Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 08:30 AM EDT

PDB ID	:	4I0I
Title	:	SPR and structural analysis yield insight towards mechanism of inhibition of BACE inhibitors
Authors	:	Yao, N.; Brecht, E.
Deposited on	:	2012-11-16
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

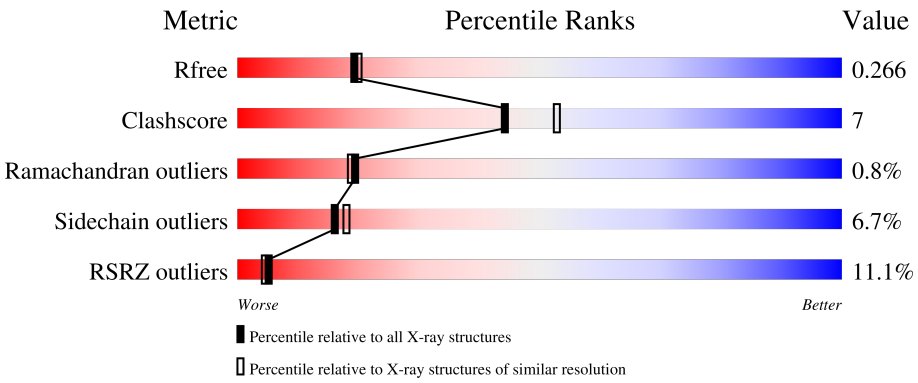
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	406	9% 75% 13% • • 8%
1	B	406	11% 71% 18% • 7%
1	C	406	11% 80% 10% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9293 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
			Total	C	N	O	S			
1	A	372	2928	1876	487	551	14	0	0	0
1	B	376	2958	1900	491	553	14	0	0	0
1	C	376	2958	1898	492	554	14	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P56817
A	399	ARG	-	EXPRESSION TAG	UNP P56817
A	400	SER	-	EXPRESSION TAG	UNP P56817
A	401	HIS	-	EXPRESSION TAG	UNP P56817
A	402	HIS	-	EXPRESSION TAG	UNP P56817
A	403	HIS	-	EXPRESSION TAG	UNP P56817
A	404	HIS	-	EXPRESSION TAG	UNP P56817
A	405	HIS	-	EXPRESSION TAG	UNP P56817
A	406	HIS	-	EXPRESSION TAG	UNP P56817
B	1	MET	-	EXPRESSION TAG	UNP P56817
B	399	ARG	-	EXPRESSION TAG	UNP P56817
B	400	SER	-	EXPRESSION TAG	UNP P56817
B	401	HIS	-	EXPRESSION TAG	UNP P56817
B	402	HIS	-	EXPRESSION TAG	UNP P56817
B	403	HIS	-	EXPRESSION TAG	UNP P56817
B	404	HIS	-	EXPRESSION TAG	UNP P56817
B	405	HIS	-	EXPRESSION TAG	UNP P56817
B	406	HIS	-	EXPRESSION TAG	UNP P56817
C	1	MET	-	EXPRESSION TAG	UNP P56817
C	399	ARG	-	EXPRESSION TAG	UNP P56817
C	400	SER	-	EXPRESSION TAG	UNP P56817
C	401	HIS	-	EXPRESSION TAG	UNP P56817
C	402	HIS	-	EXPRESSION TAG	UNP P56817

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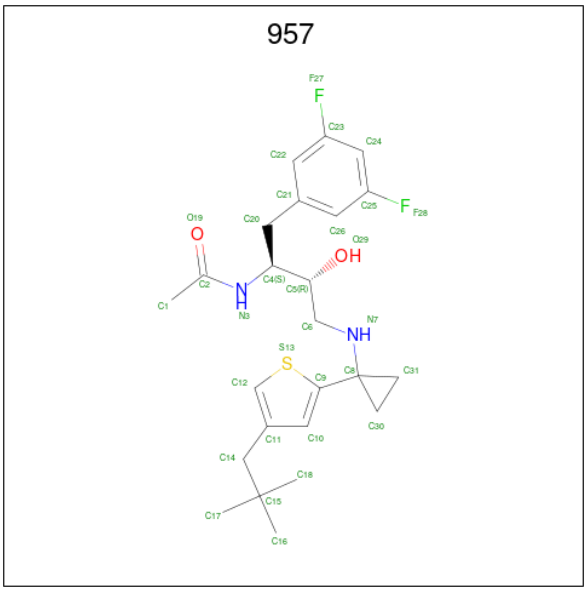
Chain	Residue	Modelled	Actual	Comment	Reference
C	403	HIS	-	EXPRESSION TAG	UNP P56817
C	404	HIS	-	EXPRESSION TAG	UNP P56817
C	405	HIS	-	EXPRESSION TAG	UNP P56817
C	406	HIS	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is N-[(1S,2R)-1-(3,5-difluorobenzyl)-3-({1-[4-(2,2-dimethylpropyl)thiophen-2-yl]cyclopropyl}amino)-2-hydroxypropyl]acetamide (three-letter code: 957) (formula: $C_{24}H_{32}F_2N_2O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	31	24	2	2	2	1	0	0
			Total	C	F	N	O	S		
2	B	1	31	24	2	2	2	1	0	0
			Total	C	F	N	O	S		
2	C	1	31	24	2	2	2	1	0	0

- Molecule 3 is water.

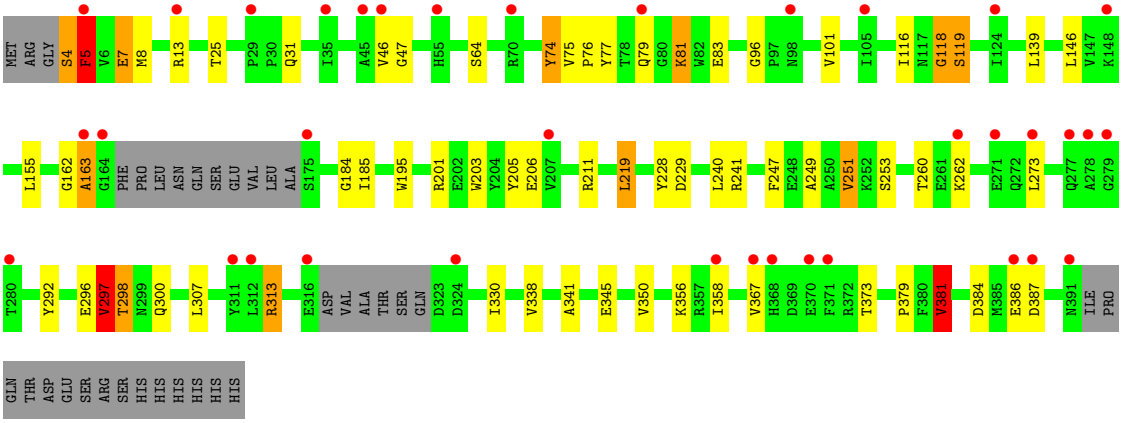
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	121	121	121	0	0
			Total	O		
3	B	108	108	108	0	0
			Total	O		
3	C	127	127	127	0	0

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.

