



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 PM UTC

PDB ID : 2G20 / pdb_00002g20
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

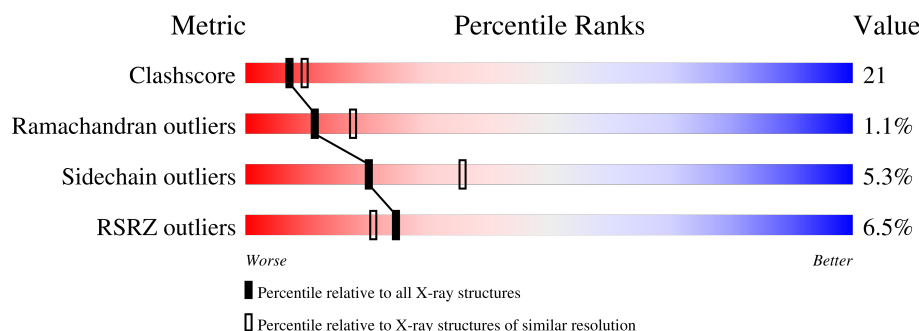
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	A	333	7% 65% 30% 5%
1	B	333	6% 59% 37% • •

2 Entry composition [i](#)

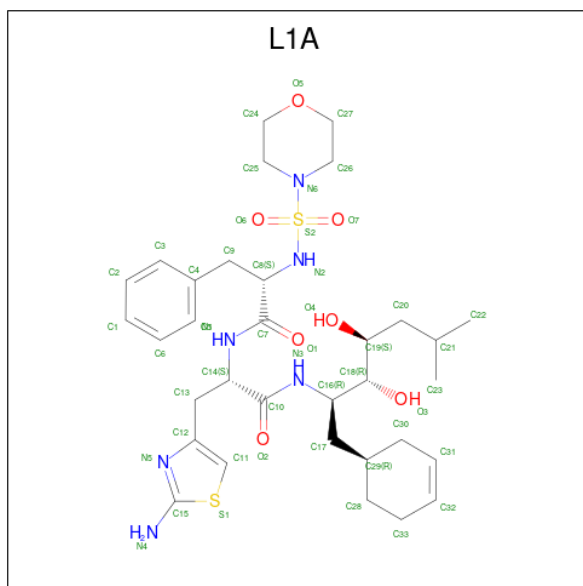
There are 3 unique types of molecules in this entry. The entry contains 5343 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	333	Total	C	N	O	S	0	0	0
			2572	1642	416	500	14			
1	B	333	Total	C	N	O	S	0	0	0
			2572	1642	416	500	14			

- 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 (CCD ID: L1A) (formula: $C_{33}H_{50}N_6O_7S_2$).



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

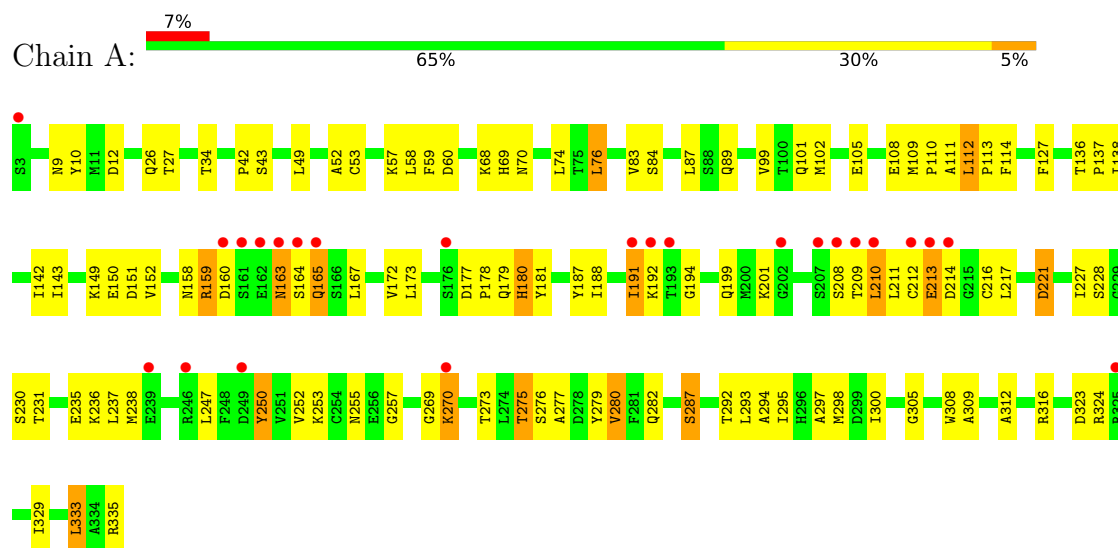
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total 61	O 61	0	0
3	B	42	Total 42	O 42	0	0

