



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:31 AM UTC

PDB ID : 2E2B / pdb\_00002e2b  
Title : Crystal structure of the c-Abl kinase domain in complex with INNO-406  
Authors : Horio, T.; Hamasaki, T.; Wakayama, T.; Takagaki, K.; Ohgi, T.  
Deposited on : 2006-11-10  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

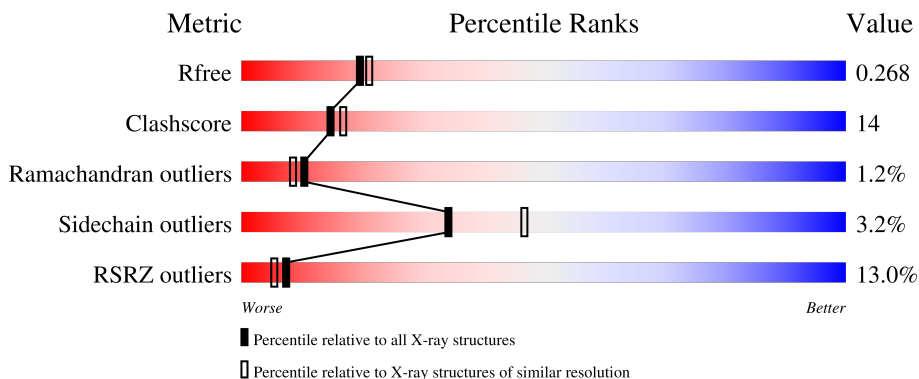
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	293	 9% 69% 20% • 8%
1	B	293	 15% 60% 29% • 11%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4545 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.

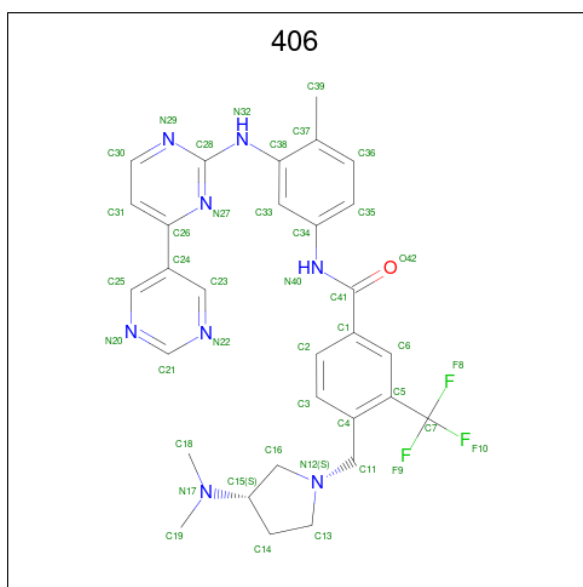
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2191	1414	358	402	17	0	0	0
1	B	262	2135	1380	346	393	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLY	-	cloning artifact	UNP P00519
A	224	ALA	-	cloning artifact	UNP P00519
A	225	MET	-	cloning artifact	UNP P00519
A	226	ASP	-	cloning artifact	UNP P00519
A	227	PRO	-	cloning artifact	UNP P00519
A	228	SER	-	cloning artifact	UNP P00519
B	223	GLY	-	cloning artifact	UNP P00519
B	224	ALA	-	cloning artifact	UNP P00519
B	225	MET	-	cloning artifact	UNP P00519
B	226	ASP	-	cloning artifact	UNP P00519
B	227	PRO	-	cloning artifact	UNP P00519
B	228	SER	-	cloning artifact	UNP P00519

- Molecule 2 is N-[3-(4,5'-BIPYRIMIDIN-2-YLAMINO)-4-METHYLPHENYL]-4-[[[(3S)-3-(DIMETHYLAMINO)PYRROLIDIN-1-YL]METHYL]-3-(TRIFLUOROMETHYL) BENZAMIDE (CCD ID: 406) (formula: C<sub>30</sub>H<sub>31</sub>F<sub>3</sub>N<sub>8</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	A	1	Total	C	F	N	O	0	0
			42	30	3	8	1		
2	B	1	Total	C	F	N	O	0	0
			42	30	3	8	1		