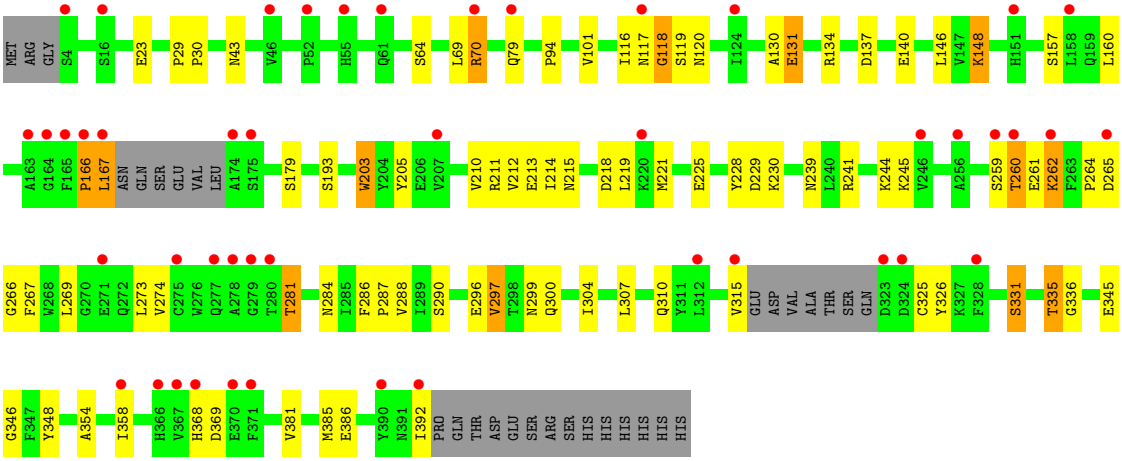
• Molecule 1: Beta-secretase 1

Chain A:



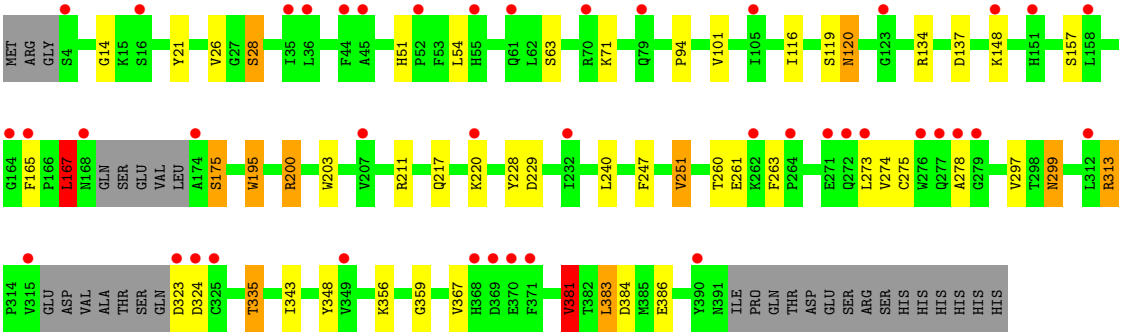
• Molecule 1: Beta-secretase 1

Chain B:



• Molecule 1: Beta-secretase 1

Chain C:


MET
ARG
GLY
S4
G14
K15
S16
Y21
V26
G27
S28
I35
L36
F44
A45
H51
P52
F53
L54
H55
Q61
L62
S63
R70
K71
Q79
P94
V101
I105
I116
S119
N120
G123
R134
D137
K148
H151
S157
L158
G164
F165
P166
L167
N168
GLN
SER
GLU
VAL
LEU
A174
S175
W195
R200
W203
V207
R211
Q217
K220
Y228
D229
I232
L240
F247
V251
T260
E261
K262
F263
P264
E271
Q272
L273
V274
C275
W276
Q277
A278
G279
V297
T298
N299
L312
R313
P314
V315
GLU
ASP
VAL
ALA
THR
SER
GLN
D323
D324
C325
T335
I343
Y348
V349
K356
G359
V367
H368
D369
E370
F371
V381
T382
L383
D384
M385
E386
Y390
N391
ILE
PRO
GLN
THR
ASP
GLU
SER
ARG
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.16Å 104.59Å 100.16Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-2.20) 96.5 (19.90-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.231 , 0.279 0.220 , 0.266	Depositor DCC
R_{free} test set	4011 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9293	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 957

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	1.08	5/3002 (0.2%)	0.98	5/4077 (0.1%)
1	B	1.09	3/3034 (0.1%)	0.97	2/4122 (0.0%)
1	C	1.05	1/3034 (0.0%)	0.99	12/4122 (0.3%)
All	All	1.07	9/9070 (0.1%)	0.98	19/12321 (0.2%)

