



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:14 PM EDT

PDB ID : 4K9H / pdb_00004k9h
Title : Bace-1 inhibitor complex
Authors : Jordan, S.R.
Deposited on : 2013-04-19
Resolution : 2.29 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

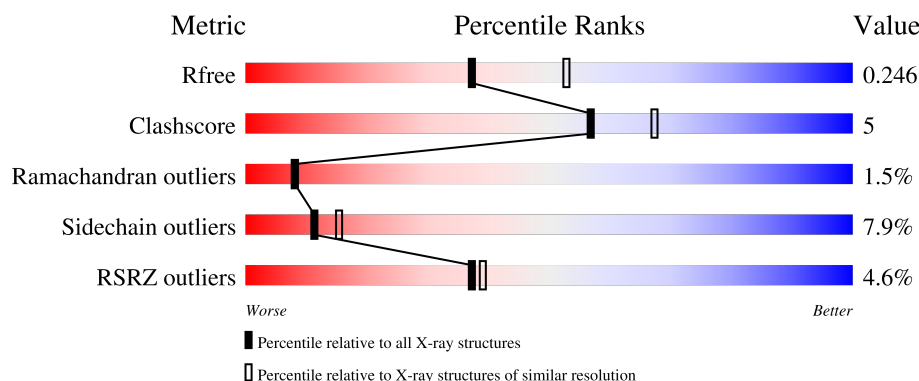
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	388	5% 78% 14% • • 5%
1	B	388	3% 79% 14% • • 5%
1	C	388	5% 78% 15% • • 5%

2 Entry composition [i](#)

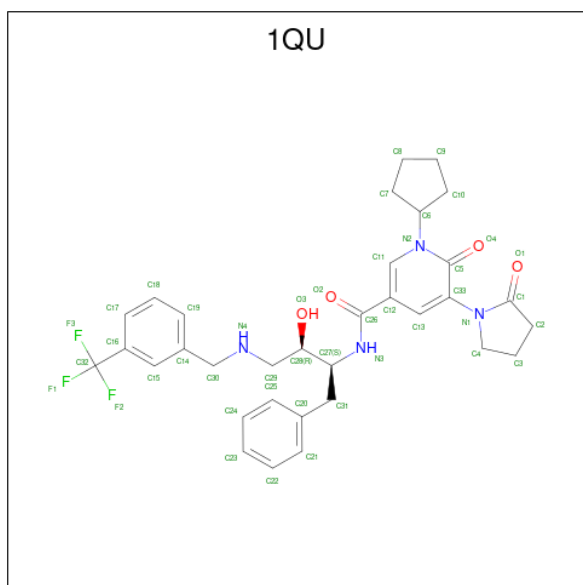
There are 3 unique types of molecules in this entry. The entry contains 8879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2915	1869	485	547	14			
1	B	369	Total	C	N	O	S	0	0	0
			2909	1866	484	545	14			
1	C	370	Total	C	N	O	S	0	0	0
			2915	1869	485	547	14			

- Molecule 2 is 1-cyclopentyl-N-[(2S,3R)-3-hydroxy-1-phenyl-4-{[3-(trifluoromethyl)benzyl]amino}butan-2-yl]-6-oxo-5-(2-oxopyrrolidin-1-yl)-1,6-dihydropyridine-3-carboxamide (CCD ID: 1QU) (formula: C₃₃H₃₇F₃N₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			44	33	3	4	4		
2	B	1	Total	C	F	N	O	0	0
			44	33	3	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	0
			44	33	3	4	4		

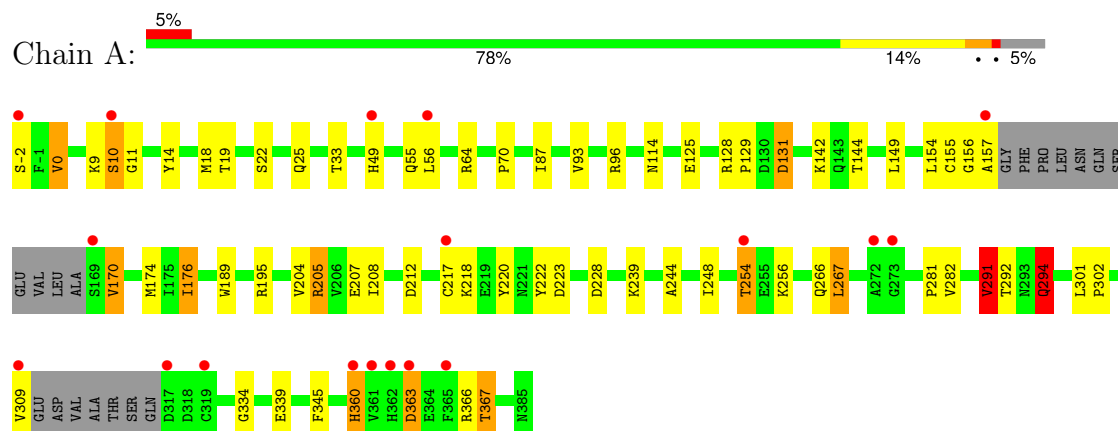
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	3	Total	O	0	0
			3	3		
3	C	3	Total	O	0	0
			3	3		

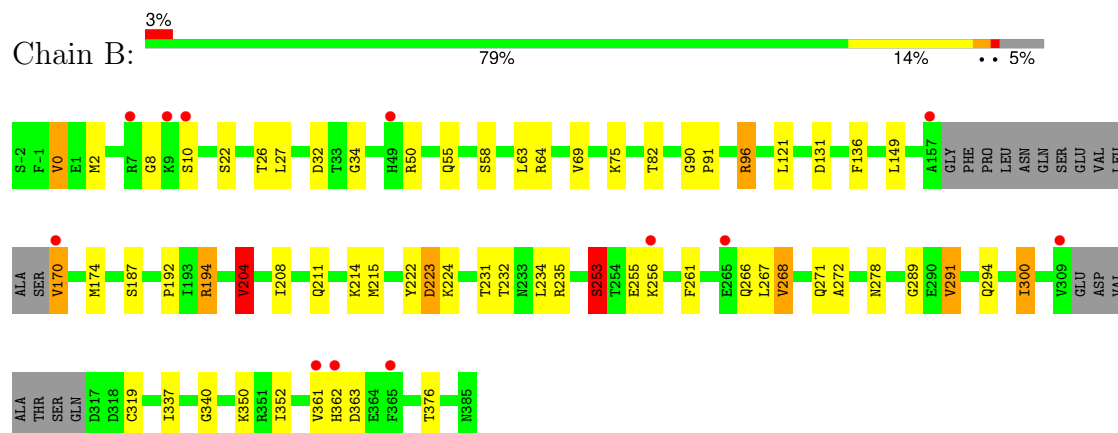
3 Residue-property plots [i](#)

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.