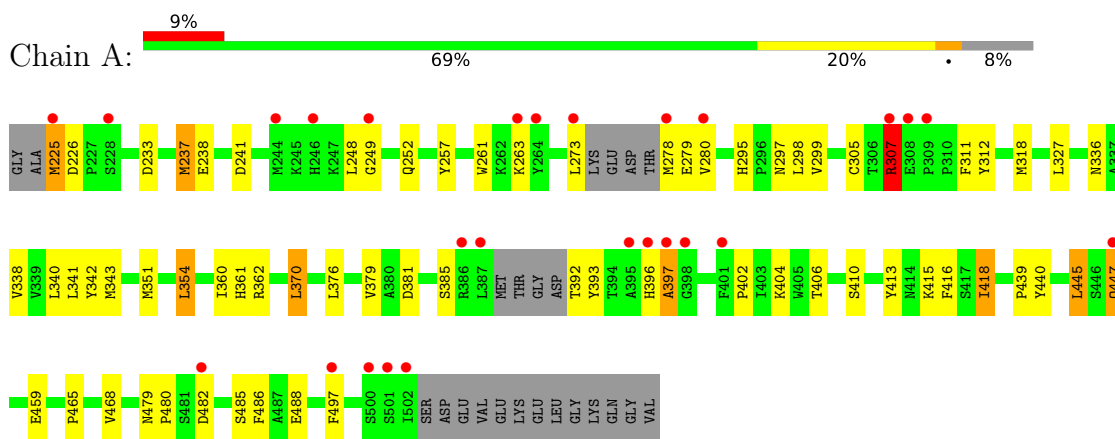
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	88	Total	O	0	0
			88	88		
3	B	47	Total	O	0	0
			47	47		

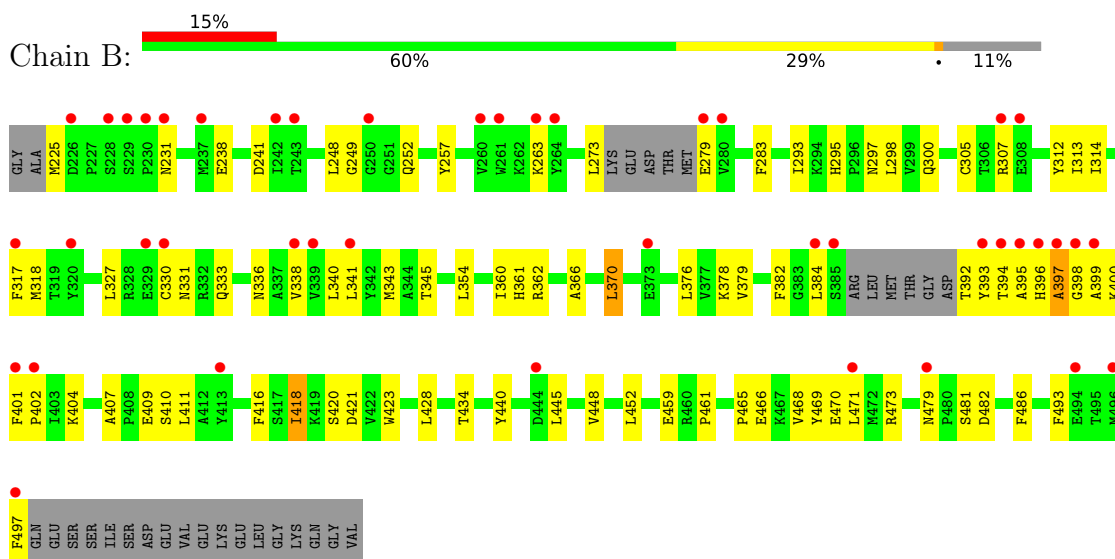
### 3 Residue-property plots [i](#)

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: Proto-oncogene tyrosine-protein kinase ABL1



- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.82Å 147.58Å 152.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.20) 98.6 (50.00-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.89 (at 2.20Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.236 , 0.270 0.233 , 0.268	Depositor DCC
$R_{free}$ test set	1563 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.047 for -h,l,k 0.013 for -1/2*k-1/2*1,-h-1/2*k+1/2*1,-h+1/2*k-1/2*1 0.007 for 1/2*k+1/2*1,h-1/2*k+1/2*1,h+1/2*k-1/2*1 0.013 for -1/2*k+1/2*1,-h-1/2*k-1/2*1,h-1/2*k-1/2*1 0.014 for 1/2*k-1/2*1,h-1/2*k-1/2*1,-h-1/2*k-1/2*1	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 406

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.55	0/2248	0.92	2/3043 (0.1%)
1	B	0.49	0/2192	0.90	8/2968 (0.3%)
All	All	0.52	0/4440	0.91	10/6011 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	GLN	N-CA-C	6.42	119.08	109.25
1	A	307	ARG	N-CA-C	-6.29	103.73	111.40
1	A	279	GLU	N-CA-C	-5.84	106.20	113.15
1	B	421	ASP	N-CA-C	-5.70	105.14	111.36
1	B	330	CYS	N-CA-C	5.32	117.39	110.53
1	B	420	SER	N-CA-C	-5.26	106.36	112.89
1	B	307	ARG	N-CA-C	-5.21	105.51	111.14
1	B	407	ALA	CA-C-N	5.13	124.58	119.24
1	B	407	ALA	C-N-CA	5.13	124.58	119.24
1	B	293	ILE	N-CA-C	5.08	115.80	108.48

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2191	0	2132	55	0
1	B	2135	0	2083	66	0
2	A	42	0	31	4	0
2	B	42	0	31	3	0
3	A	88	0	0	0	0
3	B	47	0	0	1	0
All	All	4545	0	4277	121	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 14.