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	A	0	2
1	B	0	3
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	TRP	CE3-CZ3	6.64	1.49	1.38
1	B	386	GLU	CG-CD	6.45	1.61	1.51
1	B	354	ALA	CA-CB	5.87	1.64	1.52
1	A	201	ARG	CG-CD	5.84	1.66	1.51
1	A	297	VAL	CB-CG1	-5.67	1.41	1.52
1	A	206	GLU	CG-CD	5.62	1.60	1.51
1	A	74	TYR	CD2-CE2	5.60	1.47	1.39
1	B	386	GLU	CB-CG	5.41	1.62	1.52
1	A	249	ALA	CA-CB	5.27	1.63	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	200	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	C	167	LEU	CA-CB-CG	8.53	134.92	115.30
1	A	381	VAL	CB-CA-C	-6.94	98.21	111.40
1	C	381	VAL	CB-CA-C	-6.73	98.61	111.40
1	C	200	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	C	175	SER	N-CA-C	6.59	128.79	111.00
1	C	211	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	118	GLY	N-CA-C	-5.84	98.49	113.10
1	C	211	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	313	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	C	381	VAL	CG1-CB-CG2	5.54	119.77	110.90
1	A	201	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	C	134	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	C	137	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	201	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	137	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	119	SER	N-CA-C	5.27	125.22	111.00
1	C	313	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	313	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLY	Peptide
1	A	4	SER	Peptide
1	B	117	ASN	Peptide
1	B	203	TRP	Peptide
1	B	346	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	2928	0	2839	43	0
1	B	2958	0	2876	56	0
1	C	2958	0	2871	23	0
2	A	31	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	32	1	0
2	C	31	0	32	0	0
3	A	121	0	0	5	0
3	B	108	0	0	9	1
3	C	127	0	0	2	1
All	All	9293	0	8682	117	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (117) 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:A:5:PHE:HB3	3:A:695:HOH:O	1.48	1.10
1:B:215:ASN:HA	3:B:604:HOH:O	1.58	1.01
1:B:166:PRO:O	1:B:167:LEU:HB2	1.70	0.91
1:C:335:THR:HG23	3:C:704:HOH:O	1.69	0.91
1:A:381:VAL:HG22	1:C:381:VAL:HG22	1.56	0.88
1:B:118:GLY:CA	3:B:632:HOH:O	2.21	0.88
1:B:119:SER:HA	3:B:632:HOH:O	1.78	0.84
1:A:155:LEU:HD22	1:A:184:GLY:HA2	1.61	0.83
1:B:214:ILE:HD12	1:B:219:LEU:HD13	1.62	0.79
1:B:43:ASN:HD21	1:B:134:ARG:H	1.33	0.75
1:B:118:GLY:HA3	3:B:632:HOH:O	1.85	0.70
1:A:296:GLU:H	1:A:300:GLN:HE22	1.39	0.70
1:B:119:SER:CA	3:B:632:HOH:O	2.39	0.69
1:B:23:GLU:HG2	1:B:94:PRO:HG2	1.74	0.69
1:C:260:THR:O	1:C:261:GLU:HG3	1.92	0.67
1:A:4:SER:O	1:A:4:SER:OG	2.01	0.67
1:A:155:LEU:CD2	1:A:184:GLY:HA2	2.24	0.67
1:A:247:PHE:O	1:A:251:VAL:CG1	2.45	0.65
1:B:213:GLU:OE1	3:B:627:HOH:O	2.13	0.64
1:C:275:CYS:HA	1:C:324:ASP:O	1.99	0.62
1:B:214:ILE:HD12	1:B:219:LEU:CD1	2.30	0.62
1:A:116:ILE:O	1:A:119:SER:HB2	1.98	0.62
1:A:8:MET:HG2	1:A:96:GLY:HA2	1.83	0.61
1:B:166:PRO:O	1:B:167:LEU:CB	2.46	0.61
1:A:247:PHE:O	1:A:251:VAL:HG13	2.01	0.59
1:B:211:ARG:NH1	1:C:384:ASP:OD1	2.35	0.59
1:A:162:GLY:O	1:A:163:ALA:HB3	2.04	0.58
1:A:356:LYS:HD3	3:A:666:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:VAL:O	1:B:325:CYS:HB2	2.04	0.57
1:A:7:GLU:HB2	3:A:695:HOH:O	2.04	0.56
1:C:119:SER:O	1:C:120:ASN:HB2	2.06	0.56
1:C:247:PHE:O	1:C:251:VAL:HG13	2.06	0.56
1:B:335:THR:HG23	3:B:679:HOH:O	2.05	0.56
1:C:157:SER:HB2	1:C:348:TYR:CE1	2.40	0.56
1:B:296:GLU:H	1:B:300:GLN:HE22	1.53	0.55
1:B:281:THR:HG21	1:B:326:TYR:CE1	2.41	0.54
1:B:335:THR:CG2	3:B:679:HOH:O	2.55	0.54
1:B:239:ASN:HD22	1:B:331:SER:HB3	1.72	0.54
1:A:5:PHE:CB	3:A:695:HOH:O	2.27	0.54
1:C:299:ASN:HB3	1:C:381:VAL:HG13	1.89	0.54
1:B:116:ILE:O	1:B:119:SER:HB3	2.08	0.52
1:C:299:ASN:HA	1:C:381:VAL:HA	1.91	0.52
1:B:210:VAL:HG11	1:B:385:MET:HG2	1.92	0.52
1:B:221:MET:HE2	1:B:225:GLU:CB	2.40	0.52
1:B:140:GLU:OE1	1:B:148:LYS:HE3	2.09	0.52
1:C:28:SER:O	1:C:63:SER:HA	2.09	0.52
1:A:195:TRP:CZ3	1:B:297:VAL:HG13	2.45	0.52
1:A:241:ARG:HB2	1:A:338:VAL:HB	1.92	0.52
1:A:25:THR:HA	1:A:31:GLN:O	2.11	0.51
1:A:247:PHE:O	1:A:251:VAL:HG12	2.11	0.51
1:A:240:LEU:O	1:A:330:ILE:HA	2.12	0.50
1:A:162:GLY:O	1:A:163:ALA:CB	2.59	0.50
1:A:101:VAL:HG11	1:A:146:LEU:HA	1.93	0.50
2:B:501:957:H18A	2:B:501:957:C10	2.42	0.50
1:B:211:ARG:HG2	1:B:212:VAL:N	2.26	0.50
1:A:4:SER:N	1:A:185:ILE:O	2.45	0.49
1:A:5:PHE:HD1	3:A:695:HOH:O	1.96	0.49
1:B:211:ARG:NH2	1:B:218:ASP:HB2	2.27	0.49
1:B:160:LEU:O	1:B:345:GLU:HA	2.13	0.49
1:B:288:VAL:HG12	1:B:307:LEU:HD23	1.94	0.48
1:A:155:LEU:CD2	1:A:184:GLY:CA	2.91	0.48
1:C:165:PHE:O	1:C:167:LEU:HD22	2.13	0.47
1:C:14:GLY:HA2	1:C:21:TYR:CE2	2.49	0.47
1:C:195:TRP:O	1:C:359:GLY:HA2	2.16	0.46
1:A:384:ASP:HB3	1:A:387:ASP:OD1	2.14	0.46
1:A:298:THR:HG23	3:B:657:HOH:O	2.15	0.46
1:B:221:MET:HE2	1:B:225:GLU:HB2	1.98	0.46
1:B:281:THR:CG2	1:B:326:TYR:CE1	2.98	0.46
1:B:392:ILE:H	1:B:392:ILE:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ILE:HB	1:C:119:SER:HB3	1.98	0.46
1:A:298:THR:HG21	1:B:193:SER:HB3	1.98	0.46
1:B:267:PHE:CD1	1:B:274:VAL:HG23	2.51	0.46
1:A:46:VAL:O	1:A:47:GLY:C	2.52	0.45
1:A:77:TYR:CG	2:A:501:957:H26	2.52	0.45
1:B:221:MET:CE	1:B:225:GLU:HG3	2.46	0.45
1:A:297:VAL:H	1:A:300:GLN:NE2	2.13	0.45
1:B:262:LYS:N	1:B:262:LYS:HD2	2.31	0.45
1:B:264:PRO:C	1:B:266:GLY:H	2.20	0.45
1:B:273:LEU:H	1:B:273:LEU:HD12	1.81	0.45
1:C:299:ASN:CB	1:C:381:VAL:HG13	2.47	0.45
1:B:307:LEU:N	1:B:310:GLN:OE1	2.49	0.44
1:C:228:TYR:HA	1:C:229:ASP:HA	1.73	0.44
1:A:76:PRO:HA	1:A:81:LYS:HB3	2.00	0.43
1:B:335:THR:HG23	1:B:335:THR:O	2.18	0.43
1:A:211:ARG:HB3	1:A:292:TYR:HB2	2.00	0.43
1:A:219:LEU:HA	1:A:219:LEU:HD12	1.60	0.43
1:B:230:LYS:O	1:B:336:GLY:HA3	2.19	0.43
1:B:273:LEU:HD12	1:B:273:LEU:N	2.33	0.43
1:B:259:SER:O	1:B:261:GLU:N	2.51	0.43
1:A:74:TYR:HA	1:A:83:GLU:HA	2.01	0.43
1:B:241:ARG:HA	1:B:331:SER:O	2.19	0.43
1:C:299:ASN:C	1:C:299:ASN:HD22	2.22	0.43
1:B:381:VAL:CG2	1:C:383:LEU:HD13	2.49	0.43
1:B:286:PHE:HA	1:B:287:PRO:HD3	1.89	0.42
1:B:101:VAL:HG11	1:B:146:LEU:HA	2.01	0.42
1:A:139:LEU:HD12	1:A:139:LEU:HA	1.91	0.42
1:B:157:SER:HB2	1:B:348:TYR:CE1	2.54	0.42
1:B:299:ASN:O	1:B:381:VAL:HA	2.19	0.42
1:B:205:TYR:HB3	1:B:358:ILE:HD11	2.00	0.42
1:A:379:PRO:HG2	1:B:381:VAL:HG12	2.00	0.42
1:B:221:MET:HE2	1:B:225:GLU:HG3	2.01	0.42
1:B:228:TYR:HA	1:B:229:ASP:HA	1.77	0.42
1:A:228:TYR:HA	1:A:229:ASP:HA	1.74	0.42
1:B:130:ALA:O	1:B:131:GLU:C	2.57	0.42
1:A:296:GLU:N	1:A:300:GLN:HE22	2.12	0.41
1:A:205:TYR:HB3	1:A:358:ILE:HD11	2.02	0.41
1:B:290:SER:HA	1:B:304:ILE:O	2.20	0.41
1:C:263:PHE:CD2	1:C:274:VAL:HG21	2.56	0.41
1:A:75:VAL:HA	1:A:76:PRO:HD3	1.78	0.41
1:C:51:HIS:HB3	1:C:54:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:THR:CG2	3:C:704:HOH:O	2.46	0.41
1:A:341:ALA:O	1:A:345:GLU:HG3	2.21	0.40
1:A:350:VAL:O	1:A:358:ILE:HA	2.21	0.40
1:A:307:LEU:HD12	1:A:367:VAL:HG23	2.02	0.40
1:B:29:PRO:HA	1:B:30:PRO:HD3	1.96	0.40
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.84	0.40
1:C:240:LEU:HB2	1:C:343:ILE:HD11	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:671:HOH:O	3:C:656:HOH:O[1_455]	2.04	0.16

