOH:O	2.05	0.57
1:B:91:ILE:O	1:B:91:ILE:HG13	2.03	0.57
1:B:280:VAL:HG22	1:B:293:LEU:CD2	2.34	0.57
1:B:237:LEU:O	1:B:241:LEU:HD13	2.04	0.56
1:A:143:ILE:HD11	1:A:151:ASP:OD2	2.05	0.56
1:A:70:ASN:ND2	3:A:888:HOH:O	2.36	0.56
1:B:136:THR:HG21	1:B:141:ASN:ND2	2.21	0.56
1:A:208:SER:O	1:A:210:LEU:HG	2.06	0.55
1:B:161:SER:O	1:B:162:GLU:CB	2.55	0.55
1:B:195:VAL:HG12	1:B:197:GLN:HB2	1.88	0.55
1:A:74:LEU:HD13	1:A:87:LEU:HD21	1.87	0.55
1:B:42:PRO:HG3	1:B:109:MET:CE	2.35	0.55
1:B:129:GLU:N	1:B:129:GLU:OE1	2.36	0.55
1:B:246:ARG:HG2	1:B:247:LEU:N	2.22	0.54
1:B:221:ASP:OD1	2:B:886:L1A:O3	2.24	0.54
1:A:212:CYS:SG	1:A:212:CYS:O	2.64	0.54
1:A:191:ILE:HD11	1:A:199:GLN:HB2	1.90	0.54
1:A:228:SER:OG	1:A:309:ALA:HB3	2.07	0.54
1:A:9:ASN:HD21	1:A:12:ASP:N	2.05	0.54
1:A:89:GLN:HB2	1:A:102:MET:CE	2.37	0.54
1:B:247:LEU:HD23	1:B:248:PHE:N	2.21	0.54
1:A:201:LYS:HE2	1:A:269:GLY:H	1.73	0.54
1:B:217:LEU:CB	1:B:307:THR:HG22	2.27	0.54
1:B:225:SER:O	1:B:312:ALA:HB3	2.08	0.53
1:B:7:LEU:HD11	1:B:171:ILE:HG13	1.89	0.53
1:A:112:LEU:N	1:A:112:LEU:HD12	2.23	0.53
1:A:9:ASN:ND2	1:A:12:ASP:H	2.07	0.53
1:A:209:THR:HG22	1:A:209:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASN:HD22	1:A:163:ASN:N	1.96	0.52
1:A:27:THR:O	1:A:57:LYS:HG2	2.09	0.52
1:A:213:GLU:O	1:A:214:ASP:HB2	2.09	0.52
1:B:9:ASN:C	1:B:9:ASN:ND2	2.61	0.52
1:A:180:HIS:C	1:A:335:ARG:HG2	2.30	0.52
