



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 02:18 PM EST

PDB ID : 7LEK  
Title : Crystal structure of the second bromodomain (BD2) of human BRDT bound to ERK5-IN-1  
Authors : Chan, A.; Karim, M.R.; Schonbrunn, E.  
Deposited on : 2021-01-14  
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

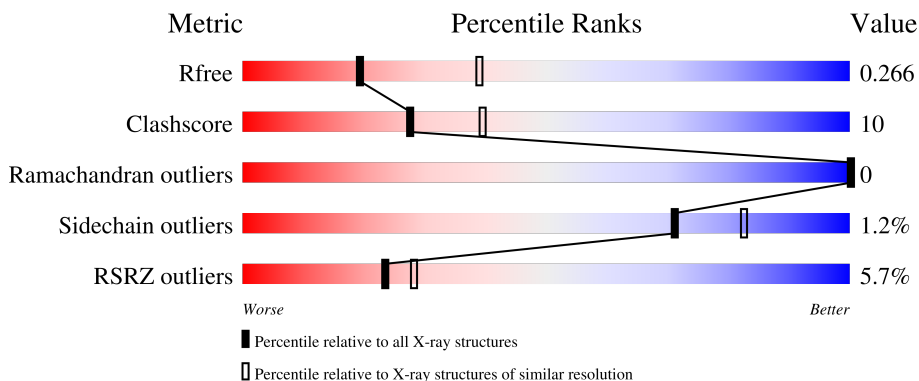
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	117	<div> <div>2%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
1	B	117	<div> <div>3%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
1	C	117	<div> <div>11%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	D	117	<div> <div>7%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3997 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.

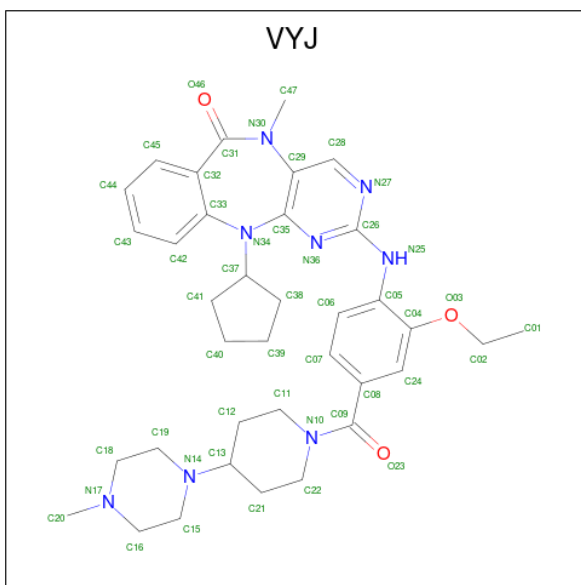
- Molecule 1 is a protein called Bromodomain testis-specific protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			928	599	152	168	9			
1	B	116	Total	C	N	O	S	0	0	0
			956	617	157	173	9			
1	C	112	Total	C	N	O	S	0	0	0
			925	598	151	167	9			
1	D	114	Total	C	N	O	S	0	0	0
			939	605	154	171	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	GLY	-	expression tag	UNP Q58F21
A	263	ALA	-	expression tag	UNP Q58F21
A	264	ALA	-	expression tag	UNP Q58F21
A	265	SER	-	expression tag	UNP Q58F21
B	262	GLY	-	expression tag	UNP Q58F21
B	263	ALA	-	expression tag	UNP Q58F21
B	264	ALA	-	expression tag	UNP Q58F21
B	265	SER	-	expression tag	UNP Q58F21
C	262	GLY	-	expression tag	UNP Q58F21
C	263	ALA	-	expression tag	UNP Q58F21
C	264	ALA	-	expression tag	UNP Q58F21
C	265	SER	-	expression tag	UNP Q58F21
D	262	GLY	-	expression tag	UNP Q58F21
D	263	ALA	-	expression tag	UNP Q58F21
D	264	ALA	-	expression tag	UNP Q58F21
D	265	SER	-	expression tag	UNP Q58F21

- Molecule 2 is 11-cyclopentyl-2-({2-ethoxy-4-[4-(4-methylpiperazin-1-yl)piperidine-1-carbonyl]phenyl}amino)-5-methyl-5,11-dihydro-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one (three-letter code: VYJ) (formula: C<sub>36</sub>H<sub>46</sub>N<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			47	36	8	3		
2	B	1	Total	C	N	O	0	0
			47	36	8	3		
2	C	1	Total	C	N	O	0	0
			47	36	8	3		
2	D	1	Total	C	N	O	0	0
			47	36	8	3		

