



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 05:19 PM EDT

PDB ID : 3VQS
Title : Crystal structure of HCV NS5B RNA polymerase with a novel piperazine inhibitor
Authors : Adachi, T.; Doi, S.; Ando, I.; Sugimoto, K.; Orita, T.; Nomura, A.; Kamada, M.
Deposited on : 2012-03-30
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4.02b-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

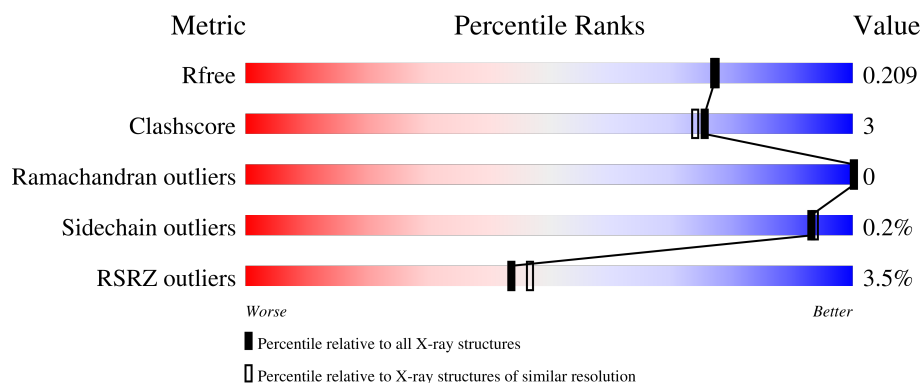
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	578	
1	B	578	
1	C	578	
1	D	578	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19445 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	21	0
			4451	2798	784	835	34			
1	B	557	Total	C	N	O	S	0	14	0
			4425	2786	780	826	33			
1	C	556	Total	C	N	O	S	0	22	0
			4477	2814	789	840	34			
1	D	553	Total	C	N	O	S	0	19	0
			4437	2790	785	827	35			

There are 32 discrepancies between the modelled and reference sequences:

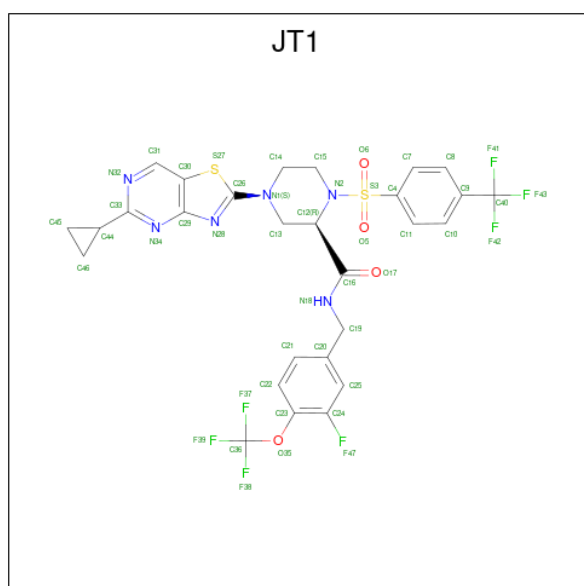
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	GLY	-	EXPRESSION TAG	UNP D0PY27
A	572	SER	-	EXPRESSION TAG	UNP D0PY27
A	573	HIS	-	EXPRESSION TAG	UNP D0PY27
A	574	HIS	-	EXPRESSION TAG	UNP D0PY27
A	575	HIS	-	EXPRESSION TAG	UNP D0PY27
A	576	HIS	-	EXPRESSION TAG	UNP D0PY27
A	577	HIS	-	EXPRESSION TAG	UNP D0PY27
A	578	HIS	-	EXPRESSION TAG	UNP D0PY27
B	571	GLY	-	EXPRESSION TAG	UNP D0PY27
B	572	SER	-	EXPRESSION TAG	UNP D0PY27
B	573	HIS	-	EXPRESSION TAG	UNP D0PY27
B	574	HIS	-	EXPRESSION TAG	UNP D0PY27
B	575	HIS	-	EXPRESSION TAG	UNP D0PY27
B	576	HIS	-	EXPRESSION TAG	UNP D0PY27
B	577	HIS	-	EXPRESSION TAG	UNP D0PY27
B	578	HIS	-	EXPRESSION TAG	UNP D0PY27
C	571	GLY	-	EXPRESSION TAG	UNP D0PY27
C	572	SER	-	EXPRESSION TAG	UNP D0PY27
C	573	HIS	-	EXPRESSION TAG	UNP D0PY27
C	574	HIS	-	EXPRESSION TAG	UNP D0PY27
C	575	HIS	-	EXPRESSION TAG	UNP D0PY27

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Chain	Residue	Modelled	Actual	Comment	Reference
C	576	HIS	-	EXPRESSION TAG	UNP D0PY27
C	577	HIS	-	EXPRESSION TAG	UNP D0PY27
C	578	HIS	-	EXPRESSION TAG	UNP D0PY27
D	571	GLY	-	EXPRESSION TAG	UNP D0PY27
D	572	SER	-	EXPRESSION TAG	UNP D0PY27
D	573	HIS	-	EXPRESSION TAG	UNP D0PY27
D	574	HIS	-	EXPRESSION TAG	UNP D0PY27
D	575	HIS	-	EXPRESSION TAG	UNP D0PY27
D	576	HIS	-	EXPRESSION TAG	UNP D0PY27
D	577	HIS	-	EXPRESSION TAG	UNP D0PY27
D	578	HIS	-	EXPRESSION TAG	UNP D0PY27

- Molecule 2 is (2R)-4-(5-cyclopropyl[1,3]thiazolo[4,5-d]pyrimidin-2-yl)-N-[3-fluoro-4-(trifluoromethoxy)benzyl]-1-{[4-(trifluoromethyl)phenyl]sulfonyl}piperazine-2-carboxamide (three-letter code: JT1) (formula: C₂₈H₂₃F₇N₆O₄S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			47	28	7	6	4	2		
2	B	1	Total	C	F	N	O	S	0	0
			47	28	7	6	4	2		
2	C	1	Total	C	F	N	O	S	0	0
			47	28	7	6	4	2		
2	D	1	Total	C	F	N	O	S	0	0
			47	28	7	6	4	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0

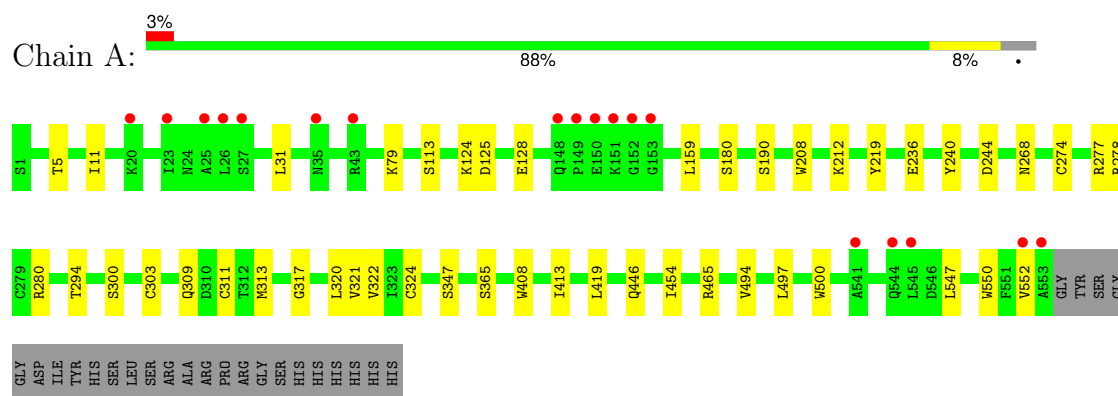
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	367	Total 367	O 367	0	0
4	B	374	Total 374	O 374	0	0
4	C	336	Total 336	O 336	0	0
4	D	388	Total 388	O 388	0	0