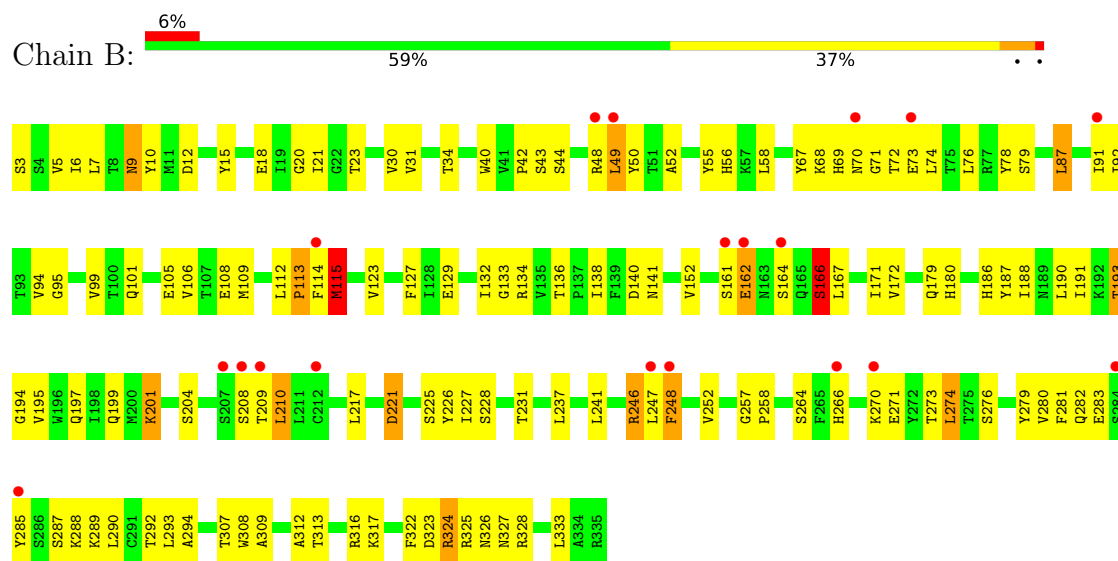
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Renin



• Molecule 1: Renin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	141.33Å 141.33Å 141.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 81.3 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.260 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5343	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage'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.*

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 ⓘ

5.1 Standard geometry ⓘ

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	0.43	0/2632	0.98	16/3568 (0.4%)
1	B	0.41	0/2632	0.99	12/3568 (0.3%)
All	All	0.42	0/5264	0.99	28/7136 (0.4%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	GLY	CA-C-N	7.77	127.43	119.82
1	B	257	GLY	C-N-CA	7.77	127.43	119.82
1	A	213	GLU	N-CA-C	-7.08	101.00	110.55
1	A	221	ASP	N-CA-C	6.93	121.27	107.62
1	A	114	PHE	N-CA-C	6.86	120.75	112.38
1	B	115	MET	N-CA-C	-6.31	105.54	113.18
1	A	159	ARG	N-CA-C	-6.21	101.74	110.50
1	A	287	SER	N-CA-C	-6.17	105.75	113.28
1	A	273	THR	N-CA-C	6.04	119.09	109.24
1	B	308	TRP	N-CA-C	-6.01	102.43	110.55
1	B	180	HIS	N-CA-C	5.92	120.20	112.92
1	B	44	SER	N-CA-C	-5.65	105.65	112.54
1	A	180	HIS	N-CA-C	5.57	119.39	112.59
1	A	177	ASP	CA-C-N	5.57	125.92	119.47
1	A	177	ASP	C-N-CA	5.57	125.92	119.47
1	A	112	LEU	N-CA-C	-5.55	100.98	109.64
1	A	308	TRP	N-CA-C	-5.54	103.39	110.53
1	B	285	TYR	N-CA-C	-5.51	105.25	112.41
1	B	289	LYS	N-CA-C	5.36	117.33	109.24
1	A	250	TYR	N-CA-C	5.32	118.39	110.14
1	B	248	PHE	N-CA-C	-5.25	106.83	114.12
1	A	227	ILE	N-CA-C	-5.24	100.90	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLN	N-CA-C	-5.24	106.41	114.16
1	A	110	PRO	N-CA-C	5.12	118.92	111.03
1	B	221	ASP	N-CA-C	5.10	116.94	108.02
1	A	34	THR	N-CA-C	-5.07	106.93	113.01
1	B	186	HIS	N-CA-C	-5.04	100.25	108.76
1	B	273	THR	N-CA-C	5.03	117.44	109.24

There are no chirality outliers.