All (121) 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:336:ASN:OD1	1:A:338:VAL:HG12	1.67	0.95
1:A:305:CYS:HB2	1:A:312:TYR:HB2	1.48	0.94
1:A:445:LEU:H	1:A:445:LEU:HD12	1.40	0.86
1:B:445:LEU:HD12	1:B:445:LEU:H	1.40	0.86
1:B:295:HIS:HD2	1:B:297:ASN:H	1.23	0.84
1:B:418:ILE:HD11	1:B:486:PHE:HD2	1.42	0.83
1:B:399:ALA:HB3	1:B:401:PHE:HE1	1.43	0.82
1:B:295:HIS:CD2	1:B:297:ASN:H	2.00	0.80
1:B:399:ALA:HB3	1:B:401:PHE:CE1	2.17	0.78
1:B:336:ASN:ND2	1:B:338:VAL:HG12	2.01	0.75
1:B:362:ARG:HD2	2:B:1002:406:H181	1.69	0.75
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.72	0.71
1:B:418:ILE:HD11	1:B:486:PHE:CD2	2.26	0.70
1:B:327:LEU:HD21	1:B:343:MET:HE1	1.74	0.70
1:A:295:HIS:HD2	1:A:297:ASN:H	1.37	0.70
1:A:295:HIS:CD2	1:A:297:ASN:H	2.11	0.68
1:B:445:LEU:H	1:B:445:LEU:CD1	2.07	0.67
1:A:445:LEU:H	1:A:445:LEU:CD1	2.09	0.66
1:A:341:LEU:HD23	1:A:497:PHE:HA	1.78	0.65
1:A:280:VAL:HG13	1:A:311:PHE:HE1	1.63	0.64
1:A:362:ARG:HD2	2:A:1001:406:H181	1.77	0.64
1:B:445:LEU:HD12	1:B:445:LEU:N	2.13	0.63
1:B:360:ILE:O	2:B:1002:406:H142	1.99	0.62
1:A:360:ILE:O	2:A:1001:406:H142	2.00	0.62
1:A:280:VAL:HG13	1:A:311:PHE:CE1	2.34	0.61
1:A:465:PRO:HG2	1:A:468:VAL:CG2	2.31	0.60
1:A:318:MET:O	2:A:1001:406:H21	2.01	0.59
1:A:318:MET:HG3	1:A:370:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:MET:HE1	1:B:231:ASN:O	2.02	0.59
1:A:341:LEU:CD2	1:A:497:PHE:HA	2.32	0.59
1:B:479:ASN:HB3	1:B:482:ASP:OD2	2.02	0.59
1:A:361:HIS:O	1:A:362:ARG:HB2	2.01	0.58
1:A:273:LEU:HD23	1:A:280:VAL:HG22	1.86	0.58
1:B:248:LEU:HD11	1:B:317:PHE:HE1	1.69	0.57
1:B:396:HIS:O	1:B:397:ALA:HB3	2.03	0.57
1:B:418:ILE:O	1:B:418:ILE:HD13	2.04	0.56
1:B:404:LYS:NZ	1:B:440:TYR:HB2	2.20	0.56
1:B:465:PRO:HG2	1:B:468:VAL:CG2	2.36	0.56
1:A:479:ASN:HB3	1:A:482:ASP:OD2	2.05	0.56
1:A:445:LEU:HD12	1:A:445:LEU:N	2.16	0.56
1:A:418:ILE:HD11	1:A:486:PHE:CD1	2.40	0.56
1:B:404:LYS:HZ2	1:B:440:TYR:HB2	1.71	0.55
1:B:318:MET:CE	1:B:378:LYS:HD2	2.38	0.54
1:B:336:ASN:HD21	1:B:338:VAL:HG12	1.72	0.54
1:A:340:LEU:HA	1:A:343:MET:HE2	1.90	0.53
1:B:397:ALA:C	1:B:399:ALA:H	2.15	0.53
1:B:361:HIS:O	1:B:362:ARG:HB2	2.08	0.53
1:A:404:LYS:NZ	1:A:440:TYR:HB2	2.23	0.53
1:A:225:MET:HE3	1:A:307:ARG:CZ	2.38	0.53
1:A:237:MET:HE1	1:A:261:TRP:CZ2	2.44	0.53
1:A:298:LEU:HD11	1:A:354:LEU:HD13	1.89	0.53
1:B:318:MET:HG3	1:B:370:LEU:CB	2.40	0.52
1:B:395:ALA:HA	1:B:399:ALA:O	2.09	0.52
1:A:318:MET:HG3	1:A:370:LEU:CB	2.40	0.52
1:A:351:MET:HB3	1:A:486:PHE:CD1	2.45	0.52
1:B:318:MET:HG3	1:B:370:LEU:HB3	1.91	0.52
1:B:336:ASN:CG	1:B:338:VAL:HG12	2.34	0.52
1:B:318:MET:O	2:B:1002:406:H21	2.07	0.52
1:A:404:LYS:HZ3	1:A:440:TYR:HB2	1.75	0.52
1:A:278:MET:C	1:A:280:VAL:H	2.17	0.51
1:B:459:GLU:HG2	3:B:28:HOH:O	2.11	0.51
1:A:249:GLY:O	1:A:252:GLN:HG2	2.11	0.50
1:A:280:VAL:CG1	1:A:311:PHE:HE1	2.24	0.50
1:A:340:LEU:HD23	1:A:343:MET:HE2	1.95	0.48