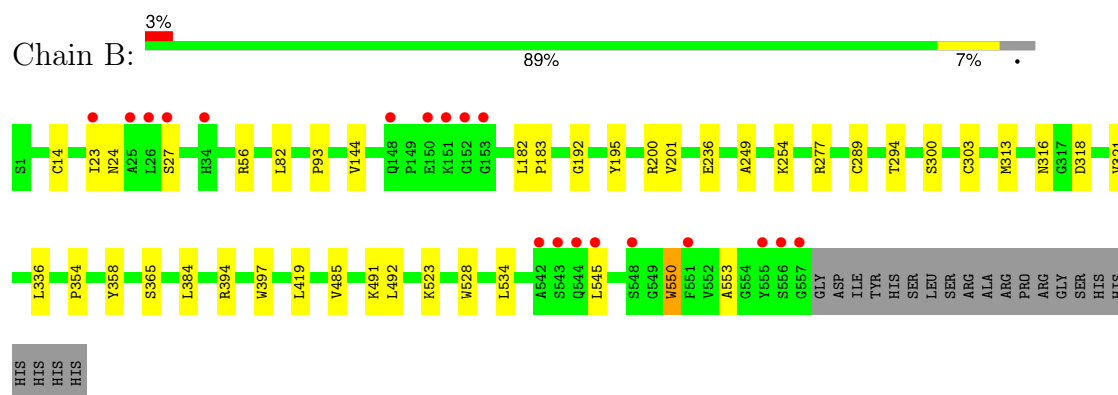
3 Residue-property plots [i](#)

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.

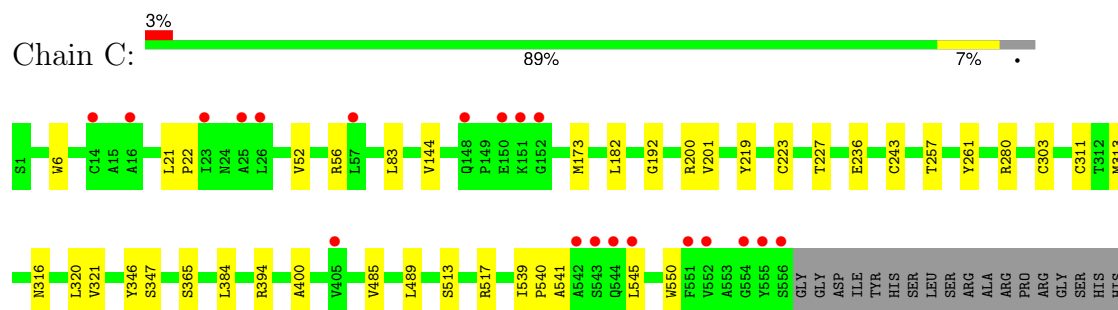
• Molecule 1: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase

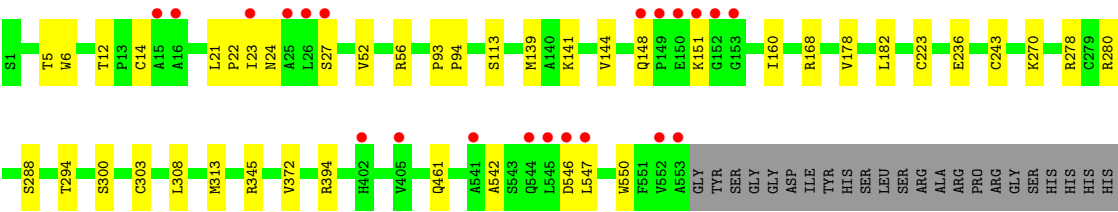
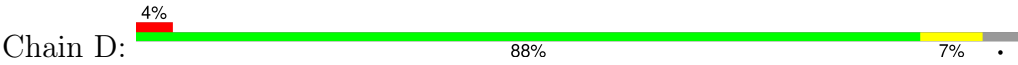


• Molecule 1: RNA-directed RNA polymerase



HIS
HIS
HIS
HIS

● Molecule 1: RNA-directed RNA polymerase



HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.12Å 101.18Å 250.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.97 – 1.90 93.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (93.97-1.90) 100.0 (93.79-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.204 0.174 , 0.209	Depositor DCC
R_{free} test set	10170 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19445	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.76% 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: CL, JT1

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	1.05	9/4544 (0.2%)	0.86	2/6168 (0.0%)
1	B	1.03	5/4519 (0.1%)	0.85	2/6134 (0.0%)
1	C	1.02	2/4571 (0.0%)	0.85	1/6207 (0.0%)
1	D	1.07	4/4531 (0.1%)	0.89	3/6149 (0.0%)
All	All	1.04	20/18165 (0.1%)	0.86	8/24658 (0.0%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	TRP	CD2-CE2	5.83	1.48	1.41
1	A	408	TRP	CG-CD1	5.76	1.44	1.36
1	B	550	TRP	CD2-CE2	5.63	1.48	1.41
1	A	500	TRP	CD2-CE2	5.51	1.48	1.41
1	A	408	TRP	CD2-CE2	5.48	1.48	1.41
1	B	195	TYR	CE1-CZ	5.45	1.45	1.38
1	A	317	GLY	N-CA	5.36	1.54	1.46
1	D	113	SER	CB-OG	5.34	1.49	1.42
1	A	550	TRP	CD2-CE2	5.34	1.47	1.41
1	B	397	TRP	CD2-CE2	5.33	1.47	1.41
1	A	113	SER	CA-CB	5.30	1.60	1.52
1	C	550	TRP	CD2-CE2	5.22	1.47	1.41
1	D	6	TRP	CD2-CE2	5.20	1.47	1.41
1	A	277	ARG	CZ-NH2	5.17	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	550	TRP	CD2-CE2	5.15	1.47	1.41
1	D	288	SER	CA-CB	5.13	1.60	1.52
1	A	208	TRP	CD2-CE2	5.07	1.47	1.41
1	A	190	SER	CB-OG	5.02	1.48	1.42
1	B	358	TYR	CE1-CZ	-5.02	1.32	1.38
1	B	528	TRP	CD2-CE2	5.00	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	280	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	D	345	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	277	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	517	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	318	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	125	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	465	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	168	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	SER	Mainchain

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	4451	0	4451	25	0
1	B	4425	0	4433	27	0
1	C	4477	0	4474	26	0
1	D	4437	0	4441	29	0
2	A	47	0	22	1	0
2	B	47	0	22	0	0
2	C	47	0	22	0	0
2	D	47	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	367	0	0	1	0
4	B	374	0	0	0	0
4	C	336	0	0	0	0
4	D	388	0	0	2	0
All	All	19445	0	17887	106	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 3.