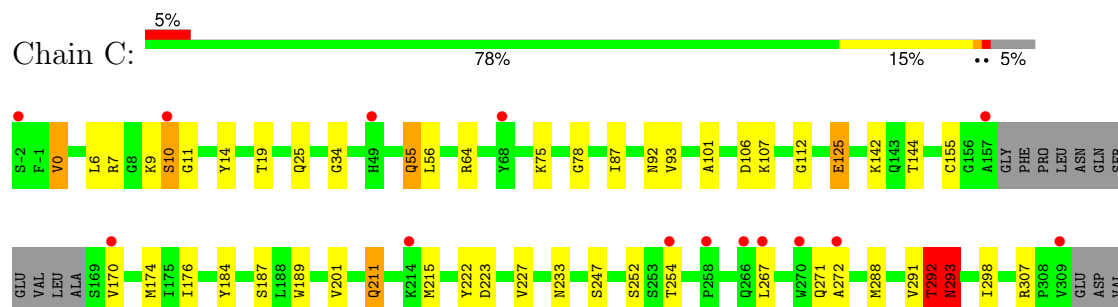
• Molecule 1: Beta-secretase 1

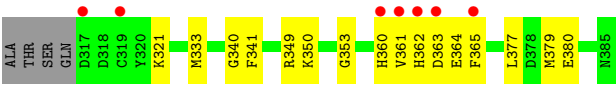


• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.54Å 103.30Å 100.86Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	44.00 – 2.29 44.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.00-2.29) 94.4 (44.00-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.199 , 0.248 0.204 , 0.246	Depositor DCC
R_{free} test set	3702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8879	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: 1QU

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	1.17	2/2989 (0.1%)	1.16	10/4060 (0.2%)
1	B	1.25	5/2983 (0.2%)	1.20	16/4052 (0.4%)
1	C	1.19	5/2989 (0.2%)	1.16	8/4060 (0.2%)
All	All	1.20	12/8961 (0.1%)	1.17	34/12172 (0.3%)

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	B	0	1
1	C	0	3
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	ARG	C-O	-6.68	1.16	1.24
1	C	292	THR	N-CA	6.45	1.54	1.46
1	C	341	PHE	CA-C	-6.04	1.45	1.52
1	C	293	ASN	N-CA	5.77	1.53	1.46
1	C	184	TYR	C-O	-5.66	1.16	1.23
1	B	136	PHE	N-CA	-5.50	1.39	1.46
1	A	176	ILE	C-O	-5.46	1.18	1.24
1	B	289	GLY	C-O	-5.33	1.18	1.23
1	B	192	PRO	C-O	-5.23	1.18	1.23
1	B	224	LYS	N-CA	5.22	1.52	1.46
1	A	149	LEU	C-O	-5.14	1.17	1.23
1	C	292	THR	C-N	-5.05	1.26	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ASP	N-CA-C	-8.40	96.64	110.17
1	A	0	VAL	CB-CA-C	-8.14	100.16	112.05
1	B	0	VAL	CB-CA-C	-7.36	102.21	112.14
1	C	0	VAL	CB-CA-C	-7.34	100.79	112.16
1	B	0	VAL	N-CA-CB	7.32	120.49	110.54
1	B	204	VAL	N-CA-CB	-7.22	102.38	112.35
1	C	252	SER	N-CA-C	6.50	119.91	112.57
1	B	300	ILE	N-CA-C	6.34	118.52	108.89
1	B	223	ASP	N-CA-C	-6.24	97.51	110.80
1	C	292	THR	N-CA-CB	6.18	120.94	110.49
1	B	204	VAL	CB-CA-C	6.00	117.42	110.88
1	C	87	ILE	CA-C-N	5.95	125.43	119.24
1	C	87	ILE	C-N-CA	5.95	125.43	119.24
1	A	292	THR	N-CA-C	5.82	118.79	110.24
1	C	56	LEU	N-CA-C	5.76	120.01	113.15
1	A	294	GLN	CB-CG-CD	-5.73	102.86	112.60
1	A	291	VAL	N-CA-CB	-5.69	102.87	112.44
1	A	281	PRO	CA-C-N	5.63	128.73	120.91
1	A	281	PRO	C-N-CA	5.63	128.73	120.91
1	B	91	PRO	CA-C-N	-5.52	114.63	122.41
1	B	91	PRO	C-N-CA	-5.52	114.63	122.41
1	C	292	THR	CA-C-N	-5.27	111.48	121.54
1	C	292	THR	C-N-CA	-5.27	111.48	121.54
1	B	363	ASP	N-CA-C	-5.25	102.71	110.48
1	A	222	TYR	CA-C-N	5.23	131.53	121.54
1	A	222	TYR	C-N-CA	5.23	131.53	121.54
1	B	69	VAL	CA-C-N	5.21	126.36	119.84
1	B	69	VAL	C-N-CA	5.21	126.36	119.84
1	B	222	TYR	O-C-N	5.21	129.55	122.57
1	B	32	ASP	N-CA-C	5.17	117.42	107.44
1	B	222	TYR	CA-C-N	5.14	131.35	121.54
1	B	222	TYR	C-N-CA	5.14	131.35	121.54
1	B	0	VAL	O-C-N	5.11	126.83	121.87
1	A	291	VAL	CB-CA-C	5.05	118.22	110.55

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	340	GLY	Peptide
1	C	222	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	C	292	THR	Peptide
1	C	340	GLY	Peptide

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	2915	0	2833	27	0
1	B	2909	0	2828	21	0
1	C	2915	0	2833	33	0
2	A	44	0	37	0	0
2	B	44	0	36	3	0
2	C	44	0	36	2	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
All	All	8879	0	8603	80	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 5.