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	366/406 (90%)	347 (95%)	16 (4%)	3 (1%)	19 19
1	B	370/406 (91%)	349 (94%)	16 (4%)	5 (1%)	11 8
1	C	370/406 (91%)	343 (93%)	26 (7%)	1 (0%)	41 46
All	All	1106/1218 (91%)	1039 (94%)	58 (5%)	9 (1%)	19 19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	PRO
1	A	118	GLY
1	B	260	THR
1	B	265	ASP
1	C	278	ALA

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Mol	Chain	Res	Type
1	A	163	ALA
1	A	5	PHE
1	B	70	ARG
1	B	369	ASP

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	317/348 (91%)	298 (94%)	19 (6%)	19 22
1	B	320/348 (92%)	300 (94%)	20 (6%)	18 20
1	C	320/348 (92%)	295 (92%)	25 (8%)	12 13
All	All	957/1044 (92%)	893 (93%)	64 (7%)	16 18

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	7	GLU
1	A	13	ARG
1	A	64	SER
1	A	79	GLN
1	A	81	LYS
1	A	203	TRP
1	A	219	LEU
1	A	251	VAL
1	A	253	SER
1	A	260	THR
1	A	262	LYS
1	A	273	LEU
1	A	297	VAL
1	A	298	THR
1	A	313	ARG
1	A	373	THR
1	A	381	VAL

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Mol	Chain	Res	Type
1	A	386	GLU
1	B	64	SER
1	B	70	ARG
1	B	79	GLN
1	B	120	ASN
1	B	131	GLU
1	B	148	LYS
1	B	167	LEU
1	B	179	SER
1	B	203	TRP
1	B	244	LYS
1	B	245	LYS
1	B	260	THR
1	B	262	LYS
1	B	269	LEU
1	B	281	THR
1	B	284	ASN
1	B	297	VAL
1	B	331	SER
1	B	335	THR
1	B	368	HIS
1	C	26	VAL
1	C	28	SER
1	C	71	LYS
1	C	94	PRO
1	C	101	VAL
1	C	120	ASN
1	C	148	LYS
1	C	167	LEU
1	C	175	SER
1	C	200	ARG
1	C	203	TRP
1	C	217	GLN
1	C	220	LYS
1	C	251	VAL
1	C	273	LEU
1	C	297	VAL
1	C	299	ASN
1	C	313	ARG
1	C	323	ASP
1	C	335	THR
1	C	356	LYS

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Mol	Chain	Res	Type
1	C	367	VAL
1	C	381	VAL
1	C	383	LEU
1	C	386	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	284	ASN
1	A	300	GLN
1	B	43	ASN
1	B	104	ASN
1	B	300	GLN
1	B	366	HIS
1	C	104	ASN
1	C	117	ASN
1	C	217	GLN
1	C	299	ASN
1	C	300	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 monosaccharides 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	957	C	501	-	31,33,33	2.30	10 (32%)	41,49,49	2.29	16 (39%)
2	957	B	501	-	31,33,33	2.33	6 (19%)	41,49,49	2.28	12 (29%)
2	957	A	501	-	31,33,33	1.85	7 (22%)	41,49,49	2.10	12 (29%)