All (106) 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:201[B]:VAL:HG12	1:C:384:LEU:HG	1.38	1.06
1:A:303[B]:CYS:SG	1:A:313:MET:CE	2.43	1.06
1:A:303[B]:CYS:SG	1:A:313:MET:HE1	1.97	1.03
1:C:201[B]:VAL:CG1	1:C:384:LEU:HG	2.03	0.89
1:D:148:GLN:HB2	1:D:151:LYS:HG3	1.59	0.85
1:A:303[B]:CYS:SG	1:A:313:MET:HE2	2.16	0.84
1:C:303[B]:CYS:HG	1:C:311[B]:CYS:HG	1.33	0.76
1:D:303[B]:CYS:SG	1:D:313:MET:CE	2.75	0.75
1:D:546:ASP:O	1:D:547:LEU:HG	1.87	0.73
1:D:303[B]:CYS:SG	1:D:313:MET:HE1	2.30	0.71
1:C:303[B]:CYS:SG	1:C:313:MET:CE	2.80	0.70
1:D:5:THR:HG23	1:D:278:ARG:HH12	1.57	0.69
1:C:303[B]:CYS:SG	1:C:313:MET:HE2	2.34	0.67
1:D:148:GLN:HB2	1:D:151:LYS:CG	2.25	0.66
1:D:303[B]:CYS:SG	1:D:313:MET:HE2	2.36	0.66
1:D:24:ASN:HB3	1:D:27:SER:HB3	1.77	0.65
1:C:236[A]:GLU:OE2	1:C:280:ARG:NH2	2.21	0.64
1:D:24:ASN:HB3	1:D:27:SER:CB	2.28	0.64
1:D:182[B]:LEU:HD12	1:D:243:CYS:SG	2.39	0.63
1:D:300:SER:HA	1:D:313:MET:HE3	1.81	0.62
1:B:24:ASN:HB3	1:B:27:SER:HB3	1.82	0.61
1:A:236[A]:GLU:OE2	1:A:280:ARG:NH2	2.26	0.61
1:D:547:LEU:O	1:D:547:LEU:HD12	2.02	0.59
1:B:93:PRO:HA	1:B:553:ALA:CB	2.33	0.59
1:C:303[B]:CYS:SG	1:C:313:MET:HE1	2.42	0.59
1:B:321[A]:VAL:CG2	1:B:365:SER:HB3	2.33	0.58
1:C:182[B]:LEU:C	1:C:182[B]:LEU:HD23	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182[B]:LEU:HD12	1:C:243:CYS:SG	2.44	0.58
1:A:5:THR:HG23	1:A:278:ARG:HH12	1.69	0.57
1:C:541:ALA:HB1	1:C:545:LEU:HD13	1.85	0.57
1:D:182[B]:LEU:C	1:D:182[B]:LEU:HD23	2.25	0.57
1:D:52:VAL:HG12	1:D:223[B]:CYS:SG	2.46	0.55
1:D:372:VAL:HG12	4:D:3293:HOH:O	2.06	0.55
1:B:200:ARG:HH12	1:B:316[A]:ASN:ND2	2.06	0.54
1:C:227:THR:HB	1:C:347:SER:O	2.08	0.54
1:C:219:TYR:HB3	1:C:320:LEU:HD23	1.91	0.53
1:B:303[B]:CYS:SG	1:B:313:MET:CE	2.97	0.53
1:B:236[A]:GLU:OE2	1:B:294:THR:OG1	2.25	0.52
1:C:52:VAL:HG12	1:C:223[B]:CYS:SG	2.49	0.52
1:B:192:GLY:HA3	1:B:316[A]:ASN:ND2	2.23	0.52
1:D:23:ILE:O	1:D:23:ILE:HG13	2.10	0.52
1:B:24:ASN:HB3	1:B:27:SER:CB	2.40	0.52
1:B:201[B]:VAL:CG2	1:B:384:LEU:HG	2.40	0.52
1:B:303[B]:CYS:SG	1:B:313:MET:HE2	2.51	0.51
1:A:347[A]:SER:O	1:A:347[A]:SER:OG	2.26	0.51
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.93	0.51
1:D:461:GLN:HB2	1:D:542:ALA:HA	1.92	0.51
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.94	0.50
1:D:236[A]:GLU:OE2	1:D:294:THR:OG1	2.27	0.50
1:C:200:ARG:HH12	1:C:316[B]:ASN:ND2	2.10	0.50
1:C:346:TYR:O	1:C:347:SER:HB3	2.11	0.49
1:D:144:VAL:HB	1:D:394:ARG:HG2	1.94	0.49
1:C:192:GLY:HA3	1:C:316[B]:ASN:ND2	2.27	0.49
1:B:321[A]:VAL:CG2	1:B:365:SER:CB	2.91	0.49
1:B:545:LEU:HD11	1:B:550:TRP:HH2	1.78	0.49
1:A:124:LYS:HE2	1:A:128[A]:GLU:OE2	2.14	0.48
1:D:24:ASN:CB	1:D:27:SER:HB3	2.43	0.47
1:C:21:LEU:HD12	1:C:22:PRO:HD2	1.97	0.47
1:C:83:LEU:HB2	1:C:173:MET:HA	1.96	0.47
1:C:321[B]:VAL:HG13	1:C:365:SER:HB3	1.96	0.47
1:D:12:THR:HG21	1:D:270:LYS:HD2	1.96	0.47
1:A:321[A]:VAL:CG2	1:A:365:SER:CB	2.94	0.46
1:B:491:LYS:HE2	1:B:492[B]:LEU:CD1	2.45	0.46
1:A:31:LEU:HB3	1:A:494:VAL:HG22	1.97	0.46
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.56	0.46
1:A:309[B]:GLN:O	1:A:324[B]:CYS:HB3	2.17	0.45
1:B:419[A]:LEU:HD22	1:B:485:VAL:HG21	1.98	0.45
1:B:523:LYS:HG3	1:B:534:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ILE:HG23	1:C:540:PRO:HD2	1.98	0.45
1:B:23:ILE:HD12	1:B:23:ILE:H	1.80	0.45
1:D:303[B]:CYS:SG	1:D:308:LEU:HD12	2.57	0.44
1:C:144:VAL:HB	1:C:394:ARG:HG2	1.99	0.44
1:B:545:LEU:HD11	1:B:550:TRP:CH2	2.52	0.44
1:B:300:SER:HA	1:B:313:MET:HE3	2.00	0.43
1:A:446:GLN:NE2	1:A:552:VAL:HG11	2.33	0.43
1:A:547:LEU:HB3	2:A:1000:JT1:H2	2.01	0.43
1:C:257:THR:HA	1:C:261:TYR:HB2	1.99	0.43
1:D:14:CYS:HB2	1:D:139:MET:CE	2.48	0.43
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.01	0.42
1:A:321[A]:VAL:HG22	1:A:365:SER:HB3	2.02	0.42
1:D:546:ASP:C	1:D:547:LEU:HG	2.40	0.42
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.59	0.42
1:A:419[B]:LEU:HD21	1:A:497:LEU:CD1	2.49	0.42
1:B:300:SER:HA	1:B:313:MET:CE	2.50	0.42
1:A:11:ILE:HD13	1:A:159:LEU:HD22	2.01	0.42
1:A:413:ILE:CD1	1:A:454[B]:ILE:HD13	2.49	0.42
4:A:3208:HOH:O	1:B:254:LYS:HE3	2.20	0.42
1:C:201[B]:VAL:HG12	1:C:384:LEU:CG	2.28	0.42
1:B:182:LEU:N	1:B:183:PRO:CD	2.84	0.41
1:A:212:LYS:HG3	1:C:513[A]:SER:O	2.19	0.41
1:B:201[B]:VAL:HG22	1:B:384:LEU:HG	2.02	0.41
1:B:303[B]:CYS:SG	1:B:313:MET:HE1	2.60	0.41
1:D:178:VAL:HG23	4:D:3088:HOH:O	2.20	0.41
1:A:236[A]:GLU:OE2	1:A:294:THR:OG1	2.34	0.41
1:A:311[B]:CYS:SG	1:A:322:VAL:CG1	3.09	0.41
1:D:93:PRO:HA	1:D:94:PRO:HD3	1.92	0.41
1:A:236[B]:GLU:HG2	1:A:240:TYR:CZ	2.56	0.41
1:D:14:CYS:HB2	1:D:139:MET:HE1	2.02	0.41
1:D:21:LEU:HD12	1:D:22:PRO:HD2	2.03	0.41
1:D:141:LYS:HD2	1:D:160[A]:ILE:HD11	2.03	0.41
1:A:300:SER:HA	1:A:313:MET:HE3	2.04	0.40
1:A:79:LYS:HA	1:A:244:ASP:HB3	2.02	0.40
1:A:236[B]:GLU:OE2	1:A:240:TYR:OH	2.34	0.40
1:B:336:LEU:HD21	1:B:354:PRO:HB2	2.03	0.40
1:C:22:PRO:HG2	1:C:400:ALA:HB1	2.03	0.40
1:C:485:VAL:O	1:C:489:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	572/578 (99%)	565 (99%)	7 (1%)	0	100	100
1	B	569/578 (98%)	563 (99%)	6 (1%)	0	100	100
1	C	576/578 (100%)	568 (99%)	8 (1%)	0	100	100
1	D	570/578 (99%)	566 (99%)	4 (1%)	0	100	100
All	All	2287/2312 (99%)	2262 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	493/492 (100%)	493 (100%)	0	100	100
1	B	488/492 (99%)	486 (100%)	2 (0%)	91	91
1	C	496/492 (101%)	495 (100%)	1 (0%)	93	94
1	D	491/492 (100%)	490 (100%)	1 (0%)	93	94
All	All	1968/1968 (100%)	1964 (100%)	4 (0%)	93	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	CYS
1	B	56	ARG