There are no planarity outliers.

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	A	2572	0	2501	102	0
1	B	2572	0	2501	112	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	214	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 21.

All (214) 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:42:PRO:HG3	1:B:109:MET:HE1	1.41	1.03
1:B:217:LEU:HB2	1:B:307:THR:HG22	1.39	1.01
1:A:89:GLN:HB2	1:A:102:MET:HE2	1.46	0.96
1:B:52:ALA:HA	1:B:115:MET:HE3	1.47	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:ND2	1:A:159:ARG:H	1.82	0.78
1:A:275:THR:HG22	1:A:277:ALA:H	1.50	0.77
1:A:163:ASN:H	1:A:163:ASN:HD22	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:9:ASN:C	1:B:9:ASN:HD22	1.94	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:52:ALA:HA	1:B:115:MET:CE	2.18	0.73
1:B:247:LEU:HD23	1:B:248:PHE:HB2	1.70	0.73
1:B:55:TYR:HB2	1:B:115:MET:HE1	1.72	0.72
1:B:201:LYS:HB2	1:B:266:HIS:HD2	1.55	0.72
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: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:A:210:LEU:HB2	1:A:236:LYS:HZ2	1.60	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:42:PRO:CG	1:B:109:MET:HE1	2.25	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:H	1:A:163:ASN:ND2	1.97	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:ASN:ND2	3:B:895:HOH:O	2.37	0.58
1:B:247:LEU:CD2	1:B:248:PHE:HB2	2.34	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:HG13	1:B:91:ILE:O	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:A:180:HIS:C	1:A:335:ARG:HG2	2.30	0.56
1:B:136:THR:HG21	1:B:141:ASN:ND2	2.21	0.56
1:B:52:ALA:CA	1:B:115:MET:HE3	2.29	0.56
1:A:208:SER:O	1:A:210:LEU:HG	2.06	0.55
1:B:140:ASP:CG	1:B:324:ARG:HH12	2.14	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:129:GLU:OE1	1:B:129:GLU:N	2.36	0.55
1:B:221:ASP:OD1	2:B:886:L1A:O3	2.24	0.54
1:B:246:ARG:HG2	1:B:247:LEU:N	2.22	0.54
1:A:191:ILE:HD11	1:A:199:GLN:HB2	1.90	0.54
1:A:212:CYS:SG	1:A:212:CYS:O	2.64	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: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:A:187:TYR:C	1:A:188:ILE:HD12	2.33	0.54
1:B:7:LEU:HD11	1:B:171:ILE:HG13	1.89	0.53
1:B:225:SER:O	1:B:312:ALA:HB3	2.08	0.53
1:A:9:ASN:ND2	1:A:12:ASP:H	2.07	0.53
1:A:112:LEU:HD12	1:A:112:LEU:N	2.23	0.53
1:A:9:ASN:C	1:A:9:ASN:HD22	2.14	0.53
1:A:209:THR:O	1:A:209:THR:HG22	2.09	0.53
1:B:164:SER:C	1:B:166:SER:H	2.17	0.53
1:A:163:ASN:HD22	1:A:163:ASN:N	1.96	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:O	1:A:57:LYS:HG2	2.09	0.52
1:A:53:CYS:SG	1:A:109:MET:HE2	2.49	0.52
1:A:213:GLU:O	1:A:214:ASP:HB2	2.09	0.52
1:B:71:GLY:O	1:B:72:THR:C	2.51	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:A:52:ALA:CB	1:A:109:MET:HE3	2.40	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:297:ALA:O	1:A:298:MET:HE2	2.10	0.50
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: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:133:GLY:C	1:B:134:ARG:HG3	2.36	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:A:294:ALA:C	1:A:295:ILE:HG13	2.36	0.50
1:B:188:ILE:N	1:B:188:ILE:HD12	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: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:238:MET:HG3	1:A:250:TYR:CD2	2.47	0.48
1:B:9:ASN:C	1:B:9:ASN:ND2	2.61	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:A:269:GLY:O	1:A:270:LYS:HB2	2.13	0.48
1:A:255:ASN:OD1	1:A:287:SER:HA	2.14	0.48
1:A:9:ASN:ND2	1:A:9:ASN:C	2.72	0.48
1:B:30:VAL:HG21	1:B:123:VAL:CG2	2.43	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:50:TYR:CZ	1:B:108:GLU:HG2	2.49	0.47
1:B:101:GLN:HE22	1:B:138:ILE:HA	1.78	0.47
1:A:26:GLN:NE2	1:A:59:PHE:HA	2.29	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:252:VAL:HG12	1:A:253:LYS:N	2.28	0.47
1:A:70:ASN:HB2	1:A:102:MET:HE1	1.97	0.46
1:B:48:ARG:N	1:B:48:ARG:HD2	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:B:127:PHE:HB2	1:B:194:GLY:HA2	1.97	0.46
1:A:99:VAL:HG21	1:A:142:ILE:CG1	2.42	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: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:6:ILE:HG23	1:B:167:LEU:HD11	1.97	0.45
1:B:127:PHE:HB3	1:B:129:GLU:OE1	2.17	0.45
1:B:282:GLN:O	1:B:283:GLU:C	2.59	0.45
1:A:298:MET:HG2	2:A:885:L1A:C11	2.47	0.45
1:B:15:TYR:O	1:B:31:VAL:HG22	2.17	0.45
1:B:228:SER:OG	1:B:309:ALA:HB3	2.17	0.45
1:A:101:GLN:NE2	1:A:138:ILE:HA	2.32	0.45
1:B:209:THR:HG22	1:B:209:THR:O	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:HD23	1:A:333:LEU:HA	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:52:ALA:HB1	1:A:109:MET:HE3	1.99	0.44
1:A:191:ILE:HD11	1:A:199:GLN:CA	2.47	0.44
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:A:208:SER:C	1:A:210:LEU:H	2.25	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: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:HG3	1:B:324:ARG:NH2	2.34	0.42
1:A:167:LEU:N	1:A:167:LEU:HD23	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: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:B:40:TRP:CZ3	1:B:109:MET:HE2	2.56	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:A:230:SER:O	1:A:231:THR:C	2.62	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:A:111:ALA:C	1:A:112:LEU:HD12	2.46	0.41
1:A:208:SER:C	1:A:210:LEU:N	2.78	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:216:CYS:C	1:A:217:LEU:HD12	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:C	1:B:50:TYR:H	2.29	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%)	10	16
1	B	331/333 (99%)	309 (93%)	19 (6%)	3 (1%)	14	22
All	All	662/666 (99%)	623 (94%)	32 (5%)	7 (1%)	11	18