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		

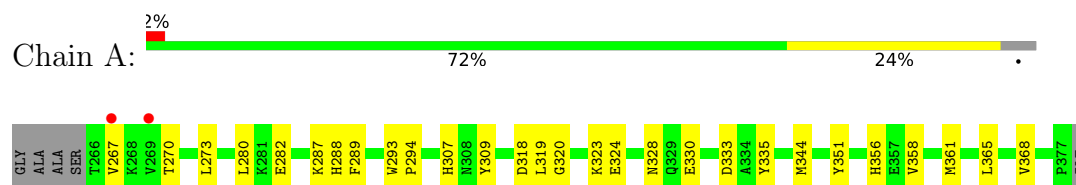
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	16	Total	O	0	0
			16	16		
5	C	11	Total	O	0	0
			11	11		
5	D	9	Total	O	0	0
			9	9		

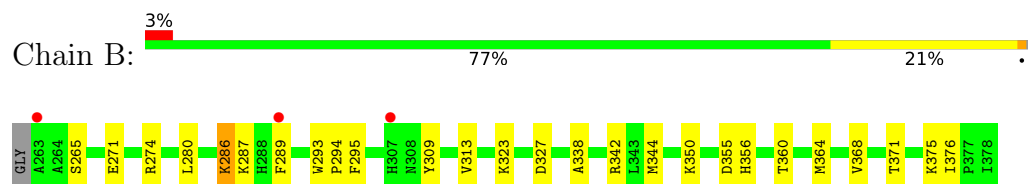
### 3 Residue-property plots [i](#)

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.

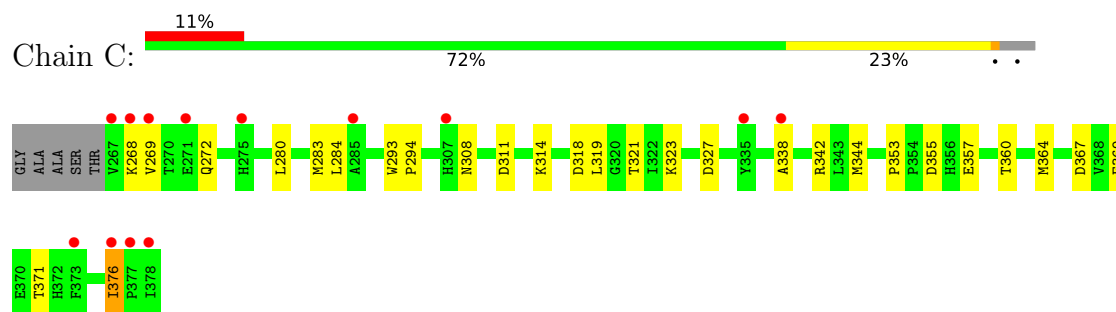
- Molecule 1: Bromodomain testis-specific protein



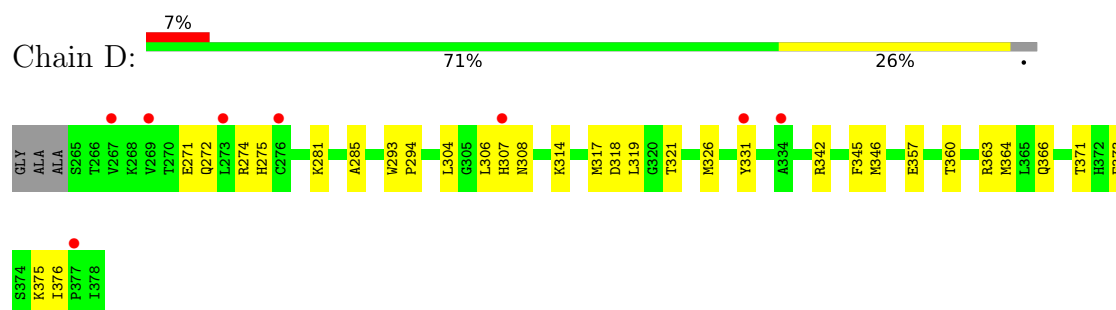
- Molecule 1: Bromodomain testis-specific protein



- Molecule 1: Bromodomain testis-specific protein



- Molecule 1: Bromodomain testis-specific protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.61Å 99.32Å 60.40Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	52.48 – 2.75 52.48 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (52.48-2.75) 99.8 (52.48-2.75)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19_4085	Depositor
R, $R_{free}$	0.213 , 0.264 0.213 , 0.266	Depositor DCC
$R_{free}$ test set	808 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.13% 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: EDO, CL, VYJ

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	0.40	0/954	0.79	1/1291 (0.1%)
1	B	0.38	0/982	0.75	0/1328
1	C	0.43	0/951	0.82	1/1288 (0.1%)
1	D	0.41	0/965	0.80	0/1306
All	All	0.41	0/3852	0.79	2/5213 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	C	376	ILE	CG1-CB-CG2	-5.19	99.99	111.40

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	928	0	898	17	0
1	B	956	0	935	16	0
1	C	925	0	891	22	0
1	D	939	0	905	21	0
2	A	47	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	47	0	0	1	0
2	C	47	0	0	1	0
2	D	47	0	0	0	0
3	B	1	0	0	0	0
4	C	4	0	6	0	0
5	A	20	0	0	0	0
5	B	16	0	0	2	0
5	C	11	0	0	0	0
5	D	9	0	0	2	0
All	All	3997	0	3635	76	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 10.