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Mol	Chain	Res	Type
1	C	56	ARG
1	D	56	ARG

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

Mol	Chain	Res	Type
1	A	49	GLN
1	B	446	GLN
1	D	446	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	JT1	C	601	-	45,52,52	1.98	11 (24%)	61,80,80	1.72	14 (22%)
2	JT1	D	1000	-	45,52,52	1.66	9 (20%)	61,80,80	1.76	13 (21%)
2	JT1	A	1000	-	45,52,52	1.87	8 (17%)	61,80,80	1.82	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	JT1	B	601	-	45,52,52	2.26	13 (28%)	61,80,80	1.93	11 (18%)

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	JT1	C	601	-	-	2/38/55/55	0/6/6/6
2	JT1	D	1000	-	-	2/38/55/55	0/6/6/6
2	JT1	A	1000	-	-	2/38/55/55	0/6/6/6
2	JT1	B	601	-	-	2/38/55/55	0/6/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	JT1	C4-S3	-6.88	1.67	1.76
2	A	1000	JT1	O6-S3	6.25	1.50	1.43
2	B	601	JT1	O5-S3	-6.14	1.37	1.43
2	B	601	JT1	C4-S3	-5.10	1.69	1.76
2	B	601	JT1	O6-S3	4.99	1.48	1.43
2	D	1000	JT1	C33-N32	4.68	1.41	1.34
2	A	1000	JT1	C4-S3	-4.33	1.70	1.76
2	B	601	JT1	C7-C4	4.21	1.45	1.38
2	A	1000	JT1	C13-C12	4.18	1.57	1.53
2	D	1000	JT1	C4-S3	-4.14	1.70	1.76
2	B	601	JT1	C23-C24	3.91	1.46	1.38
2	D	1000	JT1	O6-S3	3.81	1.47	1.43
2	B	601	JT1	C8-C7	3.75	1.44	1.38
2	C	601	JT1	C11-C4	3.67	1.44	1.38
2	B	601	JT1	C33-N32	3.42	1.39	1.34
2	C	601	JT1	O5-S3	-3.31	1.40	1.43
2	A	1000	JT1	C8-C7	3.22	1.44	1.38
2	A	1000	JT1	C29-N28	3.13	1.40	1.34
2	D	1000	JT1	S3-N2	-3.03	1.58	1.63
2	B	601	JT1	C31-N32	2.98	1.37	1.32
2	B	601	JT1	C15-N2	-2.94	1.42	1.48
2	D	1000	JT1	C13-C12	2.93	1.56	1.53
2	A	1000	JT1	O17-C16	2.91	1.29	1.23
2	B	601	JT1	C22-C21	2.70	1.43	1.38
2	C	601	JT1	O17-C16	2.69	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	JT1	C33-N32	2.64	1.38	1.34
2	B	601	JT1	C11-C4	2.63	1.43	1.38
2	C	601	JT1	F47-C24	-2.61	1.28	1.35
2	C	601	JT1	C7-C4	2.55	1.42	1.38
2	D	1000	JT1	C23-C24	2.53	1.43	1.38
2	C	601	JT1	C8-C7	2.48	1.42	1.38
2	C	601	JT1	C23-C24	2.38	1.43	1.38
2	D	1000	JT1	C22-C21	2.36	1.42	1.38
2	B	601	JT1	S3-N2	-2.33	1.59	1.63
2	A	1000	JT1	C16-N18	2.31	1.39	1.33
2	B	601	JT1	C22-C23	-2.24	1.34	1.39
2	A	1000	JT1	C7-C4	2.23	1.42	1.38
2	D	1000	JT1	C21-C20	2.13	1.43	1.38
2	C	601	JT1	C11-C10	2.10	1.42	1.38
2	D	1000	JT1	C8-C7	2.09	1.42	1.38
2	C	601	JT1	C21-C20	2.07	1.43	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	JT1	C10-C9-C8	5.72	126.56	118.03
2	D	1000	JT1	C20-C25-C24	-5.71	115.64	119.37
2	B	601	JT1	O6-S3-C4	-5.22	101.61	108.10
2	A	1000	JT1	C12-C13-N1	5.01	116.88	109.36
2	B	601	JT1	C12-C13-N1	4.95	116.80	109.36
2	D	1000	JT1	C12-C13-N1	4.92	116.75	109.36
2	C	601	JT1	C10-C9-C8	4.91	125.34	118.03
2	A	1000	JT1	C10-C9-C8	4.65	124.96	118.03
2	A	1000	JT1	C19-N18-C16	-4.55	116.03	122.29
2	B	601	JT1	C20-C19-N18	4.54	122.64	113.07
2	C	601	JT1	O6-S3-C4	-4.50	102.51	108.10
2	B	601	JT1	C7-C8-C9	-4.50	114.95	121.17
2	C	601	JT1	C11-C10-C9	-4.07	115.55	121.17
2	C	601	JT1	O35-C23-C24	3.91	119.17	116.29
2	B	601	JT1	C14-C15-N2	3.58	112.91	109.00
2	A	1000	JT1	C11-C10-C9	-3.46	116.39	121.17
2	A	1000	JT1	F43-C40-C9	3.43	120.23	112.90
2	D	1000	JT1	C10-C9-C8	3.39	123.08	118.03
2	D	1000	JT1	C21-C20-C25	3.38	123.22	118.55
2	D	1000	JT1	C7-C8-C9	-3.34	116.56	121.17
2	A	1000	JT1	O6-S3-C4	-3.31	103.98	108.10
2	D	1000	JT1	O6-S3-C4	-3.21	104.11	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	JT1	C12-C13-N1	3.16	114.11	109.36
2	D	1000	JT1	C14-C15-N2	2.95	112.23	109.00
2	A	1000	JT1	C15-N2-C12	2.94	122.45	114.89
2	A	1000	JT1	C10-C9-C40	-2.89	115.32	119.96
2	C	601	JT1	C20-C19-N18	2.85	119.08	113.07
2	C	601	JT1	C10-C9-C40	-2.83	115.41	119.96
2	A	1000	JT1	C31-N32-C33	2.83	120.74	116.06
2	C	601	JT1	C20-C25-C24	-2.71	117.60	119.37
2	B	601	JT1	C14-N1-C13	2.67	120.08	112.53
2	A	1000	JT1	C7-C8-C9	-2.62	117.56	121.17
2	B	601	JT1	O5-S3-N2	2.61	111.53	106.97
2	B	601	JT1	C8-C9-C40	-2.60	115.78	119.96
2	D	1000	JT1	C19-C20-C21	-2.52	115.80	120.94
2	C	601	JT1	C16-C12-N2	2.46	117.12	111.19
2	C	601	JT1	C14-N1-C13	2.33	119.13	112.53
2	A	1000	JT1	F47-C24-C25	2.33	123.29	118.64
2	A	1000	JT1	C22-C23-C24	2.31	121.49	118.04
2	D	1000	JT1	F41-C40-C9	2.30	117.83	112.90
2	C	601	JT1	C21-C20-C25	2.28	121.69	118.55
2	A	1000	JT1	C20-C19-N18	2.25	117.82	113.07
2	B	601	JT1	C15-N2-C12	2.22	120.61	114.89
2	B	601	JT1	O35-C23-C24	2.19	117.91	116.29
2	D	1000	JT1	C15-N2-S3	2.19	124.05	118.40
2	A	1000	JT1	C10-C11-C4	2.18	121.56	119.44
2	D	1000	JT1	C19-N18-C16	-2.18	119.29	122.29
2	C	601	JT1	C8-C7-C4	-2.12	117.37	119.44
2	D	1000	JT1	C11-C10-C9	-2.09	118.29	121.17
2	A	1000	JT1	C33-N34-C29	-2.08	113.65	115.47
2	A	1000	JT1	C25-C24-C23	-2.07	120.06	122.86
2	D	1000	JT1	C7-C4-S3	-2.05	117.70	119.73
2	C	601	JT1	C14-C15-N2	2.04	111.23	109.00
2	C	601	JT1	F43-C40-C9	2.03	117.24	112.90
2	A	1000	JT1	C14-N1-C13	2.01	118.24	112.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	JT1	C15-N2-S3-O5
2	D	1000	JT1	C15-N2-S3-O5
2	B	601	JT1	C15-N2-S3-O5
2	A	1000	JT1	C15-N2-S3-O5