1:B:274:LEU:CD2	1:B:317:LYS:HG2	2.40	0.52
1:B:179:GLN:HG2	3:B:898:HOH:O	2.10	0.51
1:B:12:ASP:O	1:B:316:ARG:NH1	2.44	0.51
1:A:42:PRO:HB2	1:A:58:LEU:HD23	1.92	0.51
1:A:127:PHE:CG	1:A:194:GLY:HA2	2.46	0.51
1:B:280:VAL:HG22	1:B:293:LEU:HD22	1.93	0.51
1:A:312:ALA:O	1:A:316:ARG:HB2	2.10	0.50
1:B:9:ASN:HD21	1:B:12:ASP:N	2.09	0.50
1:A:89:GLN:HB2	1:A:102:MET:HE2	1.94	0.50
1:B:9:ASN:ND2	1:B:12:ASP:H	2.09	0.50
1:B:67:TYR:CZ	1:B:69:HIS:HA	2.46	0.50
1:B:258:PRO:HD3	1:B:282:GLN:HE22	1.76	0.50
1:B:287:SER:OG	1:B:288:LYS:HE3	2.12	0.50
1:B:188:ILE:HD12	1:B:188:ILE:N	2.25	0.50
1:A:276:SER:O	1:A:280:VAL:CG1	2.55	0.49
1:A:309:ALA:HB3	2:A:885:L1A:HN41	1.77	0.49
1:B:20:GLY:O	1:B:92:ILE:HA	2.12	0.49
1:A:187:TYR:C	1:A:188:ILE:HD12	2.33	0.49
1:A:276:SER:HA	1:A:279:TYR:CE2	2.47	0.49
1:A:143:ILE:CD1	1:A:151:ASP:OD2	2.61	0.49
1:A:269:GLY:O	1:A:270:LYS:HB2	2.13	0.49
1:A:238:MET:HG3	1:A:250:TYR:CD2	2.47	0.48
1:A:9:ASN:C	1:A:9:ASN:HD22	2.14	0.48
1:B:309:ALA:HB3	2:B:886:L1A:HN41	1.77	0.48
1:B:30:VAL:HG21	1:B:123:VAL:HG23	1.95	0.48
1:B:140:ASP:CG	1:B:324:ARG:HH12	2.14	0.48
1:A:255:ASN:OD1	1:A:287:SER:HA	2.14	0.48
1:B:164:SER:C	1:B:166:SER:H	2.17	0.48
1:B:30:VAL:HG21	1:B:123:VAL:CG2	2.43	0.48
1:A:252:VAL:HG12	1:A:253:LYS:N	2.28	0.48
1:B:208:SER:O	1:B:210:LEU:N	2.46	0.48
1:A:9:ASN:HD22	1:A:10:TYR:N	2.12	0.47
1:B:101:GLN:HE22	1:B:138:ILE:HA	1.78	0.47
1:B:50:TYR:CZ	1:B:108:GLU:HG2	2.49	0.47