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%)	273 (96%)	11 (4%)	28	48
1	B	284/284 (100%)	265 (93%)	19 (7%)	15	26
All	All	568/568 (100%)	538 (95%)	30 (5%)	20	36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	76	LEU
1	A	113	PRO
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	280	VAL
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	115	MET
1	B	166	SER
1	B	193	THR
1	B	201	LYS
1	B	210	LEU
1	B	231	THR
1	B	274	LEU
1	B	290	LEU
1	B	324	ARG
1	B	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	GLN
1	A	89	GLN
1	A	101	GLN
1	A	141	ASN
1	A	158	ASN
1	A	163	ASN
1	A	170	GLN
1	A	184	ASN
1	A	186	HIS
1	A	189	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 ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	885	-	48,51,51	2.10	11 (22%)	60,70,70	2.54	13 (21%)
2	L1A	B	886	-	48,51,51	1.98	9 (18%)	60,70,70	2.57	13 (21%)

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	A	885	-	-	10/49/67/67	0/4/4/4
2	L1A	B	886	-	-	11/49/67/67	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	885	L1A	C32-C31	7.91	1.57	1.32
2	B	886	L1A	C32-C31	7.85	1.57	1.32
2	A	885	L1A	C12-N5	4.75	1.47	1.38
2	B	886	L1A	C12-N5	4.65	1.47	1.38
2	B	886	L1A	C15-N4	3.57	1.41	1.34
2	A	885	L1A	C16-N3	3.33	1.51	1.46
2	A	885	L1A	C15-N4	3.32	1.41	1.34
2	A	885	L1A	C15-N5	3.28	1.36	1.31
2	B	886	L1A	C15-N5	3.22	1.36	1.31
2	A	885	L1A	C18-C16	3.22	1.59	1.53
2	A	885	L1A	C30-C31	3.13	1.56	1.49
2	A	885	L1A	C10-N3	3.09	1.40	1.34
2	B	886	L1A	C30-C31	3.07	1.56	1.49
2	B	886	L1A	C18-C16	2.55	1.57	1.53
2	A	885	L1A	C15-S1	2.45	1.78	1.74
2	A	885	L1A	C19-C18	2.23	1.57	1.53
2	B	886	L1A	C33-C32	2.23	1.57	1.48
2	B	886	L1A	C16-N3	2.20	1.49	1.46
2	A	885	L1A	C33-C32	2.15	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	886	L1A	C15-S1	2.02	1.77	1.74