All (76) 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:D:314:LYS:NZ	5:D:501:HOH:O	2.12	0.82
1:D:373:PHE:O	1:D:376:ILE:HD12	1.87	0.74
1:A:328:ASN:HB3	1:A:330:GLU:HG3	1.70	0.74
1:A:356:HIS:CD2	1:A:358:VAL:HG23	2.23	0.73
1:B:271:GLU:OE2	1:B:274:ARG:NH2	2.21	0.73
1:B:371:THR:O	1:B:375:LYS:HG3	1.96	0.65
1:A:267:VAL:O	1:A:270:THR:OG1	2.11	0.64
1:D:307:HIS:O	1:D:308:ASN:ND2	2.30	0.64
1:C:269:VAL:HA	1:C:272:GLN:HG2	1.82	0.61
1:A:333:ASP:OD1	1:A:335:TYR:HB2	2.00	0.61
1:A:282:GLU:OE2	1:A:287:LYS:HD2	2.02	0.59
1:B:323:LYS:HE2	1:B:327:ASP:OD2	2.01	0.59
1:C:318:ASP:OD1	1:C:321:THR:OG1	2.20	0.58
1:D:371:THR:O	1:D:375:LYS:HG3	2.04	0.58
1:B:364:MET:O	1:B:368:VAL:HG23	2.04	0.57
1:C:283:MET:CE	1:C:369:PHE:HB2	2.34	0.57
1:B:309:TYR:CZ	1:B:313:VAL:HG21	2.41	0.56
1:B:350:LYS:NZ	5:B:502:HOH:O	2.39	0.55
1:D:326:MET:HE2	1:D:331:TYR:CD2	2.42	0.54
1:C:280:LEU:HD21	1:C:323:LYS:HA	1.89	0.54
1:A:294:PRO:HG2	1:A:361:MET:HE3	1.90	0.54
1:B:287:LYS:NZ	5:B:501:HOH:O	2.38	0.54
1:A:356:HIS:CD2	1:A:358:VAL:H	2.27	0.53
1:A:320:GLY:O	1:A:324:GLU:HG3	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:HIS:HD2	1:A:358:VAL:H	1.56	0.51
1:B:271:GLU:CD	1:B:274:ARG:HH21	2.11	0.51
1:C:269:VAL:HA	1:C:272:GLN:CG	2.41	0.51
1:C:360:THR:O	1:C:364:MET:HG3	2.10	0.51
1:D:317:MET:SD	1:D:321:THR:OG1	2.69	0.51
1:D:375:LYS:O	1:D:376:ILE:C	2.50	0.50
1:A:280:LEU:HD21	1:A:323:LYS:HA	1.94	0.50
1:D:272:GLN:O	1:D:275:HIS:HB2	2.11	0.50
1:A:294:PRO:HG2	1:A:361:MET:CE	2.42	0.49
1:C:283:MET:HE3	1:C:369:PHE:HB2	1.93	0.49
1:C:311:ASP:O	1:C:314:LYS:NZ	2.46	0.49
1:A:288:HIS:CE1	1:A:368:VAL:HG21	2.49	0.48
1:D:293:TRP:CG	1:D:294:PRO:HD3	2.49	0.48
1:D:357:GLU:H	1:D:357:GLU:CD	2.16	0.48
1:B:338:ALA:O	1:B:342:ARG:HG3	2.13	0.47
1:B:356:HIS:HE1	2:B:401:VYJ:C38	2.28	0.47
1:D:326:MET:HE2	1:D:331:TYR:HD2	1.79	0.47
1:B:375:LYS:O	1:B:376:ILE:C	2.53	0.47
1:B:360:THR:O	1:B:364:MET:HG3	2.15	0.47
1:D:363:ARG:NH2	5:D:502:HOH:O	2.47	0.47
1:C:318:ASP:HA	1:C:344:MET:SD	2.55	0.46
1:C:357:GLU:H	1:C:357:GLU:CD	2.19	0.46
1:D:318:ASP:OD1	1:D:321:THR:HG23	2.16	0.46
1:C:308:ASN:O	1:C:308:ASN:OD1	2.33	0.46
1:C:323:LYS:HE2	1:C:327:ASP:OD2	2.16	0.46
1:B:286:LYS:HE2	1:B:286:LYS:H	1.81	0.45
1:A:289:PHE:CZ	1:D:357:GLU:HG3	2.51	0.45
1:B:280:LEU:HD21	1:B:323:LYS:HA	1.98	0.45
1:A:318:ASP:HA	1:A:344:MET:SD	2.58	0.44
1:C:355:ASP:OD1	1:C:355:ASP:N	2.48	0.44
1:B:295:PHE:HB3	1:B:344:MET:SD	2.58	0.44
1:C:338:ALA:O	1:C:342:ARG:HG3	2.18	0.44
1:D:342:ARG:O	1:D:346:MET:HG2	2.18	0.44
2:C:401:VYJ:N36	2:C:401:VYJ:C06	2.81	0.44
1:B:293:TRP:CG	1:B:294:PRO:HD3	2.53	0.43
1:D:281:LYS:O	1:D:285:ALA:N	2.50	0.43
1:C:314:LYS:N	1:C:314:LYS:HD2	2.33	0.43
1:C:353:PRO:HB2	1:C:355:ASP:OD1	2.18	0.43
1:D:271:GLU:O	1:D:274:ARG:HG2	2.19	0.43
1:D:319:LEU:HD23	1:D:319:LEU:HA	1.85	0.43
1:C:367:ASP:O	1:C:371:THR:HG23	2.20	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ILE:HD13	1:C:376:ILE:HG21	1.78	0.42
1:D:304:LEU:HB2	1:D:306:LEU:HG	2.02	0.42
1:D:360:THR:O	1:D:364:MET:HG3	2.18	0.41
1:A:309:TYR:HA	1:A:351:TYR:CE1	2.55	0.41
1:C:268:LYS:O	1:C:272:GLN:HG2	2.20	0.41
1:A:293:TRP:CG	1:A:294:PRO:HD3	2.56	0.41
1:C:284:LEU:HD21	1:C:319:LEU:HB3	2.02	0.41
1:C:293:TRP:CD2	1:C:294:PRO:HD3	2.56	0.41
1:D:345:PHE:CE1	1:D:366:GLN:HA	2.55	0.41
1:A:319:LEU:HD11	1:A:365:LEU:HD21	2.03	0.41
1:C:284:LEU:HD23	1:C:284:LEU:HA	1.89	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	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
1	B	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
1	C	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
1	D	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
All	All	446/468 (95%)	436 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	102/105 (97%)	101 (99%)	1 (1%)	76	85
1	B	105/105 (100%)	101 (96%)	4 (4%)	33	53
1	C	101/105 (96%)	101 (100%)	0	100	100
1	D	103/105 (98%)	103 (100%)	0	100	100
All	All	411/420 (98%)	406 (99%)	5 (1%)	71	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	HIS
1	B	265	SER
1	B	286	LYS
1	B	289	PHE
1	B	355	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	C	308	ASN
1	C	366	GLN
1	D	308	ASN
1	D	366	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	VYJ	A	401	-	46,53,53	3.65	26 (56%)	56,76,76	4.26	12 (21%)
2	VYJ	B	401	-	46,53,53	3.61	25 (54%)	56,76,76	3.81	15 (26%)
2	VYJ	C	401	-	46,53,53	3.64	25 (54%)	56,76,76	4.19	16 (28%)
2	VYJ	D	401	-	46,53,53	3.60	27 (58%)	56,76,76	3.58	15 (26%)
4	EDO	C	402	-	3,3,3	0.49	0	2,2,2	0.29	0