1:A:26:GLN:NE2	1:A:59:PHE:HA	2.29	0.47
1:B:71:GLY:O	1:B:72:THR:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:HH11	1:A:159:ARG:HG3	1.78	0.47
1:B:161:SER:CB	1:B:164:SER:HB3	2.43	0.47
1:B:270:LYS:HG2	1:B:271:GLU:H	1.79	0.47
1:A:300:ILE:O	1:A:305:GLY:HA3	2.15	0.47
1:B:113:PRO:HG2	2:B:886:L1A:H2	1.97	0.47
1:A:26:GLN:HE22	1:A:59:PHE:HA	1.80	0.47
1:B:48:ARG:HD2	1:B:48:ARG:N	2.31	0.46
1:A:163:ASN:ND2	1:A:163:ASN:O	2.49	0.46
1:B:40:TRP:CE3	1:B:106:VAL:HG21	2.51	0.46
1:A:294:ALA:C	1:A:295:ILE:HG13	2.36	0.46
1:B:127:PHE:HB2	1:B:194:GLY:HA2	1.97	0.46
1:A:187:TYR:HA	1:A:329:ILE:O	2.14	0.46
1:A:210:LEU:CD1	1:A:211:LEU:HG	2.45	0.46
1:A:99:VAL:HG21	1:A:142:ILE:CG1	2.42	0.46
1:B:210:LEU:H	1:B:210:LEU:CD2	2.28	0.46
1:A:210:LEU:HD13	1:A:211:LEU:HG	1.97	0.46
1:A:9:ASN:HD21	1:A:12:ASP:HA	1.80	0.46
1:A:221:ASP:OD1	2:A:885:L1A:O3	2.34	0.45
1:A:231:THR:O	1:A:235:GLU:HG3	2.15	0.45
1:B:246:ARG:HD2	3:B:887:HOH:O	2.15	0.45
1:B:127:PHE:HB3	1:B:129:GLU:OE1	2.17	0.45
1:B:6:ILE:HG23	1:B:167:LEU:HD11	1.97	0.45
1:A:298:MET:HG2	2:A:885:L1A:C11	2.47	0.45
1:B:133:GLY:C	1:B:134:ARG:HG3	2.36	0.45
1:B:228:SER:OG	1:B:309:ALA:HB3	2.17	0.45
1:B:15:TYR:O	1:B:31:VAL:HG22	2.17	0.45
1:A:101:GLN:NE2	1:A:138:ILE:HA	2.32	0.45
1:B:209:THR:O	1:B:209:THR:HG22	2.16	0.45
1:B:326:ASN:HB2	1:B:328:ARG:HG2	1.99	0.45
1:B:140:ASP:OD2	1:B:140:ASP:N	2.50	0.44
1:B:281:PHE:HD1	1:B:292:THR:HG23	1.80	0.44