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	885	L1A	C24-C25-N6	8.82	114.55	108.27
2	B	886	L1A	C11-S1-C15	8.08	92.33	88.84
2	B	886	L1A	S1-C15-N5	-7.94	108.28	114.54
2	A	885	L1A	C11-S1-C15	7.93	92.26	88.84
2	A	885	L1A	S1-C15-N5	-7.92	108.30	114.54
2	B	886	L1A	C24-C25-N6	7.89	113.89	108.27
2	B	886	L1A	C27-C26-N6	6.12	112.63	108.27
2	A	885	L1A	C27-C26-N6	5.81	112.41	108.27
2	B	886	L1A	S1-C15-N4	5.48	127.36	120.99
2	A	885	L1A	S1-C15-N4	5.34	127.20	120.99
2	A	885	L1A	C16-N3-C10	4.72	131.46	123.25
2	B	886	L1A	C17-C16-N3	4.44	115.89	110.20
2	B	886	L1A	C16-N3-C10	4.20	130.55	123.25
2	B	886	L1A	C30-C31-C32	-3.54	115.49	123.18
2	A	885	L1A	C30-C31-C32	-3.45	115.68	123.18
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	-2.96	102.17	109.28
2	A	885	L1A	O3-C18-C16	-2.93	102.26	109.28
2	B	886	L1A	C11-C12-N5	-2.74	110.87	115.12
2	A	885	L1A	C17-C16-C18	2.53	116.22	112.18
2	A	885	L1A	C11-C12-N5	-2.49	111.25	115.12
2	A	885	L1A	C17-C29-C28	2.42	117.35	111.71
2	B	886	L1A	C13-C14-N1	-2.40	106.06	110.64
2	B	886	L1A	C17-C29-C28	2.14	116.70	111.71
2	A	885	L1A	C17-C16-N3	2.03	112.81	110.20

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	885	L1A	C17-C16-N3-C10
2	A	885	L1A	C16-C17-C29-C28
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

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Mol	Chain	Res	Type	Atoms
2	B	886	L1A	C26-N6-S2-O7
2	A	885	L1A	C16-C17-C29-C30
2	B	886	L1A	C16-C17-C29-C30
2	A	885	L1A	C25-N6-S2-O6
2	A	885	L1A	C26-N6-S2-O6
2	A	885	L1A	C25-N6-S2-O7
2	A	885	L1A	C26-N6-S2-O7
2	B	886	L1A	C25-N6-S2-O6
2	A	885	L1A	C12-C13-C14-C10
2	B	886	L1A	C12-C13-C14-C10
2	B	886	L1A	N3-C10-C14-N1
2	A	885	L1A	C12-C13-C14-N1
2	B	886	L1A	C12-C13-C14-N1
2	A	885	L1A	N3-C10-C14-N1
2	B	886	L1A	O2-C10-C14-N1

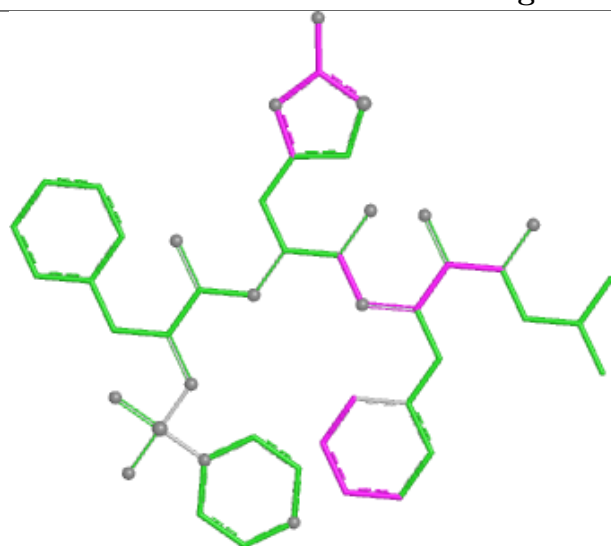
There are no ring outliers.