All (80) 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:55:GLN:H	1:C:55:GLN:HE21	1.26	0.79
1:C:10:SER:OG	1:C:11:GLY:N	2.20	0.74
1:C:227:VAL:HG22	1:C:333:MET:HE3	1.73	0.71
1:A:10:SER:OG	1:A:11:GLY:N	2.25	0.70
1:C:9:LYS:O	1:C:10:SER:HB3	1.91	0.70
1:C:363:ASP:O	1:C:365:PHE:N	2.26	0.68
1:A:205:ARG:NH2	1:A:207:GLU:OE2	2.31	0.64
1:C:9:LYS:O	1:C:10:SER:CB	2.46	0.64
1:C:55:GLN:H	1:C:55:GLN:NE2	1.97	0.63
1:B:271:GLN:OE1	1:B:271:GLN:N	2.31	0.62
1:A:266:GLN:O	1:A:267:LEU:HB2	2.00	0.61
1:A:205:ARG:NH1	1:A:212:ASP:OD2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:CYS:O	1:A:170:VAL:HG22	2.05	0.56
1:C:292:THR:O	1:C:293:ASN:CB	2.51	0.56
1:A:291:VAL:HG12	1:A:294:GLN:HB3	1.87	0.55
1:B:204:VAL:HG13	1:B:376:THR:HG21	1.89	0.55
1:C:125:GLU:O	1:C:125:GLU:HG3	2.09	0.53
1:A:93:VAL:HG21	1:A:144:THR:CG2	2.39	0.52
1:A:33:THR:HG21	1:A:345:PHE:CZ	2.44	0.52
1:C:291:VAL:O	1:C:292:THR:HG23	2.10	0.52
1:B:271:GLN:O	1:B:272:ALA:C	2.53	0.52
1:A:154:LEU:O	1:A:339:GLU:HA	2.10	0.51
1:A:205:ARG:CZ	1:A:212:ASP:OD2	2.59	0.51
1:C:155:CYS:O	1:C:170:VAL:HG13	2.11	0.50
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.94	0.49
1:B:261:PHE:CE1	1:B:268:VAL:HG23	2.49	0.48
1:A:93:VAL:HG21	1:A:144:THR:HG21	1.95	0.48
1:A:244:ALA:O	1:A:248:ILE:HG13	2.13	0.47
1:C:233:ASN:HB2	2:C:401:1QU:H3	1.96	0.47
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.97	0.46
1:A:217:CYS:HA	1:A:220:TYR:CD2	2.50	0.46
1:B:253:SER:C	1:B:255:GLU:H	2.23	0.46
1:A:291:VAL:HG12	1:A:294:GLN:CB	2.45	0.46
1:B:34:GLY:O	2:B:401:1QU:H35	2.16	0.46
1:A:56:LEU:O	1:A:56:LEU:HD12	2.16	0.46
1:B:149:LEU:HD23	1:B:149:LEU:N	2.31	0.46
1:A:18:MET:HE3	1:A:87:ILE:HG12	1.98	0.46
1:B:8:GLY:C	1:B:170:VAL:HG12	2.41	0.46
1:B:234:LEU:HB2	1:B:337:ILE:HD11	1.98	0.46
1:C:292:THR:O	1:C:293:ASN:HB3	2.16	0.45
1:C:288:MET:HE1	1:C:379:MET:HE3	1.99	0.45
1:B:26:THR:C	1:B:27:LEU:HG	2.42	0.45
1:C:78:GLY:HA3	1:C:101:ALA:O	2.17	0.45
1:B:131:ASP:OD1	1:B:131:ASP:C	2.60	0.45
1:C:189:TRP:O	1:C:353:GLY:HA2	2.17	0.45
1:C:6:LEU:O	1:C:7:ARG:NH1	2.50	0.44
1:C:349:ARG:O	1:C:350:LYS:HB2	2.17	0.44
1:A:189:TRP:CZ3	1:B:291:VAL:HG13	2.53	0.44
1:A:204:VAL:O	1:A:205:ARG:HG2	2.18	0.44
1:B:350:LYS:HB3	1:B:350:LYS:HE3	1.75	0.43
1:A:19:THR:HA	1:A:25:GLN:O	2.18	0.43
1:C:106:ASP:OD1	1:C:107:LYS:HG3	2.19	0.43
1:C:14:TYR:CE2	1:C:170:VAL:CG1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:MET:HE1	1:C:379:MET:CE	2.48	0.43
1:B:231:THR:HG23	2:B:401:1QU:H5	2.00	0.43
1:B:232:THR:OG1	2:B:401:1QU:H10	2.19	0.43
1:C:93:VAL:HG21	1:C:144:THR:HG21	2.01	0.42
1:A:363:ASP:HB3	1:A:366:ARG:H	1.83	0.42
1:C:9:LYS:HE2	1:C:112:GLY:O	2.19	0.42
1:B:121:LEU:HD11	1:B:174:MET:HE1	2.02	0.42
1:B:82:THR:HB	1:B:96:ARG:HD3	2.01	0.42
1:A:14:TYR:CE2	1:A:170:VAL:HG13	2.54	0.42
1:C:9:LYS:CE	1:C:112:GLY:O	2.68	0.42
1:C:174:MET:HE2	1:C:176:ILE:HG12	2.02	0.42
1:C:19:THR:HA	1:C:25:GLN:O	2.20	0.42
1:A:360:HIS:CE1	1:A:367:THR:HG22	2.55	0.41
1:C:93:VAL:HG21	1:C:144:THR:CG2	2.50	0.41
1:B:63:LEU:O	1:B:64:ARG:C	2.63	0.41
1:B:271:GLN:H	1:B:271:GLN:CD	2.22	0.41
1:C:14:TYR:CE2	1:C:170:VAL:HG12	2.56	0.41
1:C:379:MET:HE3	1:C:379:MET:HB2	1.92	0.41
1:A:128:ARG:HA	1:A:129:PRO:C	2.45	0.41
1:C:34:GLY:O	2:C:401:1QU:H35	2.20	0.41
1:C:211:GLN:HE21	1:C:211:GLN:HB2	1.71	0.41
1:C:298:ILE:HD13	1:C:298:ILE:HG21	1.77	0.41
1:A:228:ASP:O	1:A:334:GLY:HA2	2.21	0.40
1:C:201:VAL:HG21	1:C:333:MET:HE1	2.04	0.40
1:B:268:VAL:O	1:B:319:CYS:HA	2.21	0.40
1:B:2:MET:HG2	1:B:90:GLY:HA2	2.04	0.40
1:A:156:GLY:O	1:A:157:ALA:C	2.65	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	364/388 (94%)	342 (94%)	15 (4%)	7 (2%)	6	5
1	B	363/388 (94%)	349 (96%)	11 (3%)	3 (1%)	16	20
1	C	364/388 (94%)	343 (94%)	15 (4%)	6 (2%)	7	7
All	All	1091/1164 (94%)	1034 (95%)	41 (4%)	16 (2%)	8	8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	B	10	SER
1	B	223	ASP
1	C	10	SER
1	C	272	ALA
1	C	364	GLU
1	A	254	THR
1	A	10	SER
1	A	131	ASP
1	A	223	ASP
1	C	223	ASP
1	A	125	GLU
1	B	253	SER
1	A	70	PRO
1	C	254	THR
1	C	292	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/331 (96%)	291 (92%)	25 (8%)	11	15
1	B	315/331 (95%)	287 (91%)	28 (9%)	9	12
1	C	316/331 (96%)	294 (93%)	22 (7%)	14	19
All	All	947/993 (95%)	872 (92%)	75 (8%)	11	15