1:A:316:ARG:NH2	3:A:895:HOH:O	2.47	0.44
1:A:333:LEU:HA	1:A:333:LEU:HD23	1.69	0.44
1:B:56:HIS:HE1	1:B:114:PHE:O	1.99	0.44
1:B:78:TYR:HB3	2:B:886:L1A:H171	1.99	0.44
1:A:252:VAL:HG12	1:A:253:LYS:O	2.18	0.44
1:A:191:ILE:HD11	1:A:199:GLN:CA	2.47	0.44
1:A:9:ASN:ND2	1:A:9:ASN:C	2.72	0.43
1:A:216:CYS:HB2	3:A:919:HOH:O	2.18	0.43
1:B:172:VAL:HG23	3:B:903:HOH:O	2.17	0.43
1:B:79:SER:OG	2:B:886:L1A:H132	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:MET:HG3	1:A:250:TYR:CE2	2.54	0.43
1:A:76:LEU:HB2	1:A:83:VAL:HG23	2.01	0.43
1:B:76:LEU:HD23	1:B:132:ILE:HD12	1.99	0.43
1:B:40:TRP:HZ3	1:B:109:MET:HE1	1.84	0.43
1:B:191:ILE:HD11	1:B:199:GLN:N	2.33	0.43
1:A:149:LYS:HG2	1:A:150:GLU:HG3	2.00	0.43
1:B:23:THR:OG1	1:B:91:ILE:HD11	2.18	0.43
1:B:74:LEU:HD13	1:B:87:LEU:HD11	2.01	0.43
1:A:163:ASN:O	1:A:165:GLN:N	2.48	0.43
1:A:252:VAL:CG1	1:A:253:LYS:N	2.81	0.43
1:B:201:LYS:HB2	1:B:266:HIS:CD2	2.44	0.43
1:A:136:THR:HA	1:A:137:PRO:HD3	1.87	0.42
1:A:275:THR:CG2	1:A:276:SER:N	2.82	0.42
1:B:324:ARG:NH2	1:B:324:ARG:HG3	2.34	0.42
1:A:167:LEU:HD23	1:A:167:LEU:N	2.34	0.42
1:A:178:PRO:HG3	3:A:902:HOH:O	2.18	0.42
1:A:9:ASN:HD21	1:A:12:ASP:CA	2.33	0.42
1:A:297:ALA:O	1:A:298:MET:HE2	2.20	0.42
1:A:26:GLN:NE2	3:A:939:HOH:O	2.52	0.41
1:B:140:ASP:OD2	1:B:324:ARG:NH1	2.40	0.41
1:B:34:THR:HG21	1:B:322:PHE:CZ	2.55	0.41
1:A:102:MET:HB2	3:A:925:HOH:O	2.19	0.41