1:B:382:PHE:HB2	1:B:384:LEU:HG	1.95	0.48
1:A:413:TYR:HB2	1:A:415:LYS:HG3	1.95	0.48
1:B:283:PHE:CZ	1:B:313:ILE:HG13	2.48	0.48
1:B:318:MET:SD	1:B:378:LYS:HD2	2.53	0.48
1:B:273:LEU:HD11	1:B:279:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LEU:HD23	1:B:343:MET:HE2	1.95	0.48
1:A:273:LEU:CD2	1:A:280:VAL:HG22	2.44	0.47
1:B:362:ARG:HG2	1:B:416:PHE:CD2	2.50	0.47
1:B:249:GLY:O	1:B:252:GLN:HG2	2.14	0.47
1:B:393:TYR:CD2	1:B:402:PRO:HD3	2.49	0.47
1:B:466:GLU:O	1:B:470:GLU:HG3	2.15	0.47
1:A:327:LEU:HD21	1:A:343:MET:HE1	1.97	0.47
1:B:295:HIS:HD2	1:B:297:ASN:N	2.00	0.47
1:A:362:ARG:HG2	1:A:416:PHE:CD2	2.50	0.46
1:A:447:GLN:HE21	1:A:447:GLN:HB3	1.52	0.46
1:B:394:THR:O	1:B:400:LYS:HA	2.15	0.46
1:A:381:ASP:OD2	2:A:1001:406:H192	2.16	0.46
1:B:238:GLU:HB3	1:B:241:ASP:CG	2.41	0.46
1:B:341:LEU:HD23	1:B:497:PHE:HD1	1.80	0.46
1:B:409:GLU:HG2	1:B:410:SER:N	2.31	0.46
1:A:248:LEU:HA	1:A:248:LEU:HD12	1.66	0.45
1:B:393:TYR:CE2	1:B:402:PRO:HD3	2.52	0.45
1:A:396:HIS:O	1:A:397:ALA:C	2.60	0.45
1:B:396:HIS:HE1	1:B:411:LEU:O	2.00	0.45
1:B:448:VAL:O	1:B:452:LEU:HG	2.17	0.44
1:A:298:LEU:HD23	1:A:379:VAL:HB	1.99	0.44
1:B:345:THR:OG1	1:B:493:PHE:HB3	2.17	0.44
1:B:366:ALA:N	1:B:428:LEU:HD13	2.33	0.44
1:B:479:ASN:ND2	1:B:481:SER:OG	2.50	0.44
1:B:298:LEU:HD23	1:B:379:VAL:HB	2.00	0.43
1:B:396:HIS:CE1	1:B:411:LEU:O	2.71	0.43
1:A:342:TYR:HB2	1:A:497:PHE:CE2	2.53	0.43
1:B:396:HIS:O	1:B:397:ALA:CB	2.65	0.43
1:B:397:ALA:O	1:B:399:ALA:N	2.52	0.43
1:A:298:LEU:O	1:A:299:VAL:C	2.61	0.42
1:A:342:TYR:HB2	1:A:497:PHE:HE2	1.84	0.42
1:A:392:THR:O	1:A:402:PRO:HA	2.19	0.42
1:B:434:THR:HG22	1:B:461:PRO:HB3	2.01	0.42
1:B:257:TYR:CD1	1:B:257:TYR:N	2.87	0.42
1:B:465:PRO:HG2	1:B:468:VAL:HG23	2.01	0.42
1:A:351:MET:HB3	1:A:486:PHE:CE1	2.54	0.42
1:A:238:GLU:HB3	1:A:241:ASP:CG	2.45	0.42
1:A:439:PRO:O	1:A:440:TYR:C	2.63	0.42
1:B:423:TRP:CD1	1:B:423:TRP:C	2.98	0.42
1:A:465:PRO:HG2	1:A:468:VAL:HG23	2.02	0.41
1:B:469:TYR:CZ	1:B:473:ARG:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ILE:HD12	1:B:314:ILE:N	2.35	0.41
1:A:485:SER:OG	1:A:488:GLU:HG3	2.21	0.41
1:B:331:ASN:OD1	1:B:333:GLN:HB2	2.21	0.41
1:A:225:MET:SD	1:A:233:ASP:N	2.86	0.41
1:A:479:ASN:HA	1:A:480:PRO:HD2	1.96	0.41
1:A:406:THR:HG22	1:A:410:SER:HB2	2.03	0.41
1:A:393:TYR:CE2	1:A:402:PRO:HD3	2.56	0.40
1:B:327:LEU:CD2	1:B:343:MET:HE1	2.49	0.40
1:A:257:TYR:CD1	1:A:257:TYR:N	2.89	0.40
1:B:392:THR:O	1:B:402:PRO:HA	2.22	0.40
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.96	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	264/293 (90%)	248 (94%)	13 (5%)	3 (1%)	11	10
1	B	256/293 (87%)	241 (94%)	12 (5%)	3 (1%)	10	8
All	All	520/586 (89%)	489 (94%)	25 (5%)	6 (1%)	10	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	ALA
1	B	263	LYS
1	B	397	ALA
1	A	263	LYS
1	A	385	SER
1	B	398	GLY