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	0	VAL
1	A	9	LYS
1	A	22	SER
1	A	49	HIS
1	A	55	GLN
1	A	64	ARG
1	A	96	ARG
1	A	114	ASN
1	A	131	ASP
1	A	142	LYS
1	A	170	VAL
1	A	195	ARG
1	A	205	ARG
1	A	208	ILE
1	A	218	LYS
1	A	239	LYS
1	A	254	THR
1	A	256	LYS
1	A	282	VAL
1	A	291	VAL
1	A	294	GLN
1	A	309	VAL
1	A	360	HIS
1	A	367	THR
1	B	0	VAL
1	B	22	SER
1	B	50	ARG
1	B	55	GLN
1	B	58	SER
1	B	75	LYS
1	B	96	ARG
1	B	170	VAL
1	B	187	SER
1	B	194	ARG
1	B	204	VAL
1	B	208	ILE
1	B	211	GLN
1	B	214	LYS
1	B	215	MET
1	B	235	ARG
1	B	253	SER
1	B	256	LYS

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Mol	Chain	Res	Type
1	B	266	GLN
1	B	267	LEU
1	B	268	VAL
1	B	278	ASN
1	B	291	VAL
1	B	294	GLN
1	B	300	ILE
1	B	352	ILE
1	B	361	VAL
1	B	362	HIS
1	C	0	VAL
1	C	55	GLN
1	C	64	ARG
1	C	75	LYS
1	C	92	ASN
1	C	125	GLU
1	C	142	LYS
1	C	187	SER
1	C	211	GLN
1	C	215	MET
1	C	247	SER
1	C	267	LEU
1	C	271	GLN
1	C	292	THR
1	C	293	ASN
1	C	307	ARG
1	C	321	LYS
1	C	360	HIS
1	C	361	VAL
1	C	362	HIS
1	C	377	LEU
1	C	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	111	ASN
1	A	271	GLN
1	A	293	ASN
1	A	304	GLN
1	A	360	HIS

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Mol	Chain	Res	Type
1	B	28	ASN
1	B	73	GLN
1	B	111	ASN
1	B	233	ASN
1	B	278	ASN
1	C	12	GLN
1	C	28	ASN
1	C	53	GLN
1	C	55	GLN
1	C	111	ASN
1	C	266	GLN
1	C	271	GLN
1	C	326	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	1QU	C	401	-	47,48,48	1.34	6 (12%)	61,68,68	2.45	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1QU	A	401	-	47,48,48	1.30	5 (10%)	61,68,68	1.40	8 (13%)
2	1QU	B	401	-	47,48,48	1.51	7 (14%)	61,68,68	2.22	15 (24%)