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	957	C	501	-	-	1/19/33/33	0/3/3/3
2	957	B	501	-	-	0/19/33/33	0/3/3/3
2	957	A	501	-	-	0/19/33/33	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	957	C12-C11	8.12	1.42	1.37
2	C	501	957	C12-C11	6.43	1.41	1.37
2	A	501	957	F28-C25	5.80	1.50	1.36
2	B	501	957	F28-C25	5.59	1.49	1.36
2	B	501	957	F27-C23	5.46	1.49	1.36
2	C	501	957	F28-C25	5.43	1.49	1.36
2	C	501	957	F27-C23	4.90	1.48	1.36
2	A	501	957	F27-C23	3.78	1.45	1.36
2	A	501	957	C12-C11	3.74	1.39	1.37
2	B	501	957	C31-C8	3.60	1.55	1.51
2	C	501	957	C12-S13	3.28	1.75	1.70
2	C	501	957	C26-C25	3.19	1.43	1.37
2	C	501	957	C30-C8	3.02	1.54	1.51
2	A	501	957	C30-C8	2.70	1.54	1.51
2	C	501	957	C31-C30	2.63	1.56	1.50
2	C	501	957	C22-C23	2.45	1.41	1.37
2	A	501	957	C31-C8	2.45	1.53	1.51
2	C	501	957	C14-C11	2.35	1.55	1.51
2	C	501	957	C31-C8	2.25	1.53	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	957	C5-C4	-2.10	1.50	1.53
2	B	501	957	C22-C23	2.07	1.41	1.37
2	A	501	957	C26-C25	2.06	1.41	1.37
2	B	501	957	C14-C15	-2.00	1.50	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	957	C14-C11-C12	-9.40	118.35	128.09
2	C	501	957	C30-C8-N7	-5.98	111.62	117.30
2	C	501	957	C31-C8-N7	5.54	122.56	117.30
2	B	501	957	C21-C20-C4	-4.92	105.06	113.40
2	C	501	957	C30-C8-C9	-4.79	111.02	119.36
2	A	501	957	C31-C8-N7	4.69	121.75	117.30
2	C	501	957	C14-C11-C12	-4.55	123.38	128.09
2	A	501	957	C21-C20-C4	-4.53	105.72	113.40
2	A	501	957	F28-C25-C26	4.52	124.70	118.28
2	A	501	957	C14-C11-C12	-4.33	123.60	128.09
2	C	501	957	C10-C9-C8	-4.26	122.62	128.15
2	B	501	957	C11-C12-S13	-3.71	107.96	112.05
2	A	501	957	C10-C9-C8	-3.69	123.36	128.15
2	A	501	957	F27-C23-C22	3.34	123.02	118.28
2	A	501	957	C26-C25-C24	-3.27	119.53	123.50
2	B	501	957	C25-C24-C23	3.09	120.59	116.08
2	B	501	957	F27-C23-C22	2.97	122.50	118.28
2	C	501	957	C20-C4-N3	-2.90	105.97	110.08
2	B	501	957	C24-C23-C22	-2.81	120.08	123.50
2	B	501	957	C26-C25-C24	-2.71	120.21	123.50
2	A	501	957	C25-C24-C23	2.71	120.03	116.08
2	A	501	957	C30-C8-C9	-2.70	114.66	119.36
2	A	501	957	C14-C11-C10	-2.62	122.57	127.47
2	C	501	957	C21-C20-C4	-2.57	109.03	113.40
2	C	501	957	C14-C11-C10	-2.46	122.87	127.47
2	A	501	957	C31-C8-C9	-2.42	115.15	119.36
2	C	501	957	C31-C30-C8	-2.41	59.20	60.23
2	C	501	957	C31-C8-C9	-2.36	115.25	119.36
2	C	501	957	C26-C25-C24	-2.30	120.71	123.50
2	C	501	957	F28-C25-C26	2.26	121.49	118.28
2	C	501	957	C11-C12-S13	-2.26	109.57	112.05
2	C	501	957	C31-C8-C30	2.22	61.08	59.09
2	A	501	957	C24-C23-C22	-2.21	120.82	123.50
2	B	501	957	O19-C2-C1	-2.19	118.15	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	957	F27-C23-C22	2.19	121.39	118.28
2	B	501	957	C10-C9-C8	-2.18	125.32	128.15
2	B	501	957	C31-C8-C9	-2.11	115.69	119.36
2	B	501	957	C1-C2-N3	2.08	119.57	116.12
2	B	501	957	F28-C25-C26	2.04	121.18	118.28
2	C	501	957	C18-C15-C14	2.02	114.59	109.87

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	957	C5-C6-N7-C8

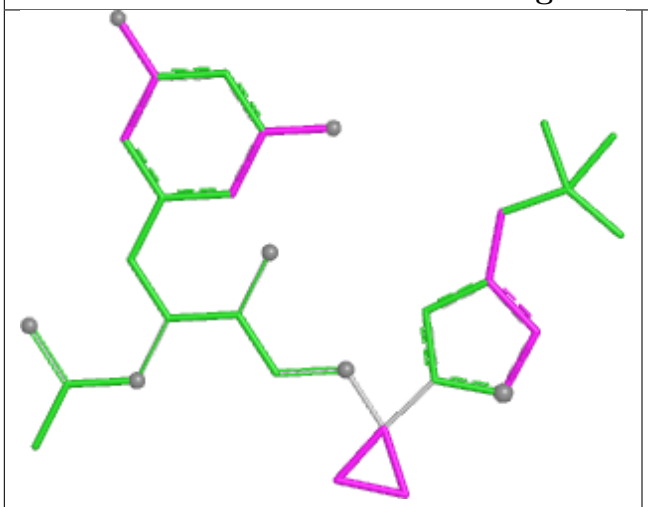
There are no ring outliers.

2 monomers are involved in 2 short contacts:

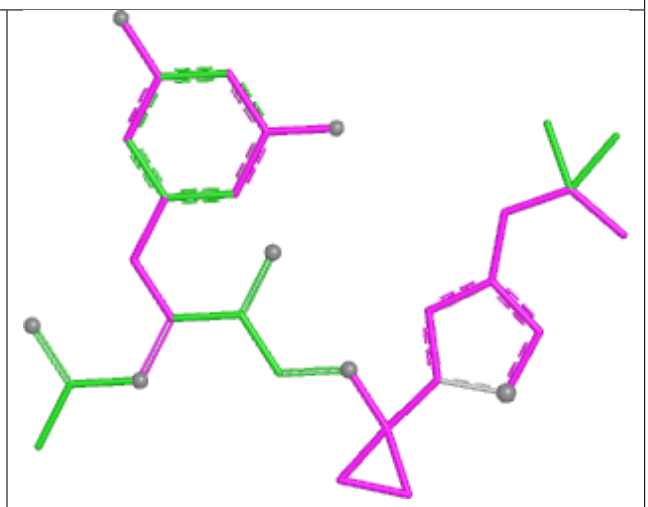
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	957	1	0
2	A	501	957	1	0

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 then 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.