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	VYJ	A	401	-	-	7/19/50/50	0/6/7/7
2	VYJ	B	401	-	-	7/19/50/50	1/6/7/7
2	VYJ	C	401	-	-	7/19/50/50	0/6/7/7
2	VYJ	D	401	-	-	6/19/50/50	0/6/7/7
4	EDO	C	402	-	-	1/1/1/1	-

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	VYJ	C20-N17	-9.96	1.23	1.46
2	D	401	VYJ	C20-N17	-9.88	1.23	1.46
2	A	401	VYJ	C20-N17	-9.86	1.23	1.46
2	B	401	VYJ	C20-N17	-9.75	1.24	1.46
2	C	401	VYJ	C26-N25	7.11	1.51	1.36
2	B	401	VYJ	C13-N14	-7.03	1.29	1.48
2	B	401	VYJ	C26-N25	7.00	1.50	1.36
2	A	401	VYJ	C09-N10	6.95	1.50	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	VYJ	C13-N14	-6.92	1.30	1.48
2	A	401	VYJ	C26-N25	6.88	1.50	1.36
2	A	401	VYJ	C15-N14	-6.80	1.33	1.47
2	D	401	VYJ	C26-N25	6.77	1.50	1.36
2	B	401	VYJ	C15-N14	-6.74	1.34	1.47
2	D	401	VYJ	C09-N10	6.73	1.49	1.34
2	D	401	VYJ	C15-N14	-6.65	1.34	1.47
2	D	401	VYJ	C13-N14	-6.60	1.31	1.48
2	C	401	VYJ	C15-N14	-6.59	1.34	1.47
2	C	401	VYJ	C09-N10	6.53	1.49	1.34
2	A	401	VYJ	C13-N14	-6.33	1.31	1.48
2	B	401	VYJ	C09-N10	6.24	1.48	1.34
2	C	401	VYJ	C18-N17	-5.89	1.33	1.46
2	D	401	VYJ	C18-N17	-5.79	1.34	1.46
2	B	401	VYJ	C18-N17	-5.77	1.34	1.46
2	A	401	VYJ	C18-N17	-5.60	1.34	1.46
2	A	401	VYJ	C43-C42	5.27	1.48	1.36
2	C	401	VYJ	C43-C42	5.24	1.48	1.36
2	D	401	VYJ	C43-C42	5.22	1.48	1.36
2	B	401	VYJ	C43-C42	5.15	1.48	1.36
2	A	401	VYJ	C26-N27	5.03	1.41	1.34
2	A	401	VYJ	C45-C32	5.02	1.51	1.41
2	B	401	VYJ	C45-C32	4.97	1.51	1.41
2	C	401	VYJ	C45-C32	4.96	1.51	1.41
2	C	401	VYJ	C26-N27	4.85	1.41	1.34
2	D	401	VYJ	C45-C32	4.82	1.50	1.41
2	B	401	VYJ	C26-N27	4.79	1.41	1.34
2	D	401	VYJ	C26-N27	4.66	1.41	1.34
2	D	401	VYJ	C07-C06	4.34	1.46	1.38
2	A	401	VYJ	C07-C06	4.33	1.46	1.38
2	B	401	VYJ	C24-C08	4.25	1.45	1.39
2	B	401	VYJ	C39-C38	-4.09	1.34	1.51
2	B	401	VYJ	C29-C35	4.06	1.45	1.40
2	C	401	VYJ	C24-C08	4.04	1.45	1.39
2	A	401	VYJ	O03-C04	4.04	1.45	1.37
2	B	401	VYJ	O03-C04	4.03	1.45	1.37
2	A	401	VYJ	C24-C08	4.01	1.45	1.39
2	C	401	VYJ	C07-C06	3.97	1.46	1.38
2	A	401	VYJ	O46-C31	-3.97	1.14	1.24
2	A	401	VYJ	C39-C38	-3.94	1.35	1.51
2	D	401	VYJ	C24-C08	3.92	1.45	1.39
2	D	401	VYJ	C39-C38	-3.90	1.35	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	VYJ	C07-C06	3.86	1.45	1.38
2	B	401	VYJ	O46-C31	-3.86	1.14	1.24
2	D	401	VYJ	O46-C31	-3.86	1.14	1.24