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	1QU	C	401	-	-	11/35/53/53	0/5/5/5
2	1QU	A	401	-	-	8/35/53/53	0/5/5/5
2	1QU	B	401	-	-	7/35/53/53	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1QU	C32-C16	4.53	1.59	1.49
2	B	401	1QU	C6-N2	-3.98	1.42	1.48
2	B	401	1QU	C33-C5	-3.78	1.39	1.47
2	C	401	1QU	C29-C28	3.75	1.57	1.52
2	A	401	1QU	C33-C5	-3.74	1.39	1.47
2	C	401	1QU	C33-C5	-3.64	1.39	1.47
2	B	401	1QU	C1-N1	-3.26	1.33	1.38
2	C	401	1QU	C31-C27	2.79	1.59	1.53
2	A	401	1QU	C30-C14	2.72	1.57	1.51
2	B	401	1QU	O3-C28	2.67	1.48	1.43
2	C	401	1QU	C29-N4	2.56	1.51	1.47
2	B	401	1QU	C4-N1	2.39	1.50	1.47
2	B	401	1QU	C13-C12	-2.32	1.39	1.43
2	B	401	1QU	C11-N2	2.31	1.41	1.38
2	A	401	1QU	C28-C27	-2.18	1.50	1.53
2	A	401	1QU	C12-C26	2.04	1.55	1.49
2	C	401	1QU	O3-C28	2.01	1.47	1.43
2	C	401	1QU	C13-C12	-2.01	1.39	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	1QU	C2-C1-N1	8.37	115.29	108.03
2	B	401	1QU	C2-C1-N1	7.83	114.83	108.03
2	B	401	1QU	C6-N2-C11	-7.04	103.90	120.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	1QU	C9-C10-C6	-6.97	88.94	104.61
2	B	401	1QU	C8-C7-C6	-6.12	90.85	104.61
2	C	401	1QU	C8-C7-C6	-5.60	92.02	104.61
2	C	401	1QU	C6-N2-C11	-5.53	107.44	120.41
2	C	401	1QU	C10-C6-N2	5.22	128.37	114.39
2	C	401	1QU	C28-C29-N4	-5.05	105.32	111.95
2	C	401	1QU	F1-C32-C16	-5.00	102.19	112.90
2	B	401	1QU	C10-C6-N2	4.93	127.60	114.39
2	B	401	1QU	F2-C32-C16	-4.62	103.00	112.90
2	C	401	1QU	C4-N1-C33	-4.26	115.62	123.25
2	A	401	1QU	C28-C27-N3	4.21	117.88	109.97
2	B	401	1QU	C9-C10-C6	-4.04	95.52	104.61
2	C	401	1QU	O1-C1-C2	-3.82	117.24	127.12
2	A	401	1QU	F1-C32-C16	-3.59	105.21	112.90
2	A	401	1QU	O1-C1-N1	3.43	127.62	123.94
2	A	401	1QU	C33-C5-N2	3.16	120.00	115.43
2	A	401	1QU	C28-C29-N4	-3.02	107.99	111.95
2	A	401	1QU	C2-C1-N1	2.71	110.39	108.03
2	B	401	1QU	C18-C19-C14	-2.64	116.91	120.61
2	C	401	1QU	C4-N1-C1	-2.63	109.57	112.82
2	B	401	1QU	O1-C1-C2	-2.57	120.48	127.12
2	B	401	1QU	C31-C27-C28	-2.56	107.49	111.66
2	B	401	1QU	C28-C29-N4	-2.56	108.59	111.95
2	A	401	1QU	O4-C5-N2	-2.51	117.42	122.45
2	C	401	1QU	F2-C32-C16	-2.45	107.66	112.90
2	B	401	1QU	C4-N1-C33	-2.35	119.04	123.25
2	C	401	1QU	C3-C2-C1	-2.27	97.67	104.41
2	B	401	1QU	C10-C6-C7	2.26	109.95	104.74
2	C	401	1QU	O1-C1-N1	2.25	126.35	123.94
2	C	401	1QU	C3-C4-N1	-2.21	100.08	102.98
2	B	401	1QU	C28-C27-N3	2.12	113.94	109.97
2	B	401	1QU	F3-C32-C16	2.09	117.37	112.90
2	B	401	1QU	C17-C18-C19	2.03	122.86	120.24
2	A	401	1QU	C18-C19-C14	-2.03	117.75	120.61
2	C	401	1QU	F3-C32-C16	2.02	117.22	112.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	1QU	C13-C12-C26-N3
2	B	401	1QU	C13-C33-N1-C4

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Mol	Chain	Res	Type	Atoms
2	B	401	1QU	C13-C12-C26-O2
2	B	401	1QU	C13-C12-C26-N3
2	C	401	1QU	C13-C33-N1-C4
2	C	401	1QU	C13-C12-C26-O2
2	C	401	1QU	O3-C28-C29-N4
2	C	401	1QU	C13-C12-C26-N3
2	B	401	1QU	C11-C12-C26-O2
2	B	401	1QU	C21-C20-C31-C27
2	A	401	1QU	C11-C12-C26-O2
2	A	401	1QU	C13-C33-N1-C4
2	B	401	1QU	C11-C12-C26-N3
2	C	401	1QU	C21-C20-C31-C27
2	B	401	1QU	C25-C20-C31-C27
2	A	401	1QU	C21-C20-C31-C27
2	C	401	1QU	C25-C20-C31-C27
2	C	401	1QU	C14-C30-N4-C29
2	C	401	1QU	C27-C28-C29-N4
2	C	401	1QU	C11-C12-C26-O2
2	A	401	1QU	C25-C20-C31-C27
2	C	401	1QU	N3-C27-C31-C20
2	A	401	1QU	C11-C12-C26-N3
2	C	401	1QU	C11-C12-C26-N3
2	A	401	1QU	C13-C12-C26-O2
2	A	401	1QU	N3-C27-C31-C20