### 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	233/255 (91%)	222 (95%)	11 (5%)	23	31
1	B	229/255 (90%)	225 (98%)	4 (2%)	53	69
All	All	462/510 (91%)	447 (97%)	15 (3%)	34	47

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	MET
1	A	226	ASP
1	A	237	MET
1	A	307	ARG
1	A	354	LEU
1	A	370	LEU
1	A	376	LEU
1	A	418	ILE
1	A	445	LEU
1	A	447	GLN
1	A	459	GLU
1	B	354	LEU
1	B	370	LEU
1	B	376	LEU
1	B	418	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	HIS
1	A	297	ASN
1	A	447	GLN
1	A	490	HIS
1	B	295	HIS
1	B	396	HIS
1	B	414	ASN

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Mol	Chain	Res	Type
1	B	479	ASN
1	B	490	HIS

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	406	A	1001	-	45,46,46	2.38	14 (31%)	62,66,66	1.78	13 (20%)
2	406	B	1002	-	45,46,46	2.53	17 (37%)	62,66,66	1.83	14 (22%)

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	406	A	1001	-	-	2/30/39/39	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	406	B	1002	-	-	2/30/39/39	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	406	C4-C5	7.11	1.49	1.40
2	A	1001	406	C4-C5	6.34	1.48	1.40
2	A	1001	406	C24-C26	-5.50	1.40	1.49
2	B	1002	406	C23-C24	5.25	1.48	1.39
2	A	1001	406	C23-C24	5.13	1.48	1.39
2	B	1002	406	C24-C26	-5.05	1.41	1.49
2	B	1002	406	C25-C24	4.72	1.47	1.39
2	B	1002	406	C31-C26	4.50	1.49	1.39
2	A	1001	406	C25-C24	4.43	1.47	1.39
2	A	1001	406	C31-C26	4.27	1.48	1.39
2	A	1001	406	C3-C4	4.13	1.46	1.39
2	B	1002	406	C7-C5	4.06	1.59	1.50
2	B	1002	406	C3-C4	3.82	1.45	1.39
2	B	1002	406	C36-C35	3.80	1.45	1.38
2	B	1002	406	C33-C34	3.70	1.45	1.39
2	A	1001	406	C33-C34	3.64	1.45	1.39
2	A	1001	406	C7-C5	3.27	1.57	1.50
2	A	1001	406	C36-C35	3.18	1.44	1.38
2	B	1002	406	C11-C4	3.14	1.57	1.51
2	A	1001	406	C11-C4	2.84	1.56	1.51
2	B	1002	406	C6-C1	2.83	1.43	1.39
2	A	1001	406	C6-C1	2.81	1.43	1.39
2	A	1001	406	C2-C1	2.72	1.43	1.39
2	B	1002	406	C31-C30	2.61	1.43	1.38
2	B	1002	406	C6-C5	2.52	1.43	1.39
2	B	1002	406	C26-N27	2.30	1.38	1.34
2	B	1002	406	C36-C37	2.22	1.44	1.39
2	B	1002	406	C2-C1	2.14	1.42	1.39
2	A	1001	406	C26-N27	2.09	1.38	1.34
2	A	1001	406	C31-C30	2.06	1.42	1.38
2	B	1002	406	C3-C2	2.03	1.42	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	406	C7-C5-C4	5.22	126.06	121.06
2	B	1002	406	C26-N27-C28	5.04	120.69	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	406	C26-N27-C28	4.83	120.53	116.81
2	A	1001	406	C7-C5-C4	4.47	125.34	121.06
2	A	1001	406	C30-N29-C28	3.85	118.64	115.42
2	A	1001	406	C4-C11-N12	3.79	119.48	112.75
2	B	1002	406	C25-C24-C26	3.76	126.85	121.29
2	B	1002	406	C4-C11-N12	3.65	119.22	112.75
2	B	1002	406	C30-N29-C28	3.62	118.44	115.42
2	A	1001	406	C25-C24-C26	3.48	126.43	121.29
2	A	1001	406	C39-C37-C38	3.15	124.80	121.23
2	B	1002	406	C13-N12-C16	3.12	107.69	104.02
2	A	1001	406	C13-N12-C16	3.07	107.63	104.02
2	B	1002	406	C31-C26-N27	-3.05	117.94	121.97
2	B	1002	406	C39-C37-C38	2.92	124.53	121.23
2	A	1001	406	C31-C26-N27	-2.75	118.34	121.97
2	B	1002	406	C25-C24-C23	-2.59	110.78	114.73
2	B	1002	406	C18-N17-C15	2.52	116.72	112.39
2	B	1002	406	C34-N40-C41	2.50	133.18	126.61
2	B	1002	406	C11-C4-C3	-2.42	115.34	120.12
2	A	1001	406	C34-N40-C41	2.33	132.73	126.61
2	A	1001	406	C25-C24-C23	-2.28	111.25	114.73
2	A	1001	406	C39-C37-C36	-2.26	115.92	120.28
2	A	1001	406	C18-N17-C15	2.23	116.22	112.39
2	B	1002	406	C39-C37-C36	-2.12	116.20	120.28
2	A	1001	406	C11-C4-C3	-2.11	115.95	120.12
2	B	1002	406	C31-C30-N29	-2.01	121.52	123.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