2	C	401	VYJ	C39-C38	-3.85	1.35	1.51
2	C	401	VYJ	O46-C31	-3.85	1.15	1.24
2	A	401	VYJ	C08-C09	3.69	1.56	1.50
2	C	401	VYJ	O03-C04	3.68	1.44	1.37
2	C	401	VYJ	C29-C35	3.67	1.44	1.40
2	A	401	VYJ	C38-C37	3.63	1.64	1.52
2	D	401	VYJ	O03-C04	3.61	1.44	1.37
2	D	401	VYJ	C29-C35	3.56	1.44	1.40
2	C	401	VYJ	C19-N14	-3.55	1.40	1.47
2	A	401	VYJ	C29-C35	3.54	1.44	1.40
2	C	401	VYJ	C16-N17	-3.50	1.38	1.46
2	C	401	VYJ	C38-C37	3.49	1.64	1.52
2	D	401	VYJ	C19-N14	-3.49	1.40	1.47
2	B	401	VYJ	C16-N17	-3.44	1.39	1.46
2	A	401	VYJ	C05-N25	3.43	1.49	1.39
2	C	401	VYJ	C05-N25	3.42	1.49	1.39
2	B	401	VYJ	C19-N14	-3.42	1.40	1.47
2	D	401	VYJ	C38-C37	3.38	1.64	1.52
2	B	401	VYJ	C38-C37	3.34	1.63	1.52
2	D	401	VYJ	C05-N25	3.32	1.49	1.39
2	D	401	VYJ	C08-C09	3.30	1.55	1.50
2	A	401	VYJ	C40-C41	-3.27	1.38	1.51
2	D	401	VYJ	C16-N17	-3.25	1.39	1.46
2	A	401	VYJ	C19-N14	-3.24	1.40	1.47
2	C	401	VYJ	C40-C41	-3.23	1.38	1.51
2	C	401	VYJ	C08-C09	3.22	1.55	1.50
2	A	401	VYJ	C16-N17	-3.21	1.39	1.46
2	D	401	VYJ	C40-C41	-3.17	1.38	1.51
2	B	401	VYJ	C08-C09	3.04	1.55	1.50
2	B	401	VYJ	C40-C41	-3.01	1.39	1.51
2	D	401	VYJ	C40-C39	2.93	1.69	1.48
2	C	401	VYJ	C40-C39	2.92	1.68	1.48
2	B	401	VYJ	C05-N25	2.92	1.48	1.39
2	B	401	VYJ	C40-C39	2.87	1.68	1.48
2	B	401	VYJ	C05-C04	2.85	1.46	1.40
2	A	401	VYJ	C40-C39	2.84	1.68	1.48
2	C	401	VYJ	C05-C04	2.70	1.46	1.40
2	C	401	VYJ	C32-C33	-2.43	1.39	1.41
2	D	401	VYJ	C05-C04	2.39	1.45	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	VYJ	C21-C22	2.39	1.59	1.52
2	A	401	VYJ	C05-C04	2.34	1.45	1.40
2	B	401	VYJ	C32-C33	-2.33	1.39	1.41
2	D	401	VYJ	C32-C33	-2.27	1.39	1.41
2	A	401	VYJ	C32-C33	-2.17	1.39	1.41
2	C	401	VYJ	C44-C43	2.14	1.43	1.38
2	D	401	VYJ	C35-N36	-2.12	1.32	1.35
2	B	401	VYJ	C44-C43	2.10	1.43	1.38
2	A	401	VYJ	C44-C43	2.07	1.43	1.38
2	D	401	VYJ	C26-N36	-2.04	1.28	1.34
2	D	401	VYJ	C21-C22	2.03	1.58	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	VYJ	C41-C37-N34	-20.85	93.41	114.19
2	C	401	VYJ	C41-C37-N34	-18.48	95.77	114.19
2	A	401	VYJ	C38-C37-N34	18.15	132.27	114.19
2	C	401	VYJ	C38-C37-N34	17.61	131.73	114.19
2	B	401	VYJ	C41-C37-N34	-15.79	98.45	114.19
2	D	401	VYJ	C38-C37-N34	15.52	129.66	114.19
2	B	401	VYJ	C38-C37-N34	14.50	128.64	114.19
2	D	401	VYJ	C41-C37-N34	-12.64	101.60	114.19