1:A:178:PRO:HA	1:A:181:TYR:CE1	2.55	0.41
1:B:69:HIS:CG	1:B:70:ASN:N	2.88	0.41
1:A:172:VAL:HG23	3:A:889:HOH:O	2.19	0.41
1:B:325:ARG:HA	1:B:325:ARG:HD2	1.77	0.41
1:B:187:TYR:HB3	1:B:328:ARG:HD2	2.03	0.41
1:B:204:SER:HB2	1:B:264:SER:HB2	2.02	0.41
1:A:270:LYS:HA	1:A:270:LYS:HD2	1.91	0.41
1:B:127:PHE:CB	1:B:194:GLY:HA2	2.50	0.41
1:A:69:HIS:CG	1:A:70:ASN:N	2.88	0.41
1:B:247:LEU:HD23	1:B:248:PHE:CB	2.47	0.41
1:A:292:THR:HG22	1:A:293:LEU:N	2.36	0.40
1:B:112:LEU:HA	1:B:113:PRO:HA	1.79	0.40
1:B:190:LEU:HG	1:B:327:ASN:O	2.21	0.40
1:B:282:GLN:O	1:B:283:GLU:C	2.59	0.40
1:A:257:GLY:HA3	1:A:282:GLN:HE22	1.85	0.40
1:A:228:SER:HB2	1:A:298:MET:HB2	2.03	0.40
1:B:3:SER:OG	1:B:95:GLY:O	2.38	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	A	331/333 (99%)	314 (95%)	13 (4%)	4 (1%)	13	19
1	B	331/333 (99%)	309 (93%)	19 (6%)	3 (1%)	17	25
All	All	662/666 (99%)	623 (94%)	32 (5%)	7 (1%)	14	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	SER
1	A	191	ILE
1	A	247	LEU
1	A	270	LYS
1	B	162	GLU
1	B	166	SER
1	B	246	ARG

### 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	A	284/284 (100%)	269 (95%)	15 (5%)	22	37
1	B	284/284 (100%)	264 (93%)	20 (7%)	15	24
All	All	568/568 (100%)	533 (94%)	35 (6%)	18	29

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	49	LEU
1	A	76	LEU
1	A	102	MET
1	A	113	PRO
1	A	140	ASP
1	A	158	ASN
1	A	163	ASN
1	A	173	LEU
1	A	179	GLN