2 monomers are involved in 8 short contacts:

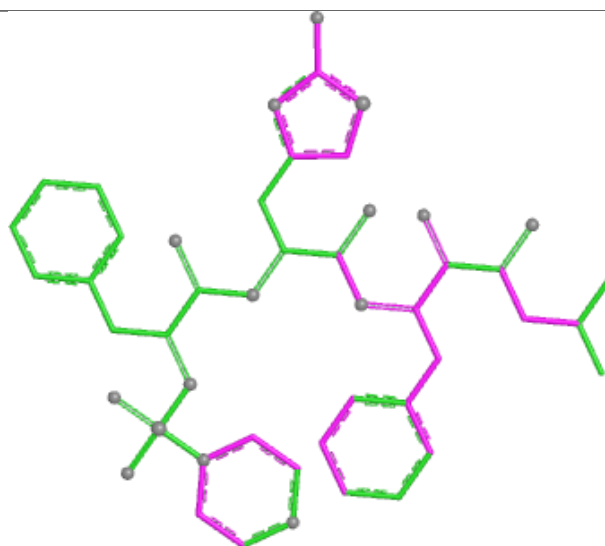
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	885	L1A	3	0
2	B	886	L1A	5	0

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.

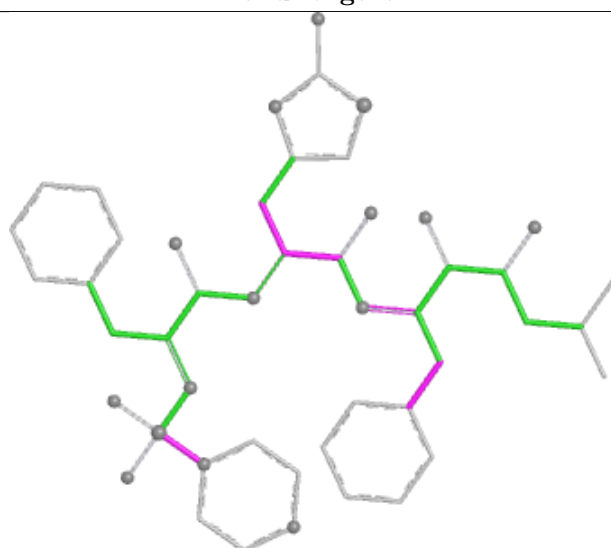
Ligand L1A A 885



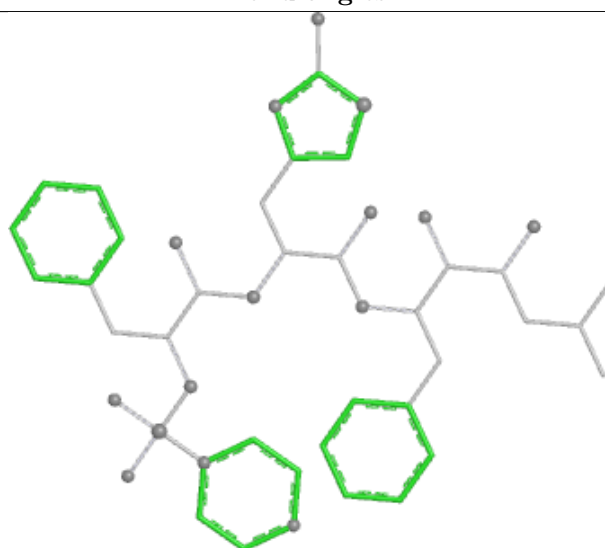
Bond lengths



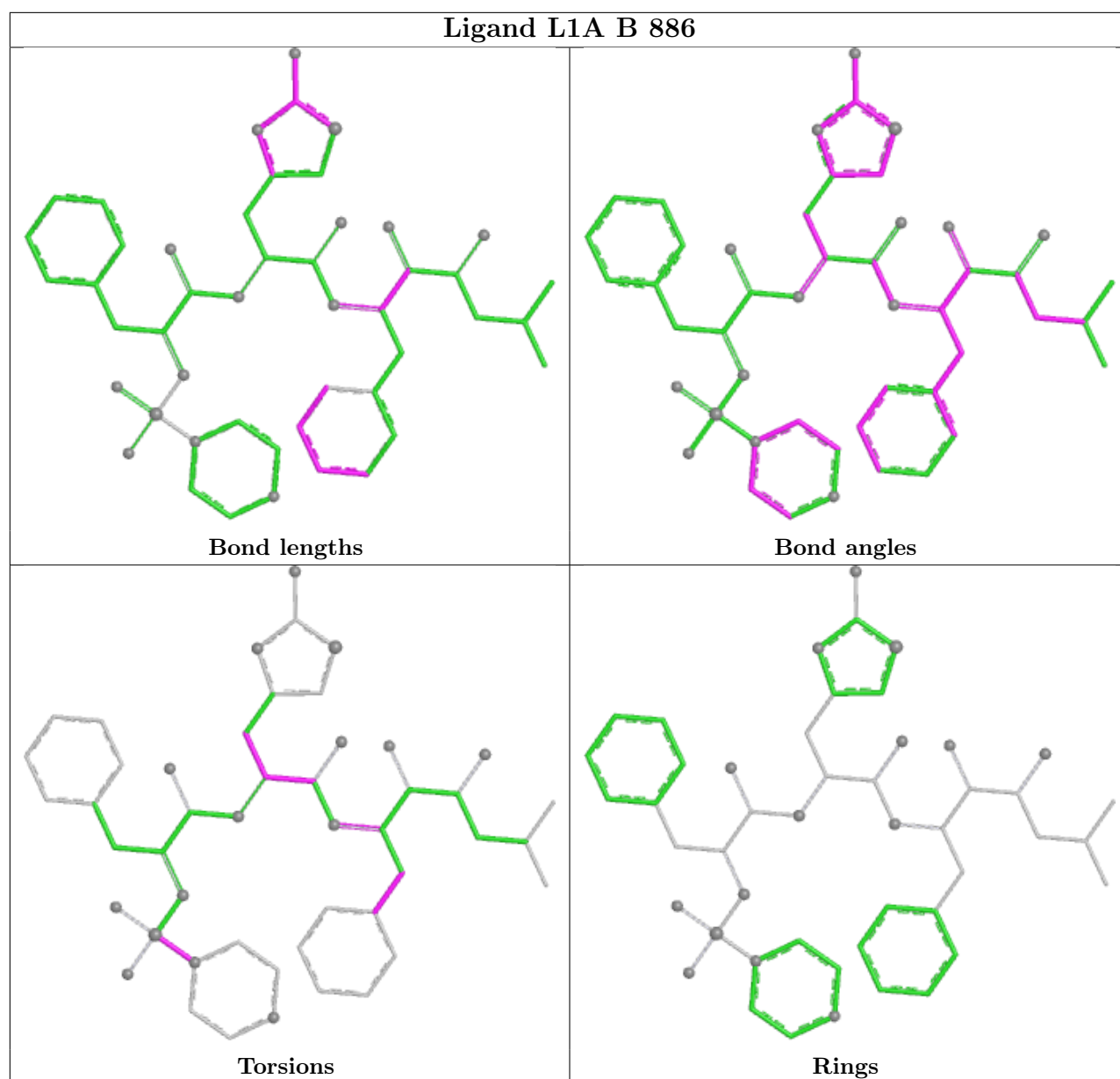
Bond angles



Torsions



Rings



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, 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	A	333/333 (100%)	0.27	24 (7%) 21 18	25, 39, 63, 84	0
1	B	333/333 (100%)	0.48	19 (5%) 29 25	27, 46, 69, 84	0
All	All	666/666 (100%)	0.38	43 (6%) 25 21	25, 43, 68, 84	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	THR	4.5