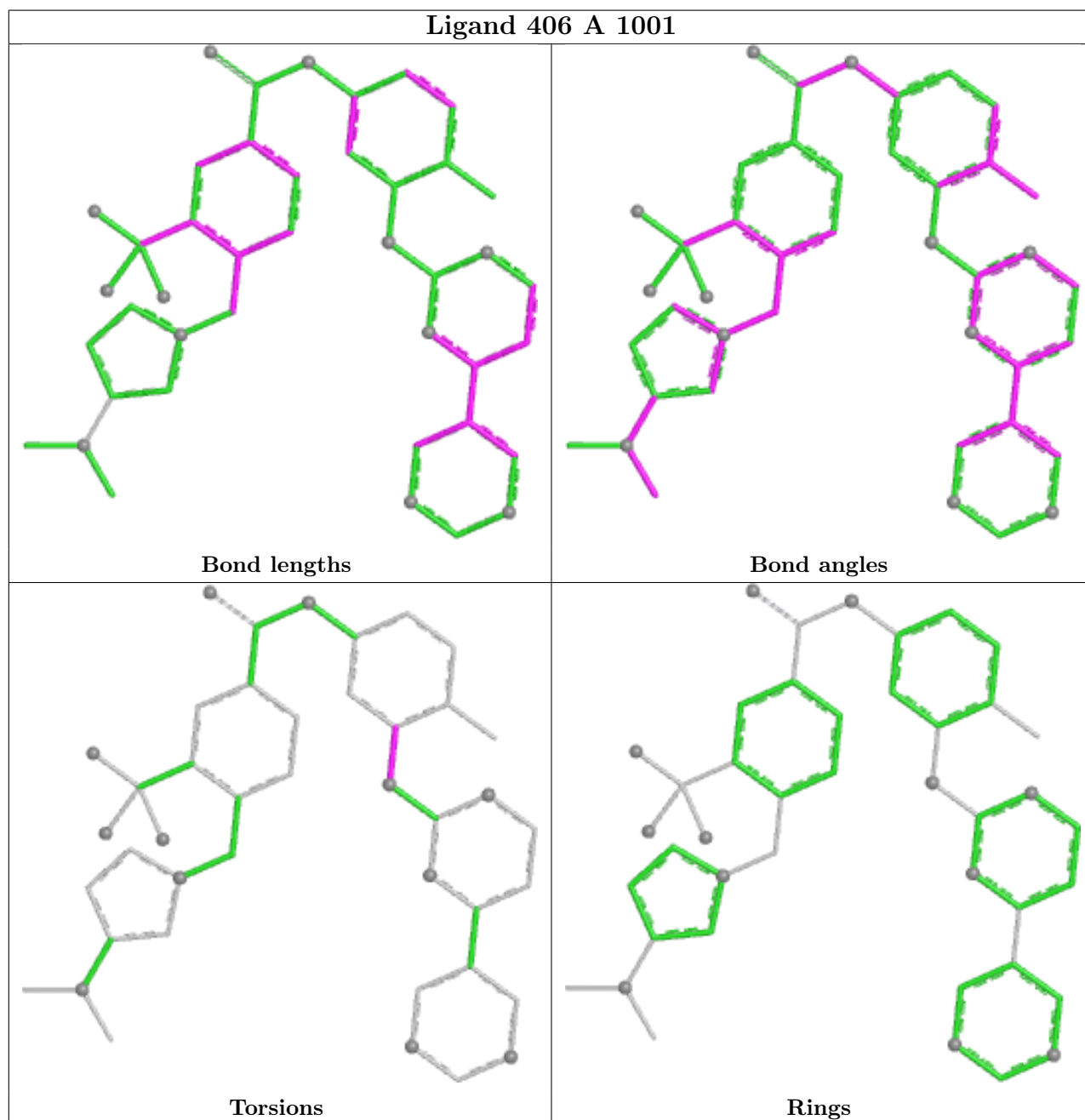
Mol	Chain	Res	Type	Atoms
2	A	1001	406	C33-C38-N32-C28
2	A	1001	406	C37-C38-N32-C28
2	B	1002	406	C33-C38-N32-C28
2	B	1002	406	C37-C38-N32-C28