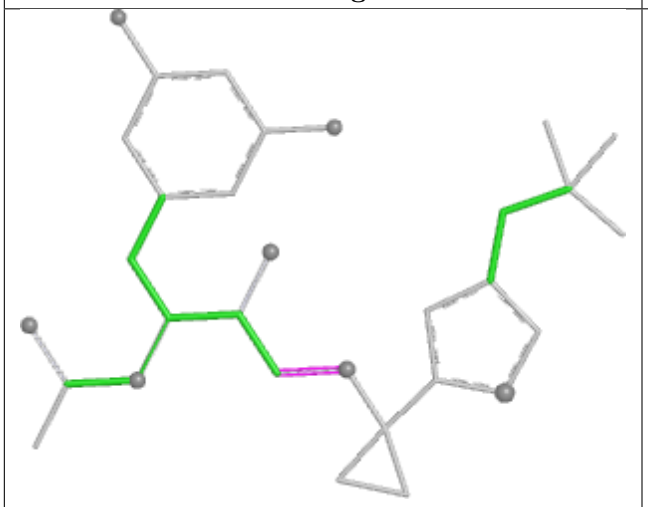
Ligand 957 C 501



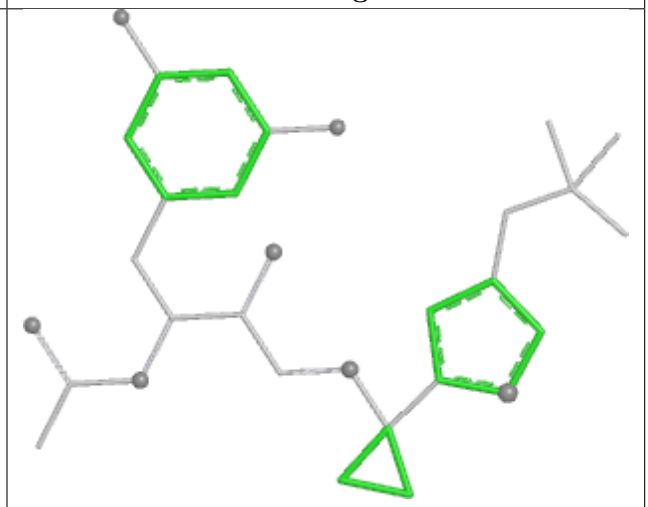
Bond lengths



Bond angles

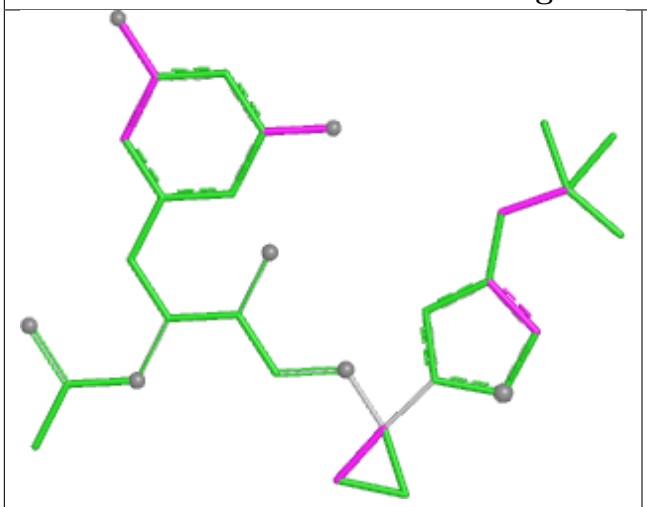


Torsions

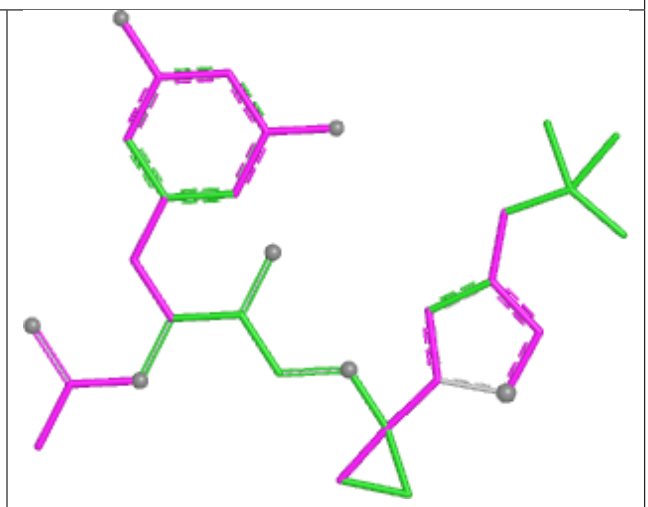


Rings

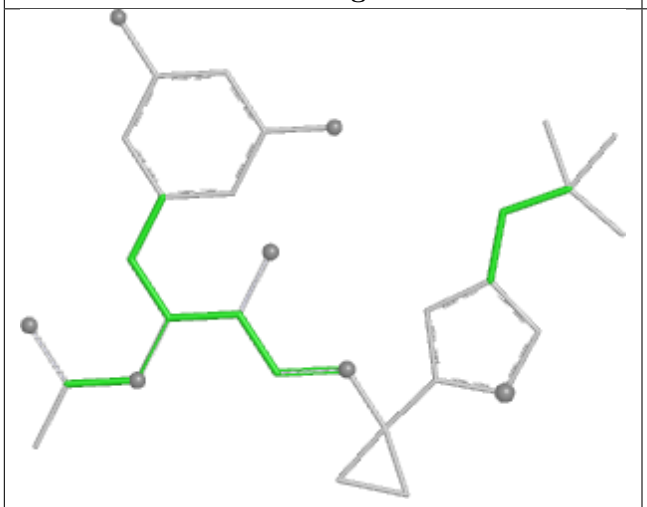
Ligand 957 B 501



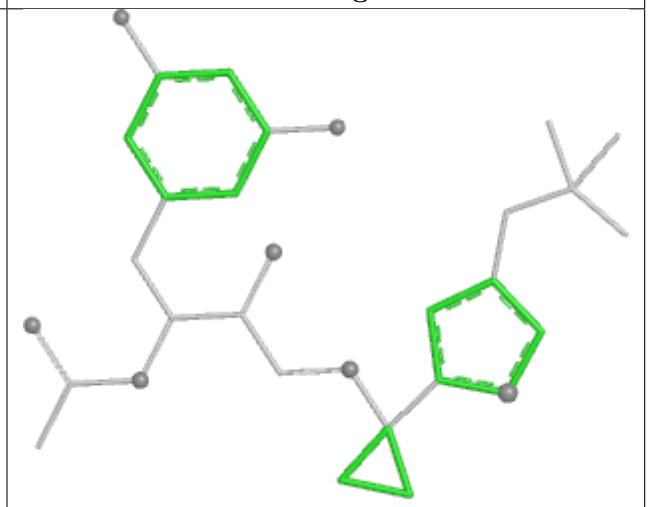
Bond lengths



Bond angles

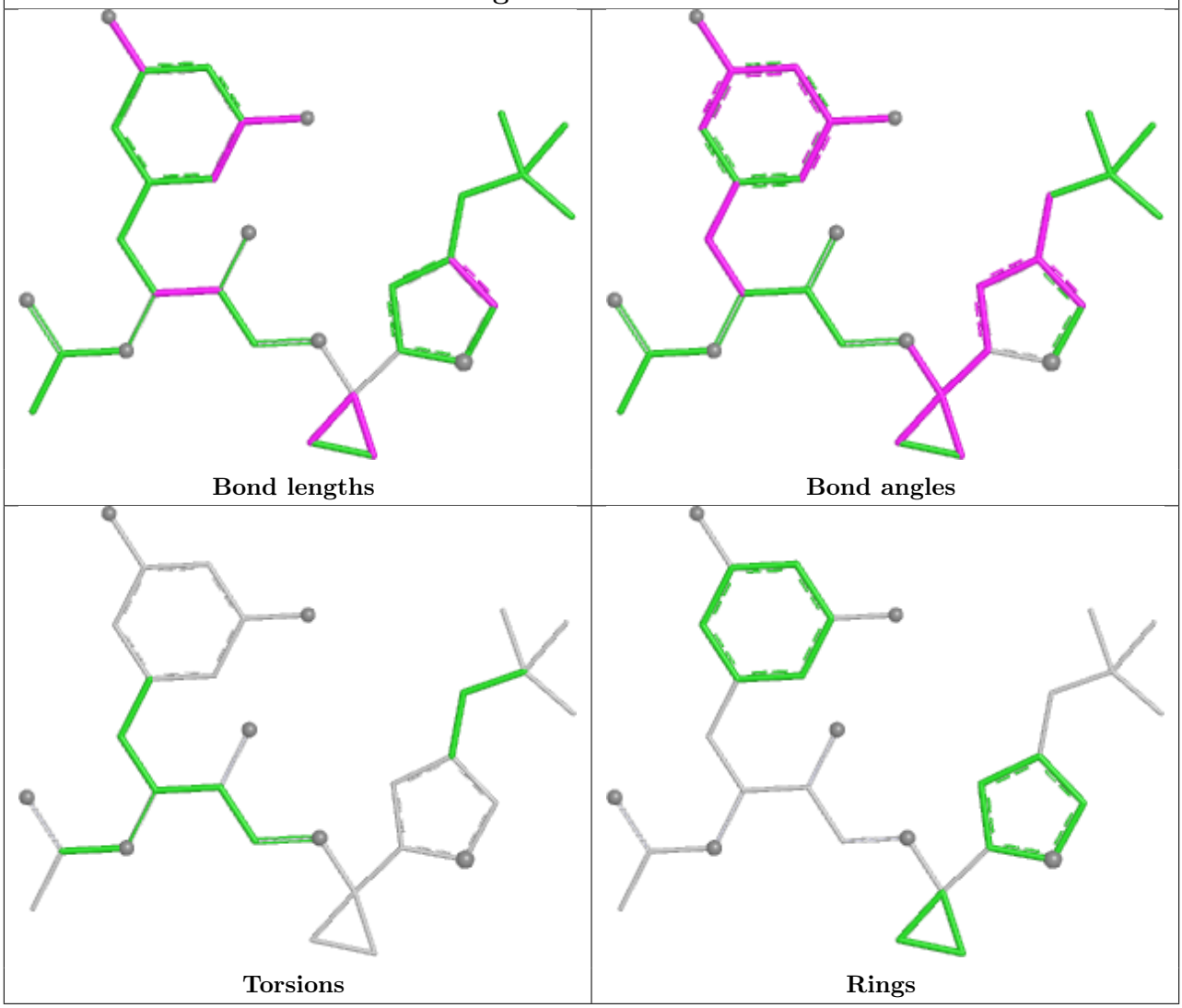


Torsions



Rings

Ligand 957 A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	372/406 (91%)	0.44	36 (9%) 7 6	34, 51, 81, 89	0
1	B	376/406 (92%)	0.57	46 (12%) 4 3	33, 52, 84, 93	0
1	C	376/406 (92%)	0.43	43 (11%) 5 4	36, 50, 81, 90	0
All	All	1124/1218 (92%)	0.48	125 (11%) 5 4	33, 51, 82, 93	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	7.3
1	C	368	HIS	6.0
1	A	164	GLY	5.8
1	C	371	PHE	5.4
1	A	279	GLY	5.3
1	B	392	ILE	5.3
1	C	325	CYS	5.1
1	C	278	ALA	5.1
1	B	260	THR	4.9
1	B	165	PHE	4.7
1	A	371	PHE	4.6
1	B	166	PRO	4.6
1	B	279	GLY	4.5
1	B	371	PHE	4.4
1	B	278	ALA	4.3
1	A	370	GLU	4.3
1	C	370	GLU	4.2
1	C	4	SER	4.0
1	A	368	HIS	4.0
1	B	164	GLY	3.9
1	B	315	VAL	3.8
1	B	4	SER	3.7
1	B	151	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	262	LYS	3.6
1	B	368	HIS	3.5
1	C	262	LYS	3.4
1	C	151	HIS	3.4
1	C	315	VAL	3.4
1	A	386	GLU	3.4
1	B	323	ASP	3.3
1	A	70	ARG	3.3
1	B	277	GLN	3.3
1	C	164	GLY	3.2
1	C	271	GLU	3.2
1	C	70	ARG	3.2
1	B	370	GLU	3.1
1	A	316	GLU	3.1
1	B	16	SER	3.1
1	C	272	GLN	3.1
1	B	52	PRO	3.1
1	B	271	GLU	3.1
1	C	16	SER	3.0
1	C	279	GLY	3.0
1	B	367	VAL	3.0