1	A	210	LEU
1	A	237	LEU
1	A	275	THR
1	A	296	HIS
1	A	333	LEU
1	B	5	VAL
1	B	9	ASN
1	B	18	GLU
1	B	49	LEU
1	B	68	LYS
1	B	73	GLU
1	B	87	LEU
1	B	94	VAL
1	B	113	PRO
1	B	140	ASP
1	B	166	SER
1	B	193	THR
1	B	201	LYS
1	B	210	LEU
1	B	219	LEU
1	B	231	THR
1	B	290	LEU
1	B	324	ARG
1	B	325	ARG
1	B	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	GLN
1	A	101	GLN
1	A	141	ASN

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Mol	Chain	Res	Type
1	A	145	GLN
1	A	158	ASN
1	A	163	ASN
1	A	170	GLN
1	A	184	ASN
1	A	197	GLN
1	A	199	GLN
1	A	282	GLN
1	B	9	ASN
1	B	26	GLN
1	B	101	GLN
1	B	141	ASN
1	B	145	GLN
1	B	170	GLN
1	B	189	ASN
1	B	266	HIS
1	B	282	GLN
1	B	327	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	L1A	B	886	-	46,51,51	2.21	11 (23%)	52,70,70	2.31	11 (21%)
2	L1A	A	885	-	46,51,51	2.34	11 (23%)	52,70,70	2.32	10 (19%)

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
2	L1A	B	886	-	-	11/49/67/67	0/4/4/4
2	L1A	A	885	-	-	9/49/67/67	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	885	L1A	C32-C31	8.26	1.57	1.32
2	B	886	L1A	C32-C31	8.20	1.57	1.32
2	A	885	L1A	S2-N2	7.95	1.72	1.61
2	B	886	L1A	S2-N2	7.32	1.71	1.61
2	B	886	L1A	S2-N6	4.82	1.74	1.62
2	A	885	L1A	S2-N6	4.75	1.74	1.62
2	A	885	L1A	C16-N3	3.21	1.51	1.46
2	A	885	L1A	C18-C16	3.03	1.59	1.53
2	A	885	L1A	C10-N3	3.01	1.40	1.34
2	A	885	L1A	C30-C31	3.01	1.56	1.49
2	B	886	L1A	C30-C31	2.95	1.56	1.49