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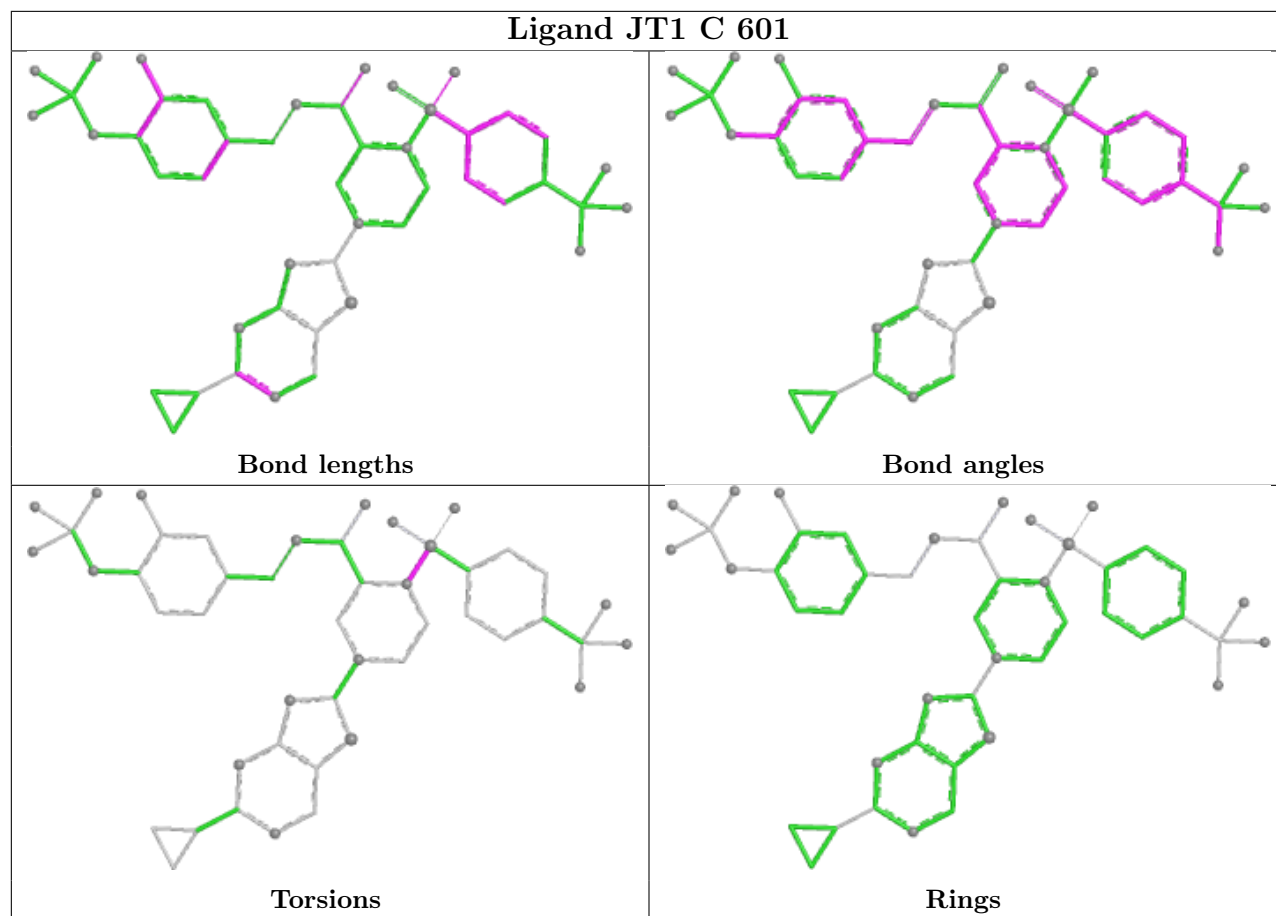
Mol	Chain	Res	Type	Atoms
2	B	601	JT1	C15-N2-S3-O6
2	D	1000	JT1	C15-N2-S3-O6
2	A	1000	JT1	C15-N2-S3-O6
2	C	601	JT1	C15-N2-S3-O6