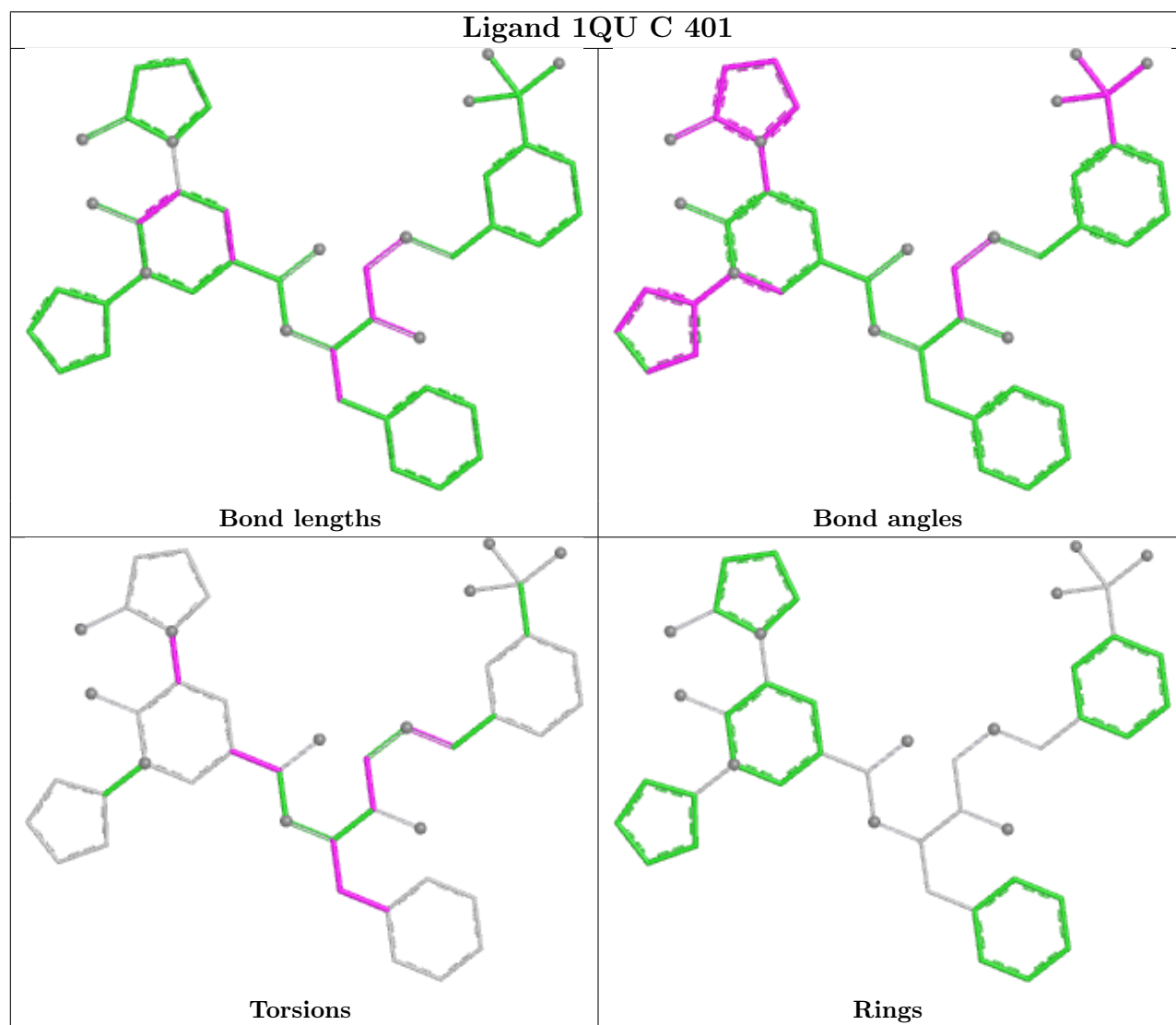
There are no ring outliers.

2 monomers are involved in 5 short contacts:

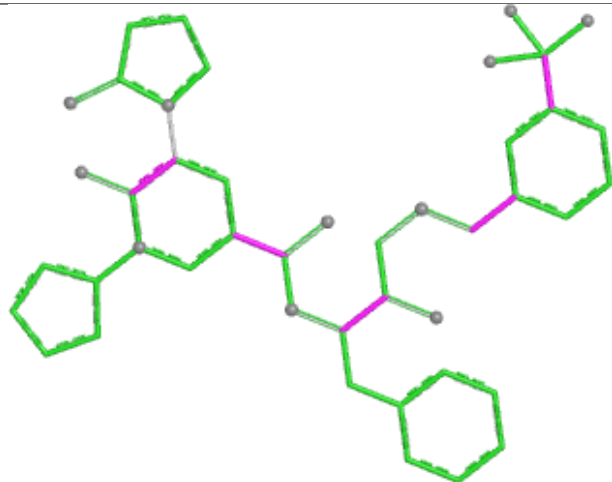
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	1QU	2	0
2	B	401	1QU	3	0

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.

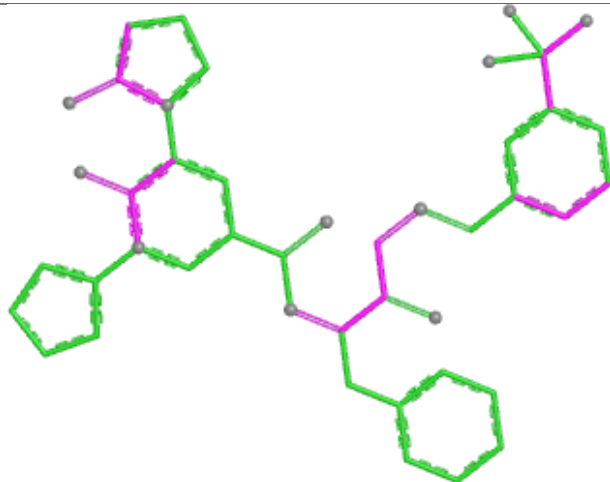
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