2	B	886	L1A	C18-C16	2.40	1.57	1.53
2	B	886	L1A	C33-C32	2.28	1.57	1.48
2	A	885	L1A	C33-C32	2.20	1.56	1.48
2	B	886	L1A	C15-N4	2.20	1.41	1.35
2	A	885	L1A	C17-C29	2.13	1.56	1.53
2	B	886	L1A	C16-N3	2.10	1.49	1.46
2	B	886	L1A	C28-C33	2.06	1.57	1.52
2	A	885	L1A	C19-C18	2.05	1.57	1.53
2	A	885	L1A	C15-N4	2.03	1.41	1.35
2	B	886	L1A	C11-S1	2.02	1.73	1.70
2	B	886	L1A	C17-C29	2.00	1.56	1.53

All (21) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	885	L1A	C24-C25-N6	10.82	114.55	108.18
2	B	886	L1A	C24-C25-N6	9.70	113.89	108.18
2	B	886	L1A	C27-C26-N6	7.56	112.63	108.18
2	A	885	L1A	C27-C26-N6	7.18	112.41	108.18
2	A	885	L1A	C16-N3-C10	4.74	131.46	123.07
2	B	886	L1A	C17-C16-N3	4.41	115.89	110.18
2	B	886	L1A	C16-N3-C10	4.23	130.55	123.07
2	B	886	L1A	C30-C31-C32	-3.41	115.49	123.19
2	A	885	L1A	C30-C31-C32	-3.33	115.68	123.19
2	A	885	L1A	C21-C20-C19	3.22	119.29	114.82
2	B	886	L1A	C21-C20-C19	3.16	119.21	114.82
2	B	886	L1A	O3-C18-C16	-2.85	102.17	108.98
2	A	885	L1A	O3-C18-C16	-2.81	102.26	108.98
2	A	885	L1A	C17-C29-C28	2.58	117.35	111.73
2	A	885	L1A	C13-C12-C11	-2.47	125.70	130.18
2	B	886	L1A	C13-C12-C11	-2.39	125.84	130.18
2	B	886	L1A	C17-C29-C28	2.28	116.70	111.73
2	B	886	L1A	C13-C14-N1	-2.25	106.06	110.79
2	A	885	L1A	C33-C32-C31	-2.17	115.61	123.02
2	B	886	L1A	C33-C32-C31	-2.15	115.68	123.02
2	A	885	L1A	C17-C16-N3	2.03	112.81	110.18