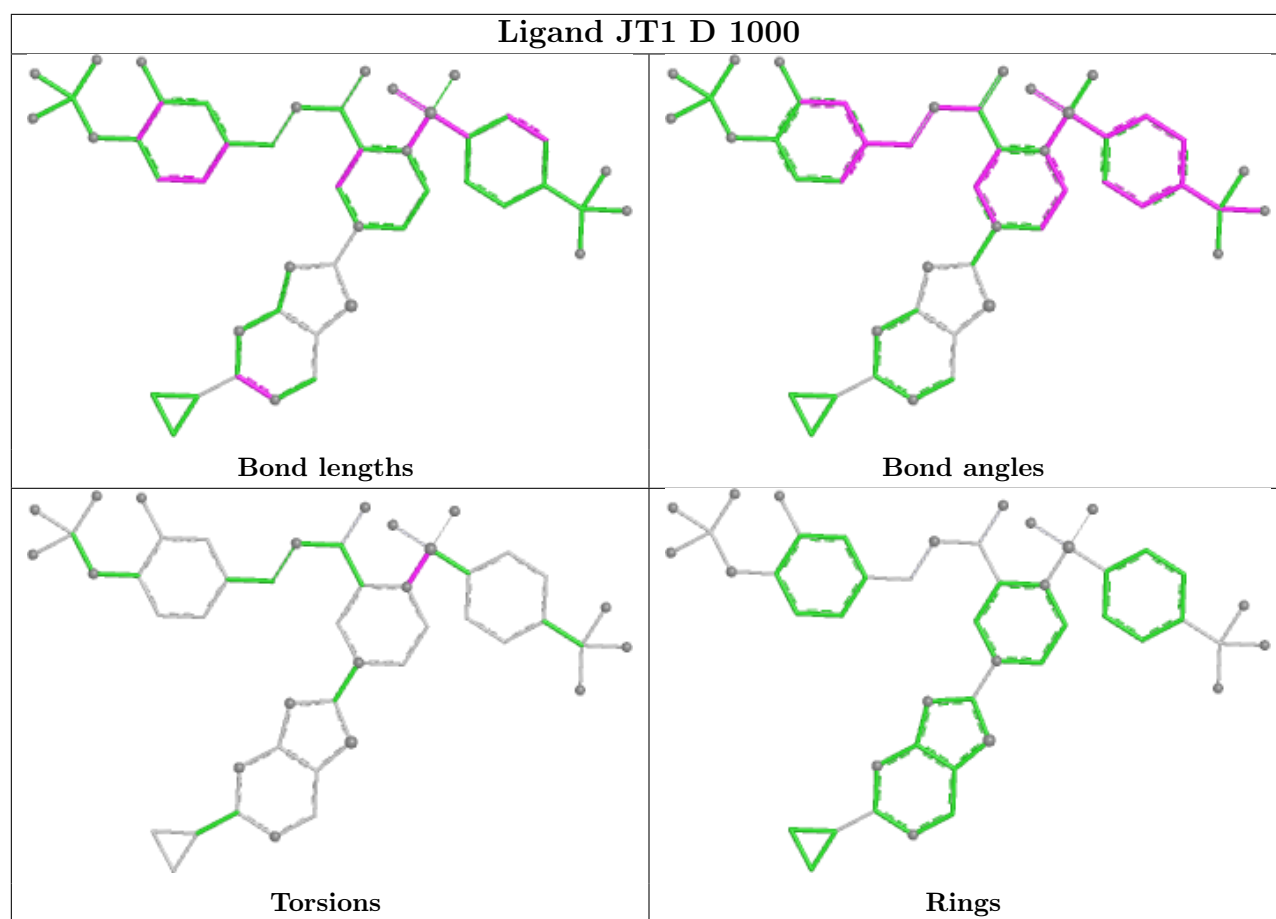
There are no ring outliers.

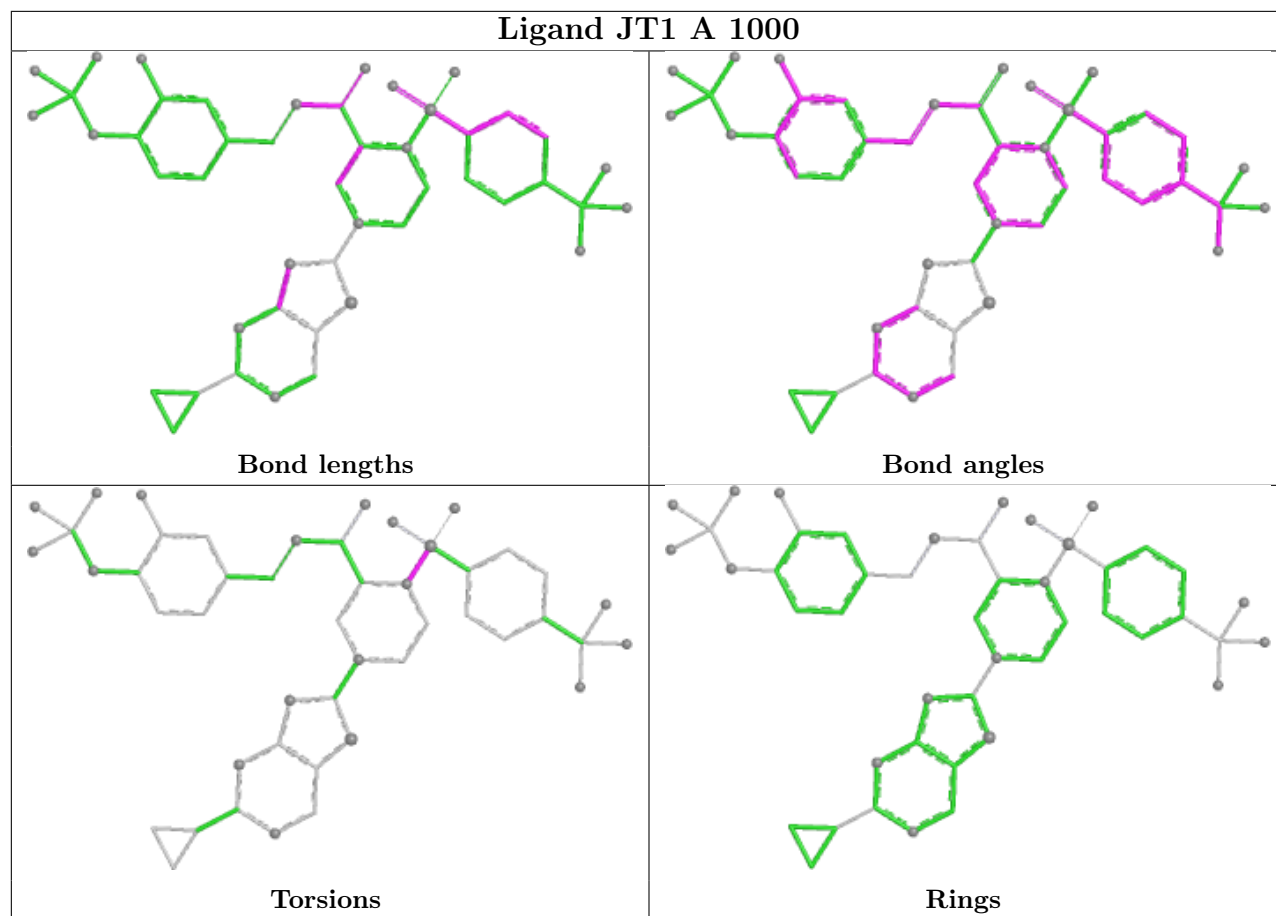
1 monomer is involved in 1 short contact:

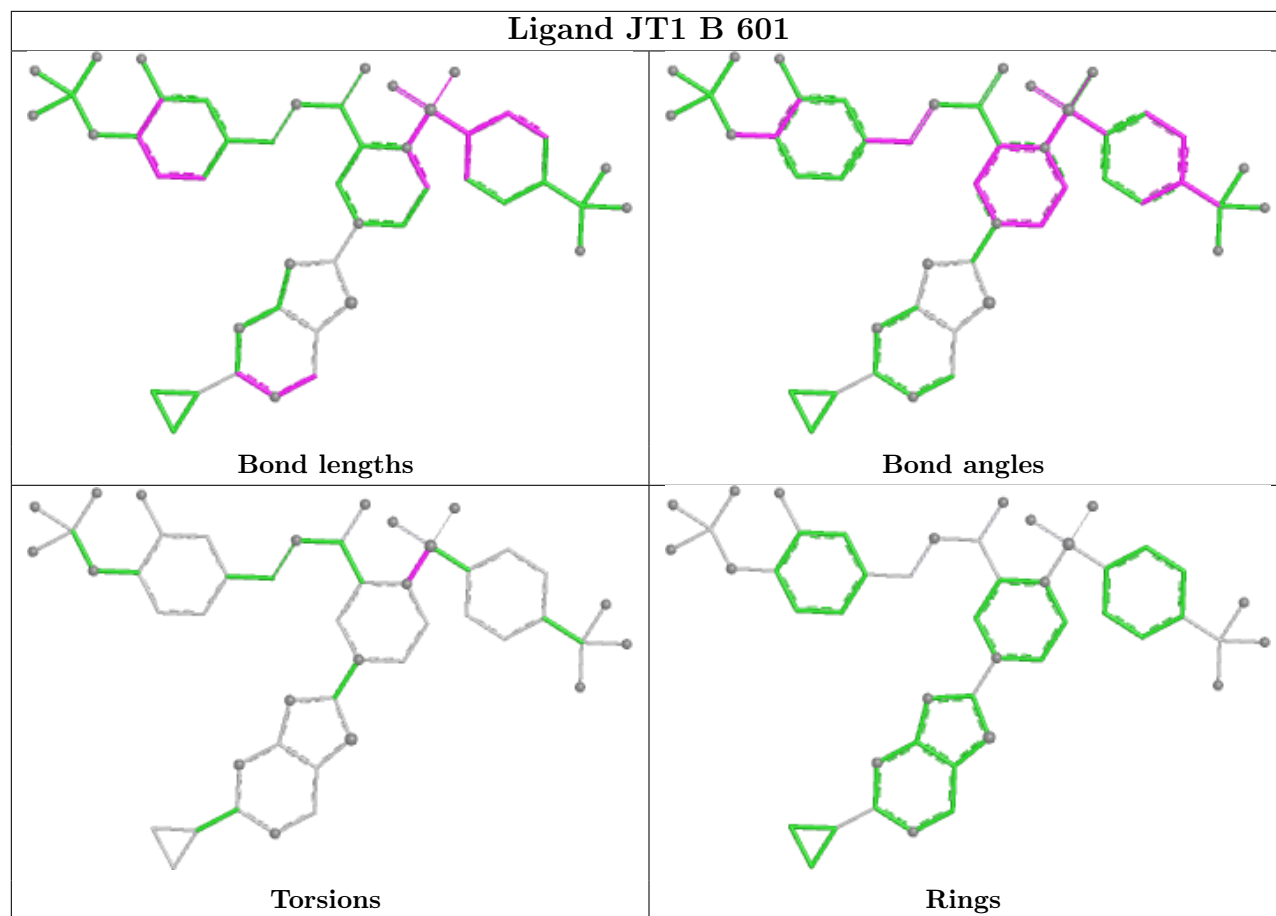
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	JT1	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	553/578 (95%)	0.08	18 (3%) 46 49	20, 35, 72, 123	0
1	B	557/578 (96%)	0.09	19 (3%) 45 48	22, 37, 70, 122	0
1	C	556/578 (96%)	0.16	20 (3%) 42 45	21, 37, 71, 128	0
1	D	553/578 (95%)	0.08	21 (3%) 40 43	21, 33, 69, 123	0
All	All	2219/2312 (95%)	0.10	78 (3%) 44 47	20, 36, 71, 128	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	GLY	8.4
1	D	23	ILE	7.7
1	B	151	LYS	7.1
1	D	544	GLN	6.8
1	A	23	ILE	6.7
1	D	152	GLY	6.5
1	B	542	ALA	6.5
1	C	543	SER	6.2
1	B	544	GLN	6.2
1	C	542	ALA	6.0
1	C	23	ILE	5.8
1	C	150	GLU	5.7
1	B	153	GLY	5.2
1	A	150	GLU	4.8
1	C	551	PHE	4.7
1	A	149	PRO	4.6
1	D	150	GLU	4.6
1	D	553	ALA	4.6
1	B	23	ILE	4.6
1	D	153	GLY	4.5
1	D	547	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	543	SER	4.4
1	C	544	GLN	4.3
1	C	555	TYR	4.2
1	A	553	ALA	4.1
1	D	148	GLN	4.0
1	C	25	ALA	4.0
1	D	27	SER	3.9
1	B	545	LEU	3.9
1	D	26	LEU	3.9
1	C	552	VAL	3.9
1	A	153	GLY	3.6
1	D	545	LEU	3.6
1	D	25	ALA	3.6
1	D	546	ASP	3.5
1	A	151	LYS	3.4
1	B	150	GLU	3.4
1	C	26	LEU	3.3
1	B	152	GLY	3.2
1	C	151	LYS	3.2
1	C	148	GLN	3.2
1	A	25	ALA	3.2
1	B	557	GLY	3.2
1	A	545	LEU	3.1
1	A	148	GLN	3.1
1	D	149	PRO	3.1
1	A	26	LEU	3.1
1	A	552	VAL	3.1
1	C	57	LEU	3.0
1	A	152	GLY	3.0
1	C	405	VAL	3.0
1	C	16	ALA	3.0
1	B	555	TYR	3.0
1	C	545	LEU	2.9
1	D	151	LYS	2.9
1	B	556[A]	SER	2.9
1	A	544	GLN	2.8
1	B	548	SER	2.8
1	B	25	ALA	2.7
1	A	35	ASN	2.7
1	D	402[A]	HIS	2.6
1	D	405	VAL	2.6
1	B	551	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	541	ALA	2.5
1	D	16	ALA	2.5
1	A	20	LYS	2.5
1	D	15	ALA	2.5
1	C	14	CYS	2.4
1	D	552	VAL	2.4
1	B	27	SER	2.3
1	B	34	HIS	2.2
1	C	554	GLY	2.2
1	C	556	SER	2.1
1	B	148	GLN	2.1
1	B	26	LEU	2.1
1	A	541	ALA	2.0
1	A	27	SER	2.0
1	A	43	ARG	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.

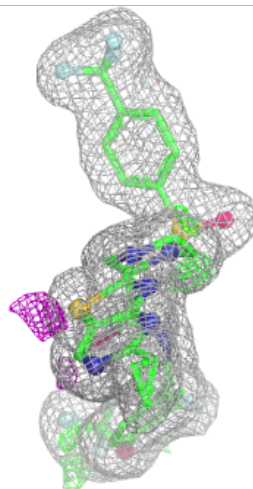
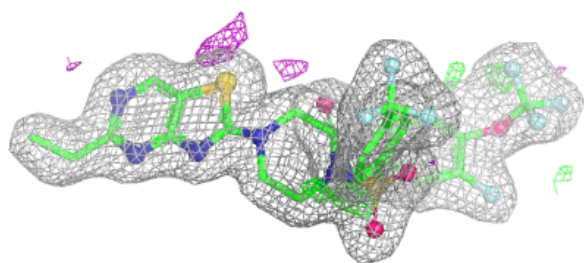
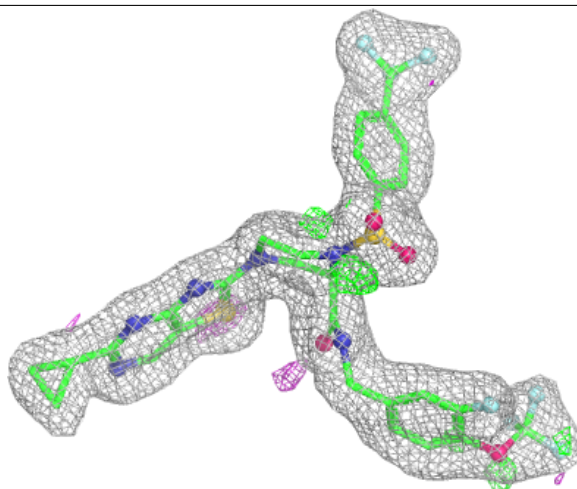
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	JT1	B	601	47/47	0.97	0.11	23,28,43,52	0
2	JT1	C	601	47/47	0.97	0.11	24,30,37,40	0
3	CL	C	602	1/1	0.97	0.09	47,47,47,47	0
2	JT1	D	1000	47/47	0.98	0.10	22,25,29,31	0
2	JT1	A	1000	47/47	0.98	0.09	21,25,31,34	0
3	CL	B	602	1/1	0.99	0.10	43,43,43,43	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.