1	A	262	LYS	3.0
1	A	277	GLN	3.0
1	C	174	ALA	2.9
1	B	124	ILE	2.9
1	A	5	PHE	2.9
1	B	175	SER	2.9
1	B	366	HIS	2.9
1	B	167	LEU	2.8
1	B	324	ASP	2.8
1	C	349	VAL	2.8
1	B	312	LEU	2.8
1	A	98	ASN	2.8
1	A	387	ASP	2.7
1	A	367	VAL	2.7
1	B	220	LYS	2.7
1	B	259	SER	2.7
1	C	79	GLN	2.7
1	C	312	LEU	2.7
1	A	105	ILE	2.6
1	A	124	ILE	2.6
1	C	168	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	55	HIS	2.6
1	B	328	PHE	2.6
1	B	265	ASP	2.6
1	B	207	VAL	2.6
1	C	369	ASP	2.6
1	B	55	HIS	2.5
1	C	207	VAL	2.5
1	B	61	GLN	2.5
1	B	79	GLN	2.5
1	A	280	THR	2.5
1	B	70	ARG	2.5
1	C	105	ILE	2.5
1	A	163	ALA	2.4
1	B	46	VAL	2.4
1	A	391	ASN	2.4
1	A	358	ILE	2.4
1	B	158	LEU	2.4
1	A	55	HIS	2.4
1	B	246	VAL	2.4
1	B	280	THR	2.4
1	A	278	ALA	2.4
1	A	175	SER	2.4
1	C	323	ASP	2.4
1	A	312	LEU	2.3
1	C	232	ILE	2.3
1	C	35	ILE	2.3
1	A	324	ASP	2.3
1	C	276	TRP	2.3
1	B	390	TYR	2.3
1	A	13	ARG	2.3
1	A	29	PRO	2.3
1	A	79	GLN	2.2
1	C	277	GLN	2.2
1	A	35	ILE	2.2
1	A	311	TYR	2.2
1	A	46	VAL	2.2
1	B	358	ILE	2.2
1	C	273	LEU	2.2
1	B	256	ALA	2.2
1	C	220	LYS	2.2
1	C	148	LYS	2.1
1	C	45	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	158	LEU	2.1
1	A	271	GLU	2.1
1	C	61	GLN	2.1
1	C	324	ASP	2.1
1	C	52	PRO	2.1
1	B	275	CYS	2.1
1	C	44	PHE	2.1
1	C	123	GLY	2.1
1	A	273	LEU	2.0
1	B	117	ASN	2.0
1	A	207	VAL	2.0
1	A	45	ALA	2.0
1	B	163	ALA	2.0
1	C	264	PRO	2.0
1	A	148	LYS	2.0
1	C	165	PHE	2.0
1	C	390	TYR	2.0
1	C	36	LEU	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 monosaccharides 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.