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	886	L1A	C17-C16-N3-C10
2	B	886	L1A	C16-C17-C29-C28
2	B	886	L1A	C26-N6-S2-O6
2	B	886	L1A	C25-N6-S2-O7
2	A	885	L1A	C17-C16-N3-C10
2	A	885	L1A	C16-C17-C29-C28
2	A	885	L1A	C16-C17-C29-C30
2	B	886	L1A	C16-C17-C29-C30
2	B	886	L1A	C12-C13-C14-C10
2	B	886	L1A	C25-N6-S2-O6
2	B	886	L1A	C26-N6-S2-O7
2	A	885	L1A	C25-N6-S2-O6
2	A	885	L1A	C12-C13-C14-C10
2	B	886	L1A	C12-C13-C14-N1
2	A	885	L1A	C12-C13-C14-N1
2	B	886	L1A	N3-C10-C14-N1
2	A	885	L1A	N3-C10-C14-N1

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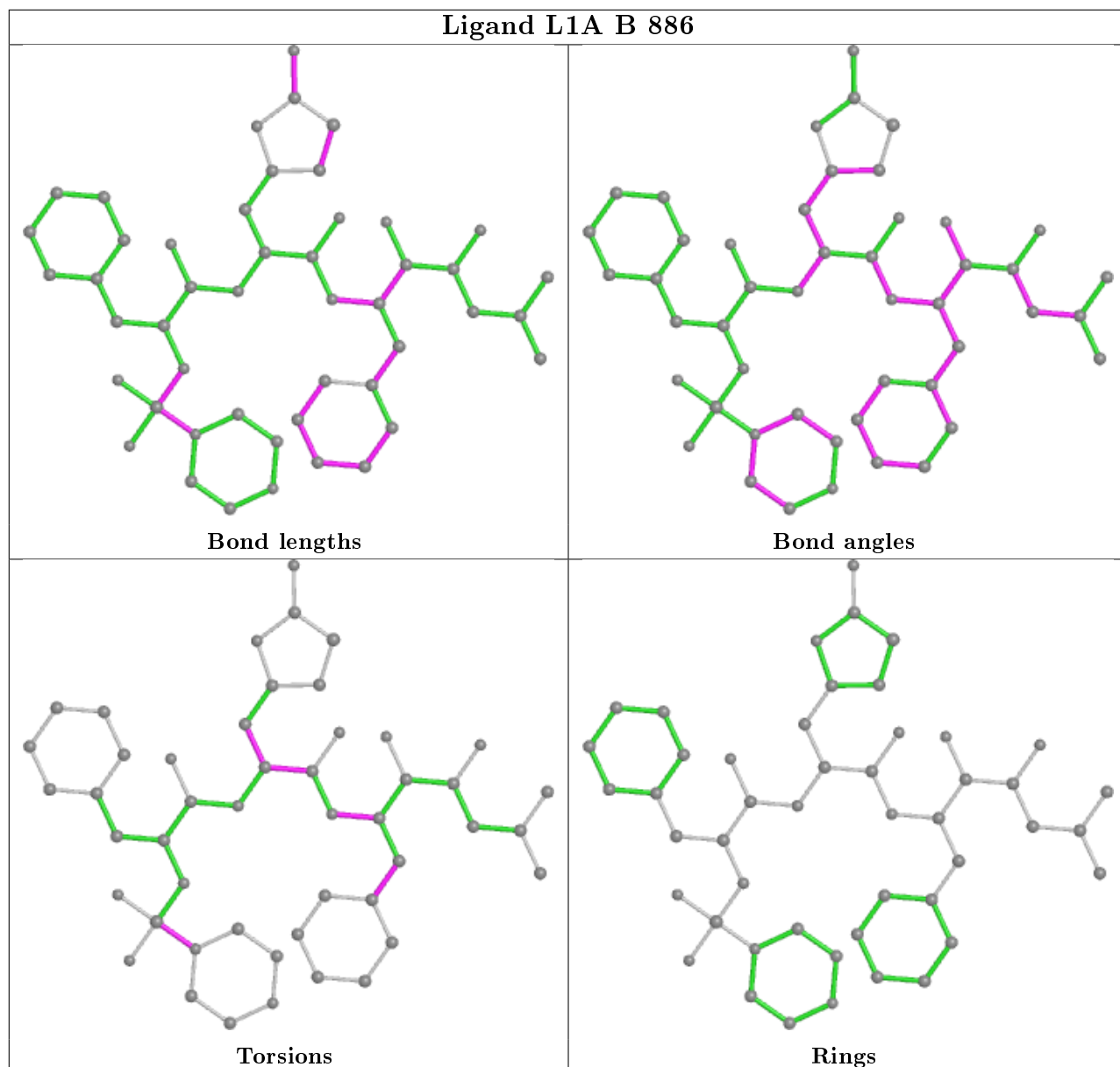
Mol	Chain	Res	Type	Atoms
2	A	885	L1A	C26-N6-S2-O6
2	A	885	L1A	C25-N6-S2-O7
2	B	886	L1A	O2-C10-C14-N1

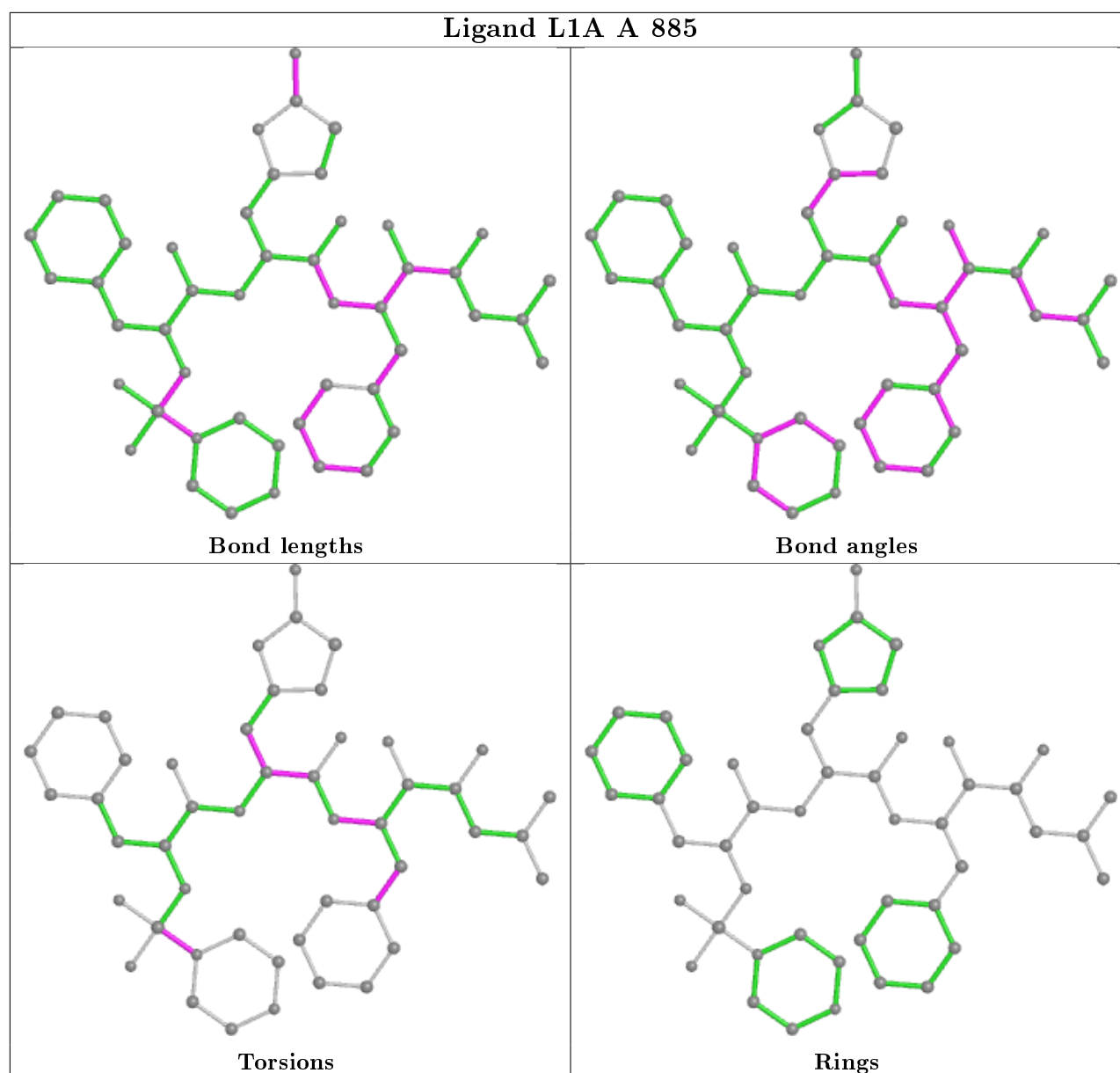
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	886	L1A	5	0
2	A	885	L1A	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

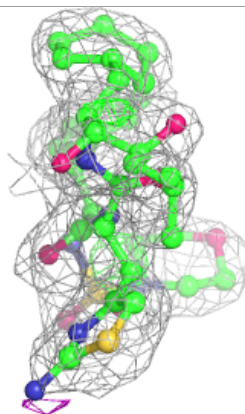
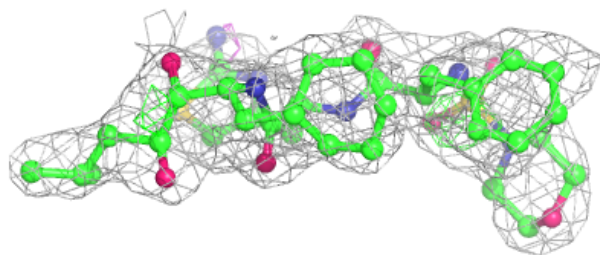
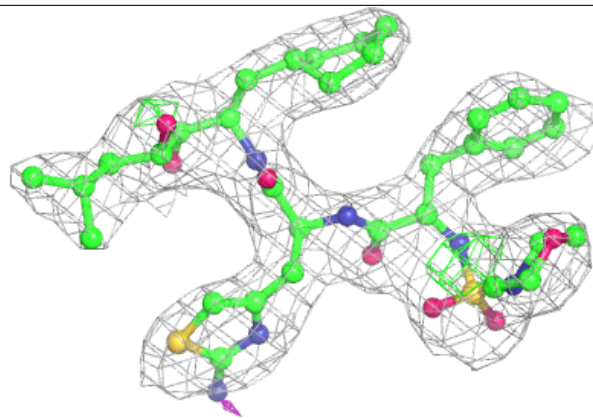
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

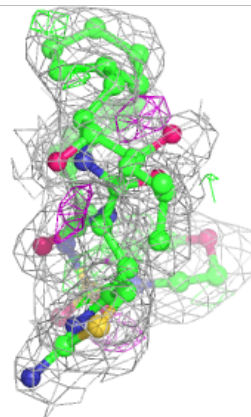
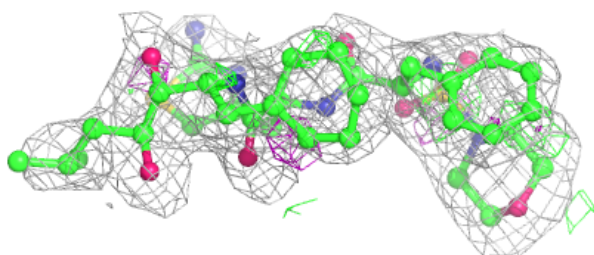
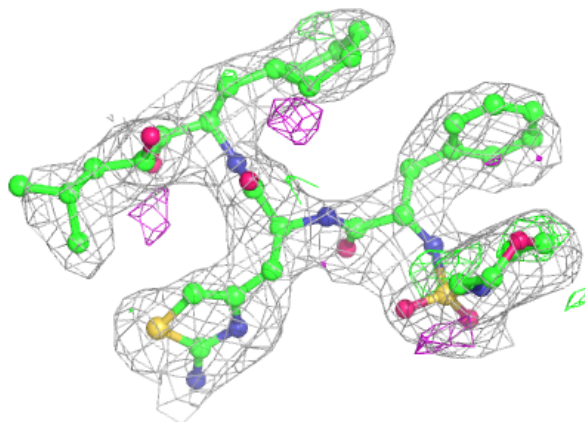
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around L1A B 886:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around L1A A 885:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.