1	B	209	THR	4.4
1	B	162	GLU	4.4
1	B	208	SER	4.3
1	A	210	LEU	3.9
1	B	247	LEU	3.9
1	B	49	LEU	3.7
1	B	207	SER	3.4
1	B	248	PHE	3.3
1	B	161	SER	3.2
1	A	214	ASP	3.1
1	A	3	SER	3.0
1	A	213	GLU	3.0
1	A	325	ARG	3.0
1	A	249	ASP	2.9
1	A	165	GLN	2.8
1	A	160	ASP	2.8
1	A	161	SER	2.7
1	A	212	CYS	2.6
1	B	266	HIS	2.6
1	A	208	SER	2.6
1	B	164	SER	2.6
1	B	285	TYR	2.5
1	A	202	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	LYS	2.4
1	A	163	ASN	2.3
1	B	284	SER	2.3
1	B	48	ARG	2.3
1	B	212	CYS	2.3
1	B	70	ASN	2.2
1	B	114	PHE	2.2
1	A	246	ARG	2.2
1	A	176	SER	2.1
1	A	207	SER	2.1
1	A	192	LYS	2.1
1	A	193	THR	2.1
1	B	91	ILE	2.1
1	A	164	SER	2.1
1	A	162	GLU	2.0
1	B	73	GLU	2.0
1	A	191	ILE	2.0
1	B	270	LYS	2.0
1	A	239	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