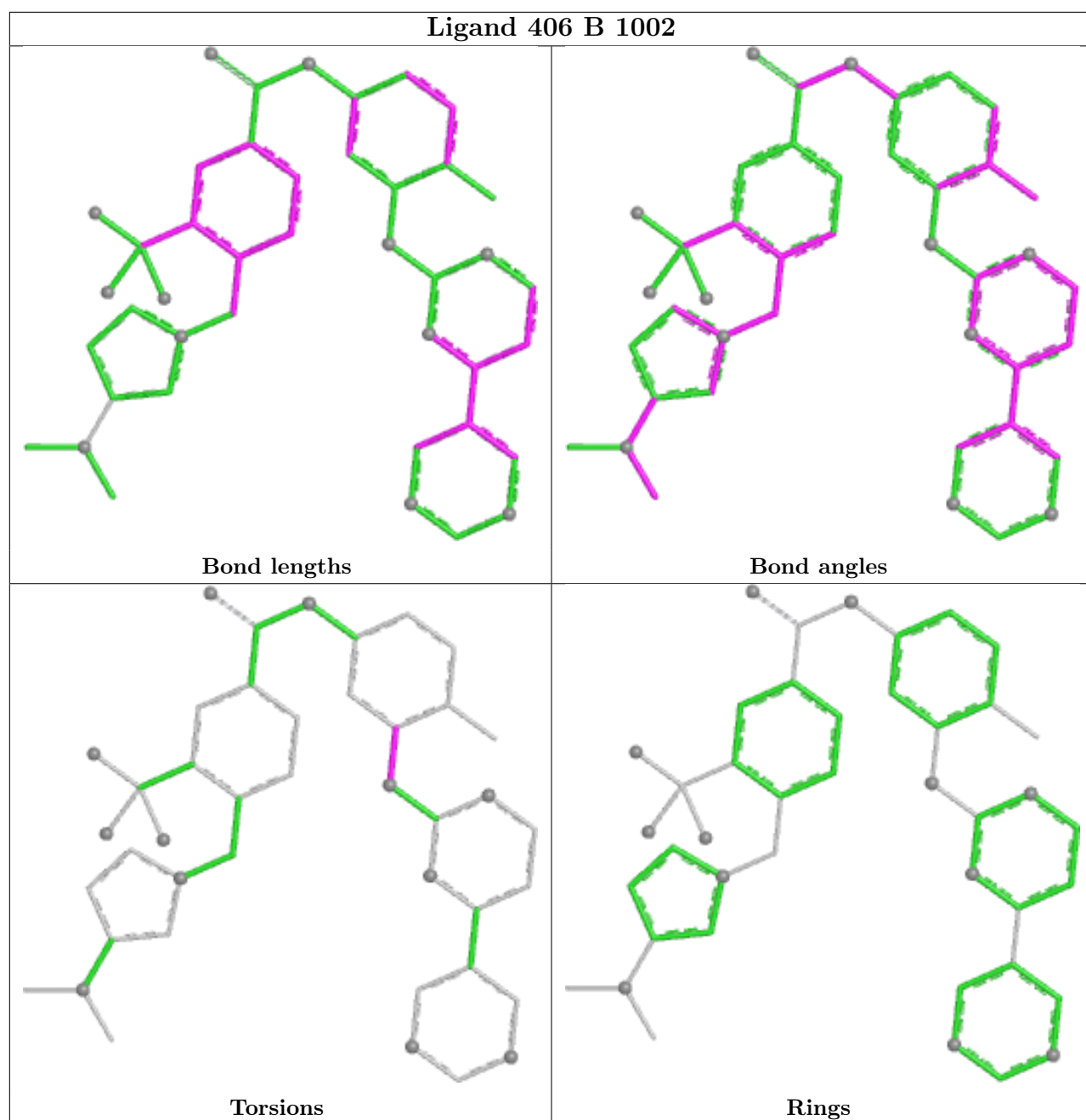
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	406	4	0
2	B	1002	406	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	270/293 (92%)	0.56	26 (9%) 13 11	22, 43, 89, 135	0
1	B	262/293 (89%)	1.00	43 (16%) 4 3	29, 51, 104, 128	0
All	All	532/586 (90%)	0.78	69 (12%) 7 5	22, 48, 101, 135	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	PHE	6.2
1	A	398	GLY	6.1
1	B	401	PHE	4.6
1	A	278	MET	4.6
1	A	502	ILE	4.5
1	A	264	TYR	4.2
1	A	501	SER	4.1
1	B	228	SER	4.0
1	B	394	THR	3.9
1	B	402	PRO	3.9
1	A	401	PHE	3.8
1	A	225	MET	3.7
1	B	396	HIS	3.6
1	A	397	ALA	3.5
1	A	395	ALA	3.4
1	B	229	SER	3.3
1	A	396	HIS	3.3
1	A	500	SER	3.3
1	B	280	VAL	3.3
1	B	264	TYR	3.3
1	A	497	PHE	3.2
1	A	307	ARG	3.1
1	B	338	VAL	3.1
1	B	397	ALA	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	260	VAL	3.0
1	B	261	TRP	3.0
1	B	398	GLY	2.9
1	A	482	ASP	2.9
1	B	395	ALA	2.8
1	B	263	LYS	2.8
1	B	444	ASP	2.8
1	A	273	LEU	2.7
1	A	447	GLN	2.7
1	B	339	VAL	2.7
1	B	237	MET	2.7
1	B	413	TYR	2.6
1	B	308	GLU	2.6
1	A	387	LEU	2.6
1	B	494	GLU	2.6
1	A	309	PRO	2.6
1	B	385	SER	2.6
1	A	386	ARG	2.5
1	B	231	ASN	2.5
1	B	320	TYR	2.4
1	B	393	TYR	2.4
1	B	496	MET	2.4
1	A	308	GLU	2.4
1	B	317	PHE	2.4
1	B	384	LEU	2.4
1	B	243	THR	2.3
1	A	263	LYS	2.3
1	B	279	GLU	2.3
1	A	280	VAL	2.3
1	B	230	PRO	2.2
1	A	249	GLY	2.2
1	B	330	CYS	2.2
1	B	242	ILE	2.1
1	B	329	GLU	2.1
1	B	479	ASN	2.1
1	A	246	HIS	2.1
1	B	307	ARG	2.1
1	B	373	GLU	2.1
1	A	228	SER	2.1
1	B	399	ALA	2.1
1	B	471	LEU	2.1
1	B	250	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	244	MET	2.0
1	B	226	ASP	2.0
1	B	341	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