2	B	401	VYJ	C21-C13-N14	-10.57	85.05	112.52
2	C	401	VYJ	C21-C13-N14	-9.81	87.04	112.52
2	D	401	VYJ	C21-C13-N14	-9.05	89.02	112.52
2	D	401	VYJ	C12-C13-N14	7.17	131.13	112.52
2	A	401	VYJ	C12-C13-N14	7.05	130.82	112.52
2	A	401	VYJ	C21-C13-N14	-7.04	94.23	112.52
2	C	401	VYJ	C45-C32-C33	6.68	120.97	117.96
2	A	401	VYJ	C45-C32-C33	6.53	120.91	117.96
2	B	401	VYJ	C45-C32-C33	6.47	120.88	117.96
2	C	401	VYJ	C12-C13-N14	6.15	128.49	112.52
2	D	401	VYJ	C45-C32-C33	6.06	120.70	117.96
2	B	401	VYJ	C19-N14-C15	6.06	120.15	109.08
2	B	401	VYJ	C12-C13-N14	5.90	127.83	112.52
2	D	401	VYJ	C26-N36-C35	5.13	121.10	115.28
2	C	401	VYJ	N27-C26-N36	-4.88	121.81	126.52
2	A	401	VYJ	C26-N36-C35	4.74	120.66	115.28
2	D	401	VYJ	N27-C26-N36	-4.43	122.24	126.52
2	C	401	VYJ	C19-N14-C15	4.34	117.02	109.08
2	A	401	VYJ	N27-C26-N36	-4.28	122.38	126.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	VYJ	C21-C22-N10	-4.10	104.58	110.82
2	C	401	VYJ	C26-N36-C35	4.08	119.91	115.28
2	D	401	VYJ	C22-C21-C13	4.01	118.44	110.81
2	B	401	VYJ	N27-C26-N36	-3.90	122.75	126.52
2	B	401	VYJ	C28-N27-C26	3.90	121.67	115.88
2	C	401	VYJ	C28-N27-C26	3.90	121.67	115.88
2	C	401	VYJ	C08-C09-N10	3.66	123.36	118.72
2	D	401	VYJ	C19-N14-C15	3.56	115.59	109.08
2	B	401	VYJ	C26-N36-C35	3.44	119.19	115.28
2	D	401	VYJ	C21-C22-N10	3.42	116.02	110.82
2	B	401	VYJ	C16-C15-N14	3.25	116.81	110.59
2	A	401	VYJ	C28-N27-C26	3.19	120.61	115.88
2	D	401	VYJ	C28-N27-C26	3.09	120.46	115.88
2	B	401	VYJ	C18-C19-N14	3.08	116.49	110.59
2	C	401	VYJ	C11-C12-C13	3.01	116.53	110.81
2	A	401	VYJ	C19-C18-N17	2.94	114.13	110.80
2	C	401	VYJ	C21-C22-N10	-2.68	106.75	110.82
2	D	401	VYJ	C12-C11-N10	-2.50	107.01	110.82
2	B	401	VYJ	O03-C04-C05	2.47	118.97	114.92
2	C	401	VYJ	O23-C09-N10	-2.34	118.47	122.34
2	A	401	VYJ	C18-C19-N14	2.25	114.90	110.59
2	C	401	VYJ	C05-N25-C26	-2.18	123.02	129.60
2	C	401	VYJ	C16-C15-N14	2.17	114.74	110.59
2	B	401	VYJ	C11-C12-C13	2.17	114.94	110.81
2	C	401	VYJ	O03-C04-C05	2.16	118.47	114.92
2	D	401	VYJ	C41-C37-C38	-2.14	101.33	104.25
2	A	401	VYJ	C18-N17-C16	2.08	112.43	109.52
2	B	401	VYJ	C19-C18-N17	2.04	113.11	110.80
2	D	401	VYJ	O03-C04-C05	2.02	118.23	114.92
2	A	401	VYJ	C19-N14-C15	2.02	112.76	109.08
2	D	401	VYJ	C05-N25-C26	-2.02	123.53	129.60