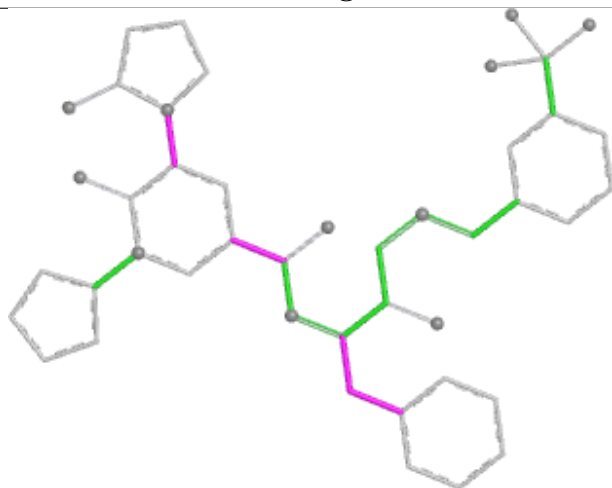
Ligand 1QU A 401



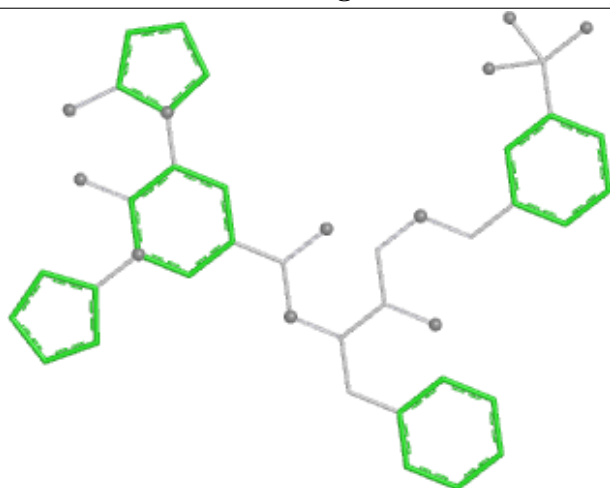
Bond lengths



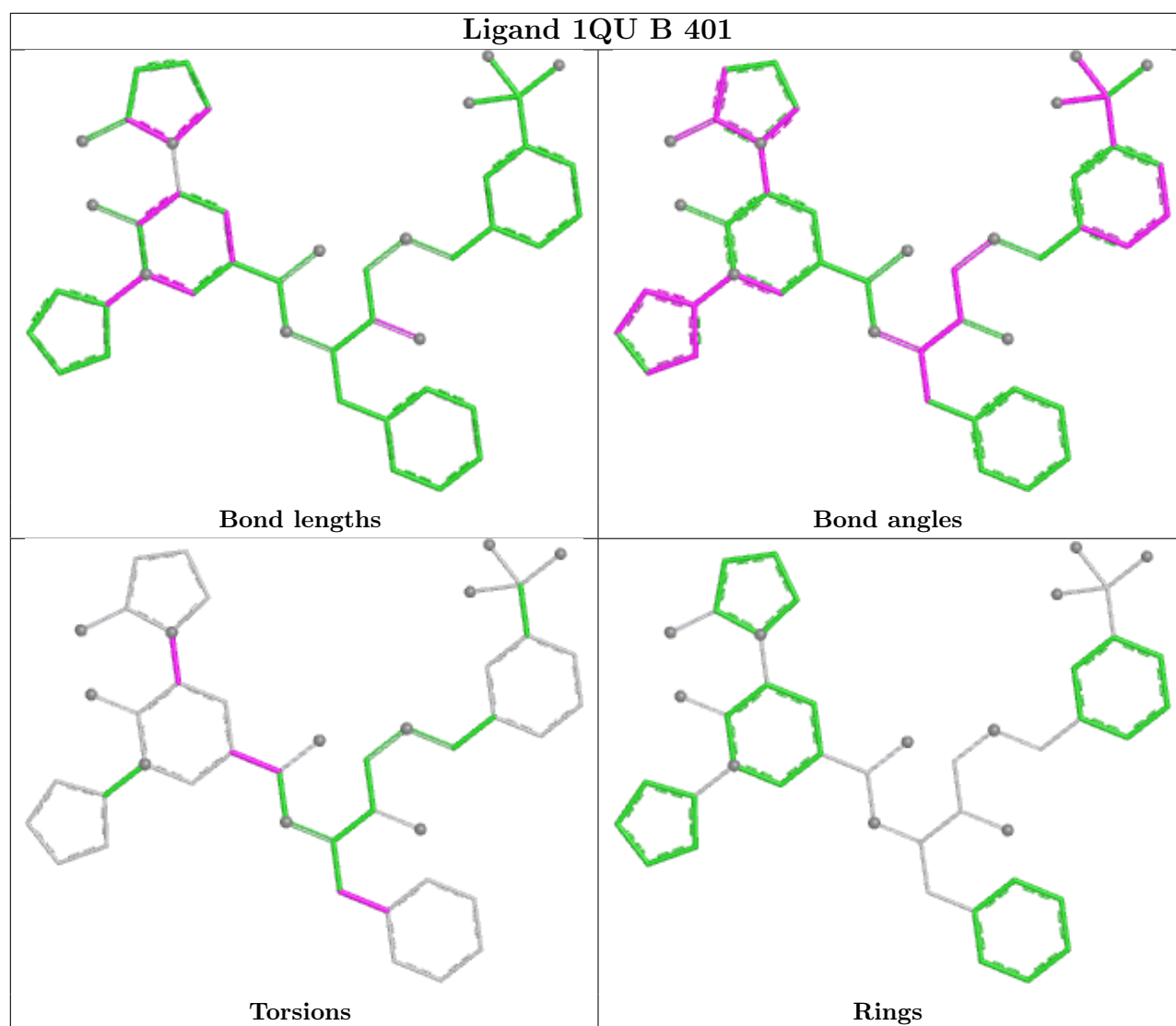
Bond angles



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	370/388 (95%)	0.24	18 (4%) 35 36	26, 45, 84, 116	0
1	B	369/388 (95%)	0.04	12 (3%) 49 51	25, 41, 72, 112	0
1	C	370/388 (95%)	0.11	21 (5%) 29 31	27, 43, 75, 104	0
All	All	1109/1164 (95%)	0.13	51 (4%) 37 39	25, 43, 78, 116	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	7.5
1	B	361	VAL	6.1
1	A	309	VAL	6.1
1	B	10	SER	5.6
1	A	361	VAL	5.0
1	C	-2	SER	4.7
1	C	361	VAL	4.7
1	C	10	SER	4.5
1	C	157	ALA	4.4
1	A	362	HIS	4.3
1	B	170	VAL	4.2
1	B	365	PHE	4.2
1	C	365	PHE	3.6
1	C	362	HIS	3.5
1	B	157	ALA	3.5
1	B	309	VAL	3.5
1	B	49	HIS	3.4
1	B	362	HIS	3.4
1	A	-2	SER	3.4
1	A	360	HIS	3.4
1	C	254	THR	3.1
1	C	170	VAL	3.0
1	A	272	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	309	VAL	2.7
1	B	7	ARG	2.7
1	A	365	PHE	2.6
1	A	273	GLY	2.6
1	A	56	LEU	2.6
1	C	319	CYS	2.6
1	A	317	ASP	2.5
1	B	9	LYS	2.5
1	C	214	LYS	2.5
1	C	360	HIS	2.5
1	A	49	HIS	2.5
1	B	256	LYS	2.3
1	A	169	SER	2.3
1	C	266	GLN	2.3
1	C	267	LEU	2.3
1	A	10	SER	2.3
1	C	272	ALA	2.3
1	C	258	PRO	2.2
1	A	319	CYS	2.2
1	B	265	GLU	2.2
1	A	254	THR	2.2
1	C	68	TYR	2.1
1	C	270	TRP	2.1
1	C	317	ASP	2.1
1	A	363	ASP	2.1
1	C	49	HIS	2.1
1	C	363	ASP	2.1
1	A	217	CYS	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,