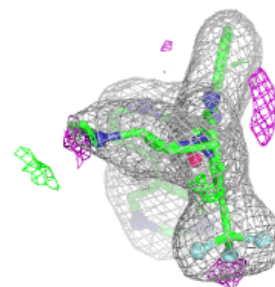
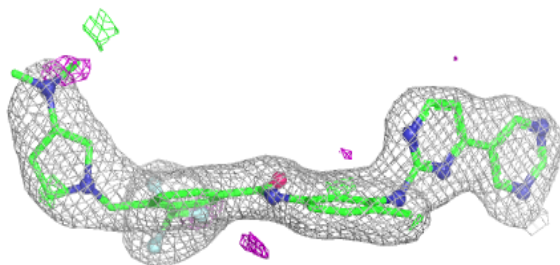
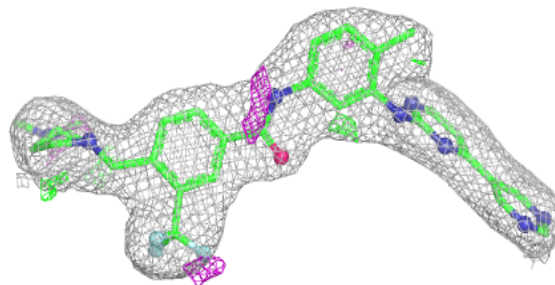
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	406	B	1002	42/42	0.89	0.13	46,47,47,48	0
2	406	A	1001	42/42	0.91	0.11	37,38,39,39	0

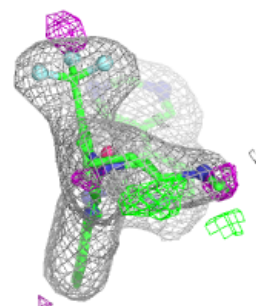
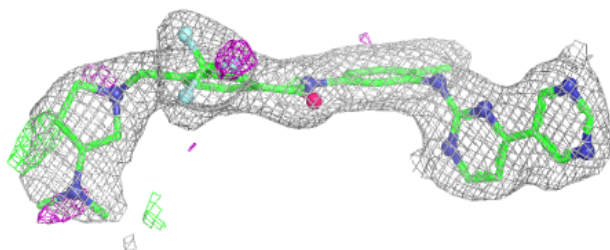
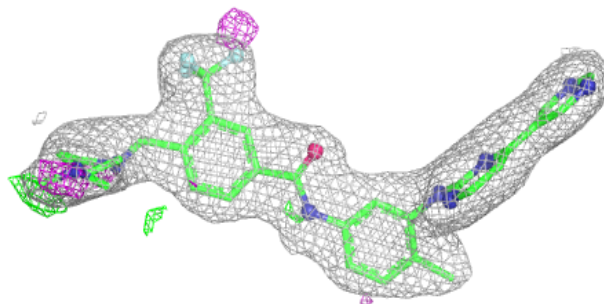
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 406 B 1002:**

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

**Electron density around 406 A 1001:**

$2mF_o-DF_c$  (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.