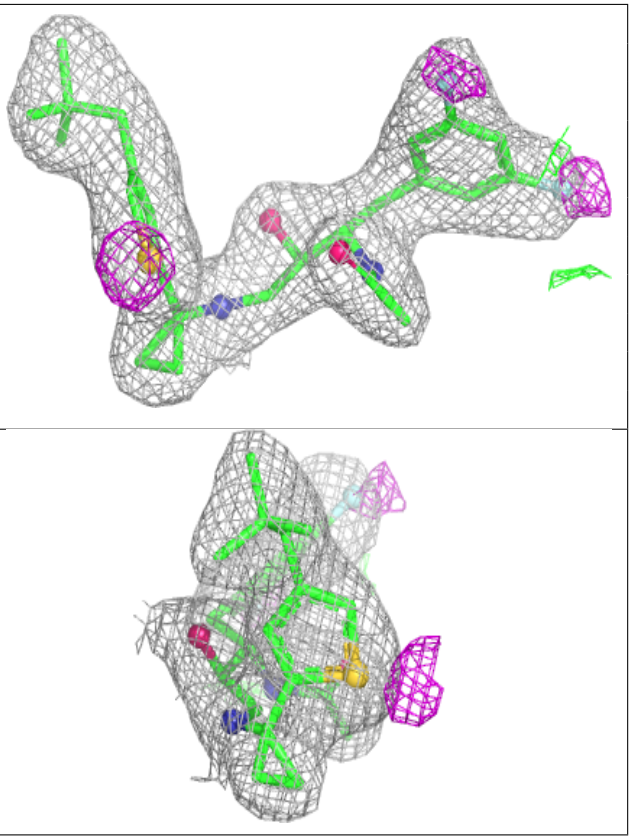
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	957	A	501	31/31	0.96	0.12	32,42,46,50	0
2	957	B	501	31/31	0.96	0.12	35,43,47,50	0
2	957	C	501	31/31	0.96	0.11	32,37,41,42	0

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.

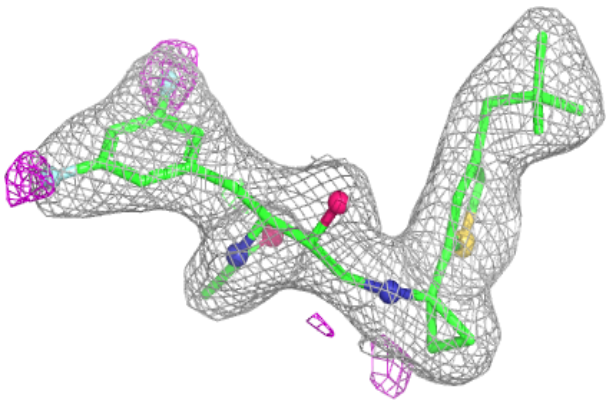
Electron density around 957 A 501:

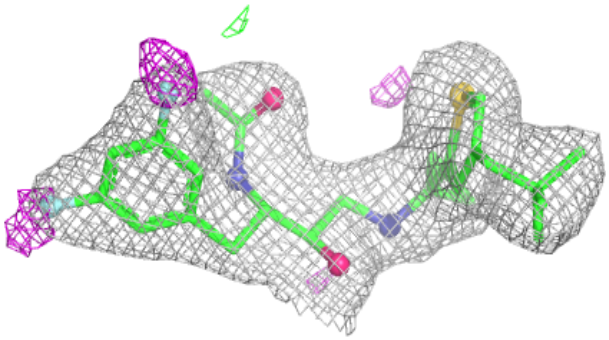
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

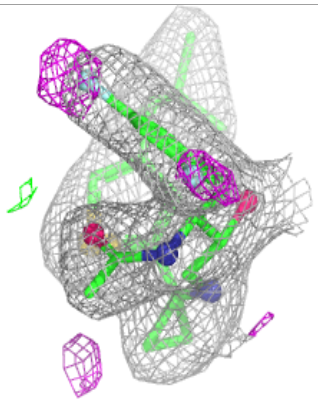


Electron density around 957 B 501:

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

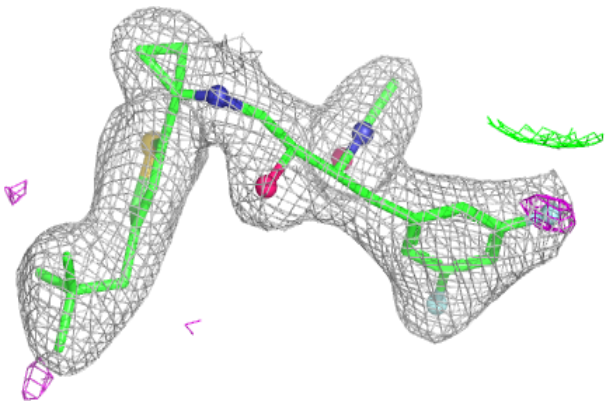


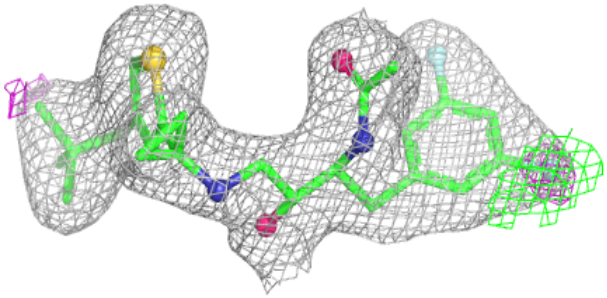




Electron density around 957 C 501:

$2mF_o$-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.