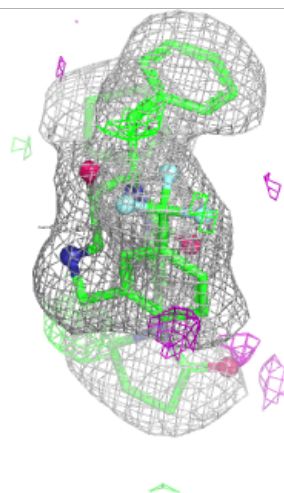
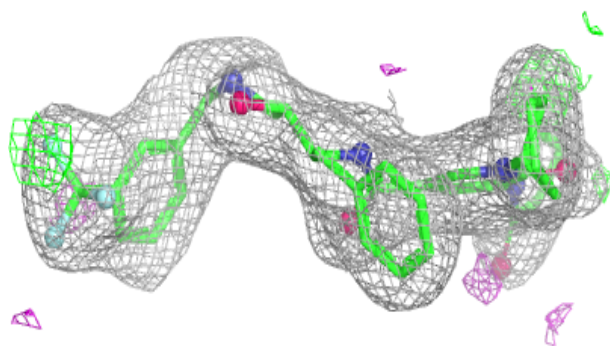
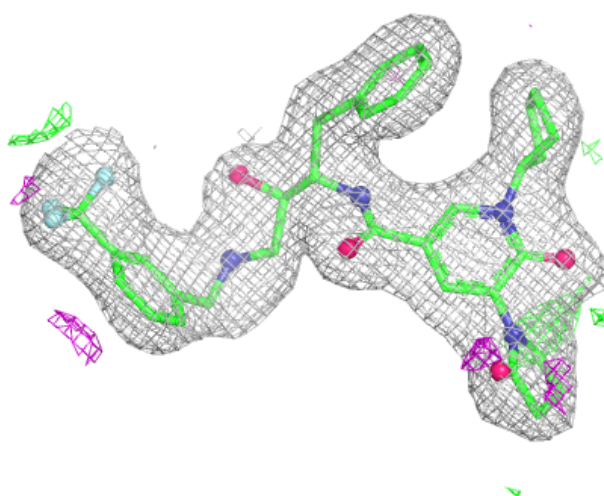
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	1QU	C	401	44/44	0.95	0.07	31,36,49,62	0
2	1QU	B	401	44/44	0.96	0.07	25,34,47,64	0
2	1QU	A	401	44/44	0.96	0.07	31,39,52,59	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.

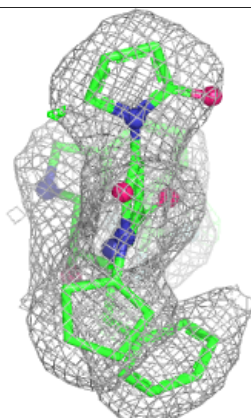
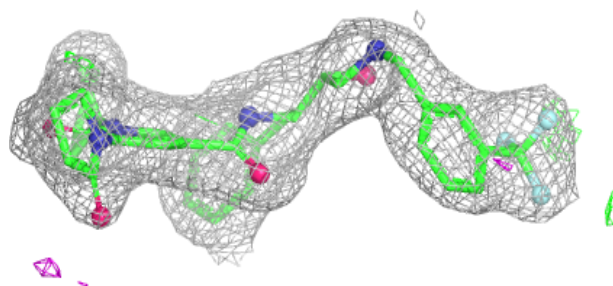
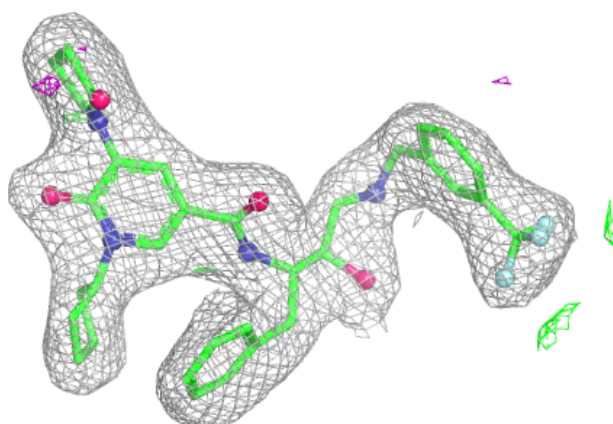
Electron density around 1QU C 401:

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

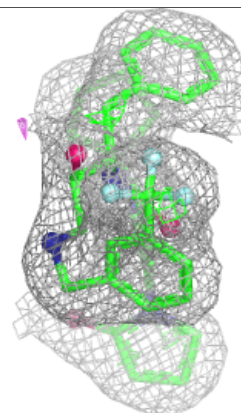
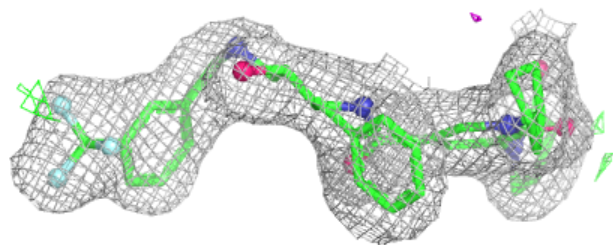
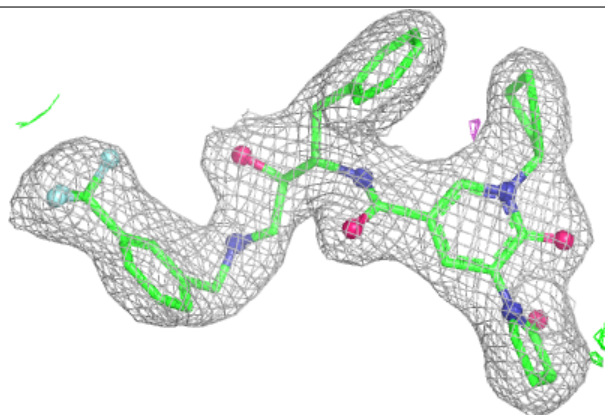


Electron density around 1QU B 401:

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

**Electron density around 1QU A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.