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	VYJ	C21-C13-N14-C15
2	A	401	VYJ	C21-C13-N14-C19
2	A	401	VYJ	C12-C13-N14-C15
2	A	401	VYJ	C12-C13-N14-C19
2	B	401	VYJ	C21-C13-N14-C15
2	B	401	VYJ	C12-C13-N14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	401	VYJ	C21-C13-N14-C15
2	C	401	VYJ	C21-C13-N14-C19
2	C	401	VYJ	C12-C13-N14-C19
2	D	401	VYJ	C21-C13-N14-C15
2	D	401	VYJ	C21-C13-N14-C19
2	D	401	VYJ	C12-C13-N14-C15
2	C	401	VYJ	C12-C13-N14-C15
2	D	401	VYJ	C12-C13-N14-C19
2	B	401	VYJ	C01-C02-O03-C04
2	A	401	VYJ	C01-C02-O03-C04
2	B	401	VYJ	C05-C04-O03-C02
2	A	401	VYJ	C05-C04-O03-C02
2	D	401	VYJ	C05-C04-O03-C02
2	B	401	VYJ	C24-C04-O03-C02
2	C	401	VYJ	C05-C04-O03-C02
2	A	401	VYJ	C24-C04-O03-C02
2	D	401	VYJ	C24-C04-O03-C02
2	C	401	VYJ	C24-C04-O03-C02
2	B	401	VYJ	C21-C13-N14-C19
4	C	402	EDO	O1-C1-C2-O2
2	C	401	VYJ	C01-C02-O03-C04
2	B	401	VYJ	C12-C13-N14-C19