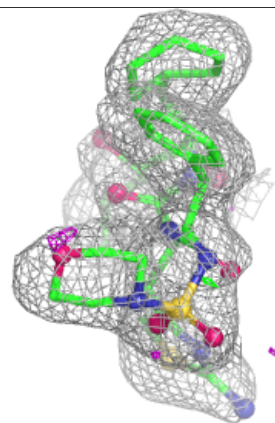
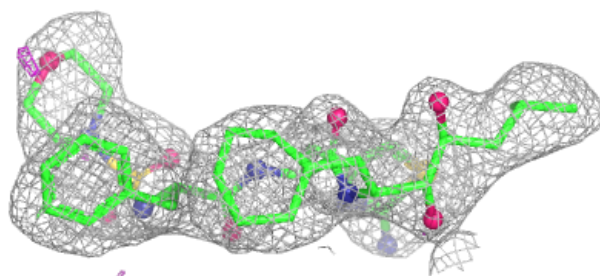
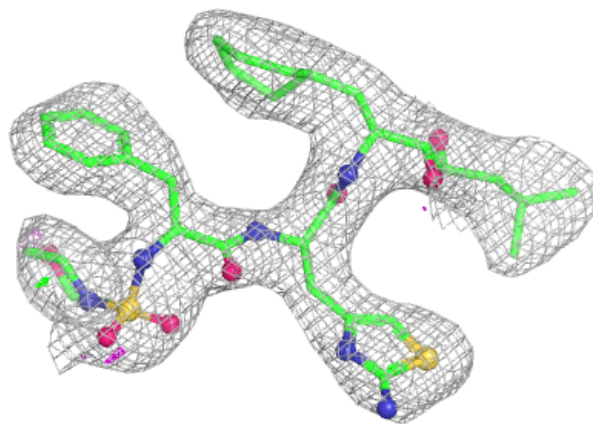
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	L1A	B	886	48/48	0.93	0.10	33,42,50,52	0
2	L1A	A	885	48/48	0.95	0.09	25,33,37,37	0

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.

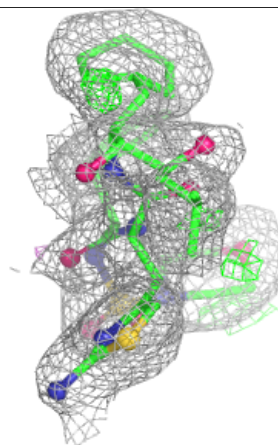
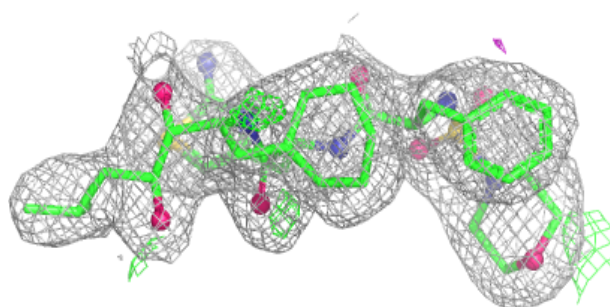
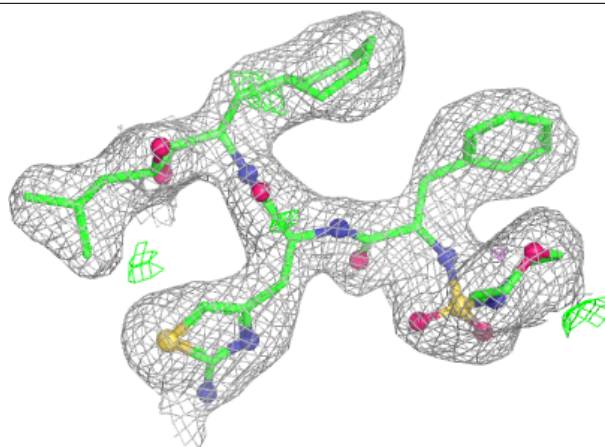
Electron density around L1A B 886:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.