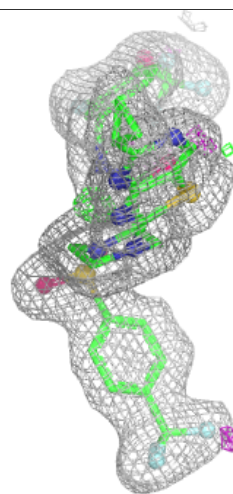
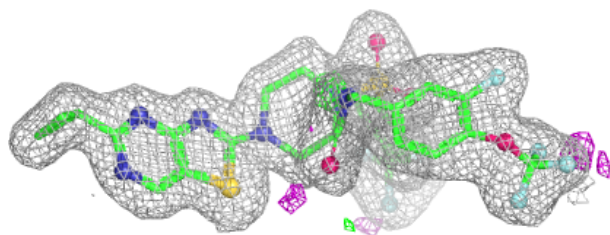
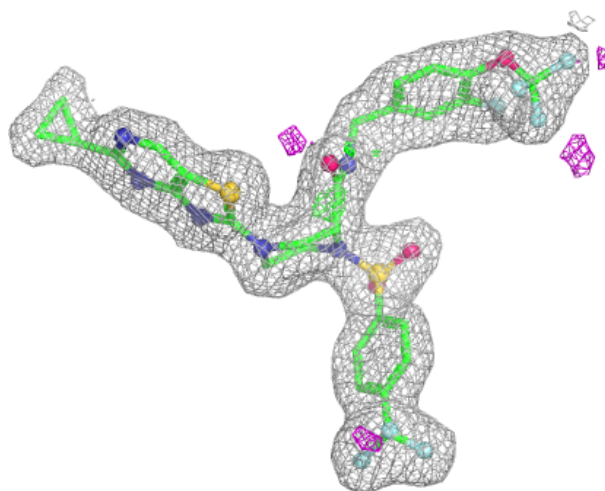
Electron density around JT1 B 601:

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



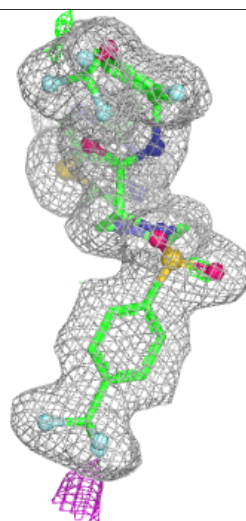
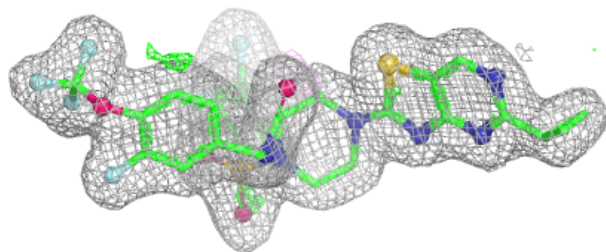
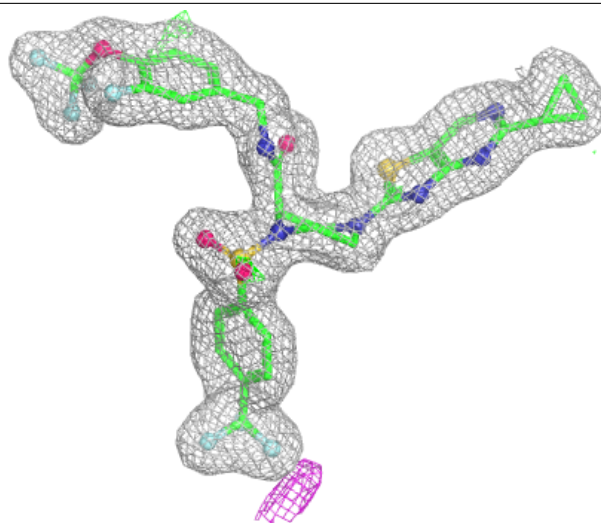
Electron density around JT1 C 601:

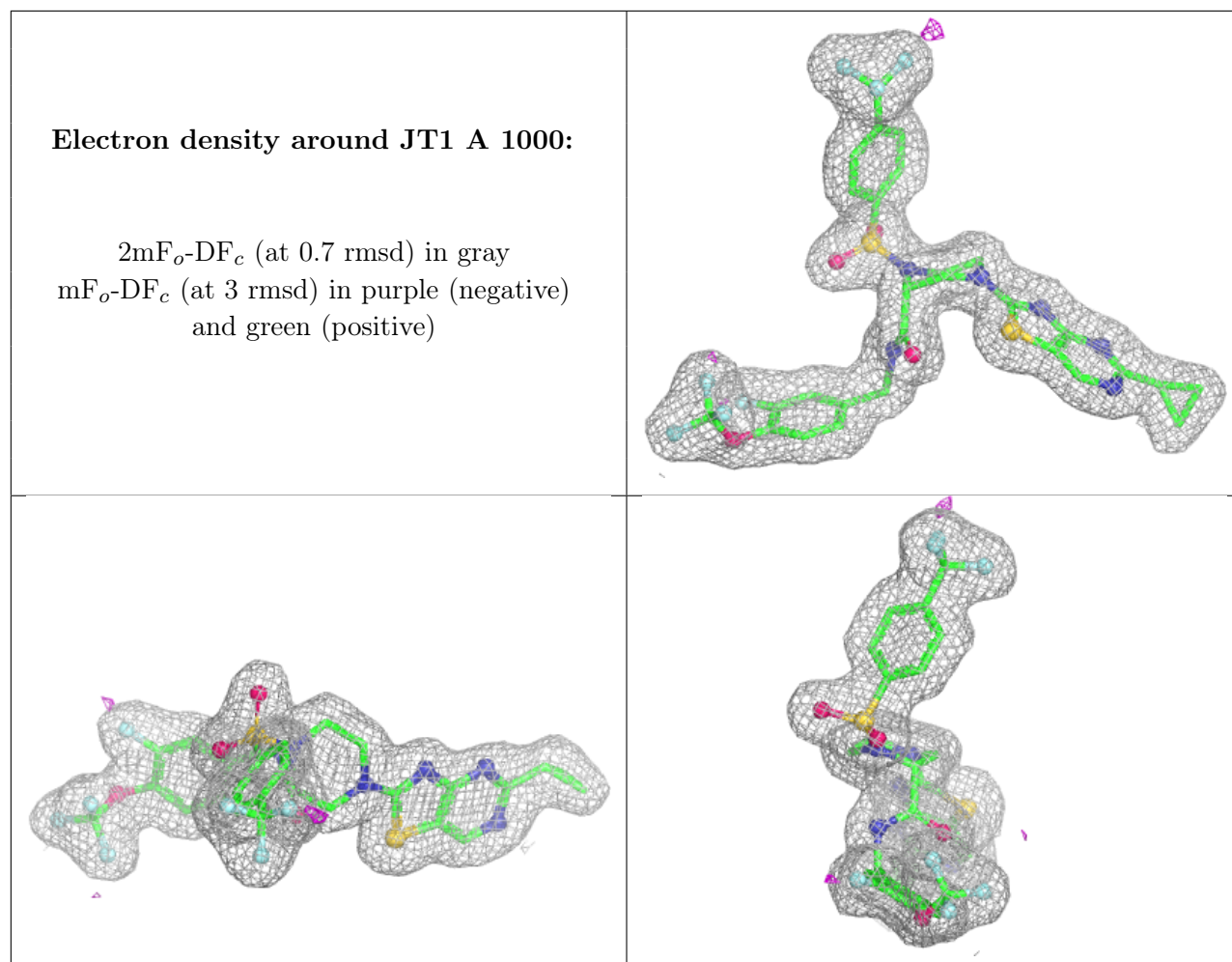
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around JT1 D 1000:

$2mF_o-DF_c$ (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.