All (1) ring outliers are listed below:

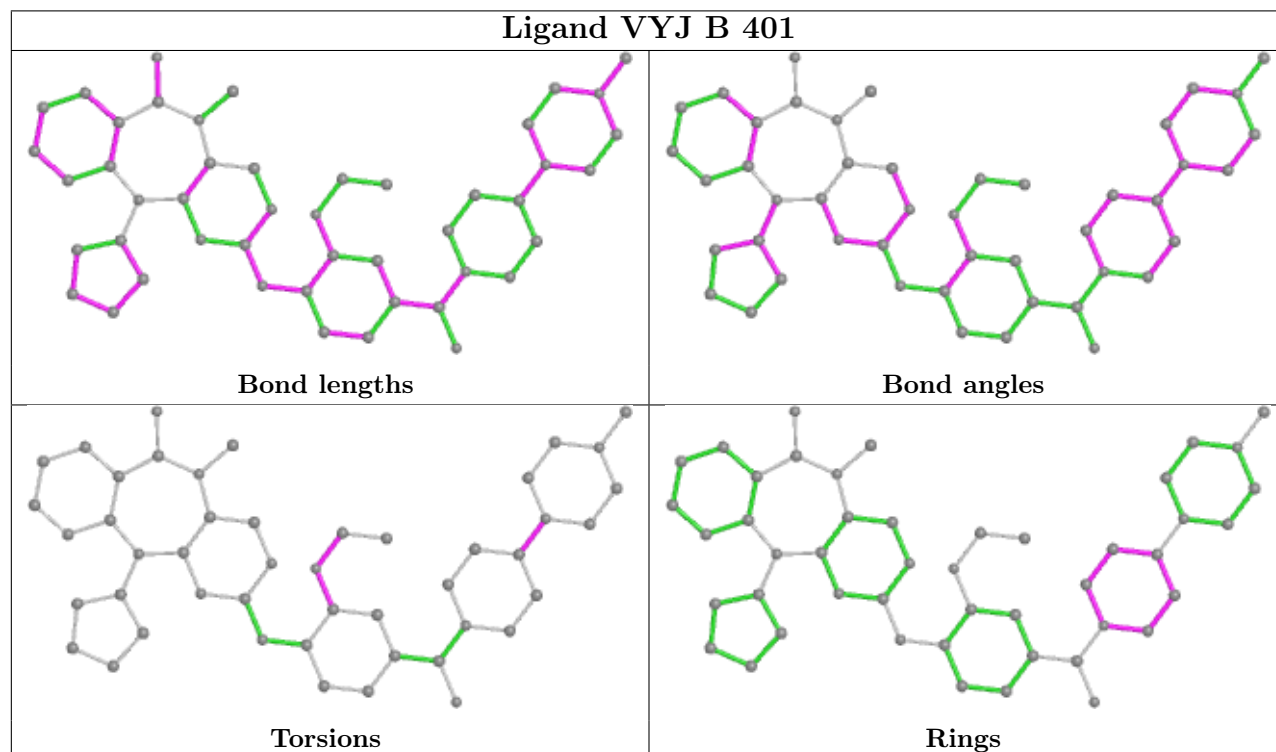
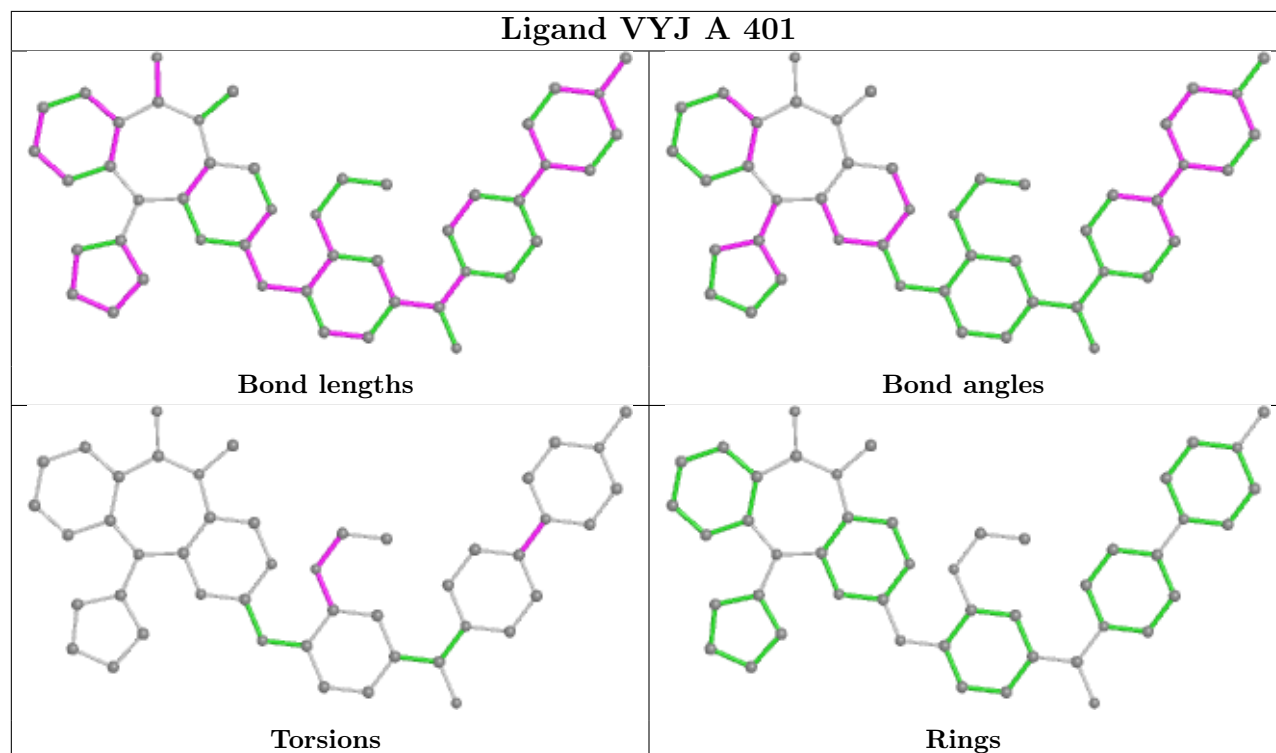
Mol	Chain	Res	Type	Atoms
2	B	401	VYJ	C11-C12-C13-C21-C22-N10

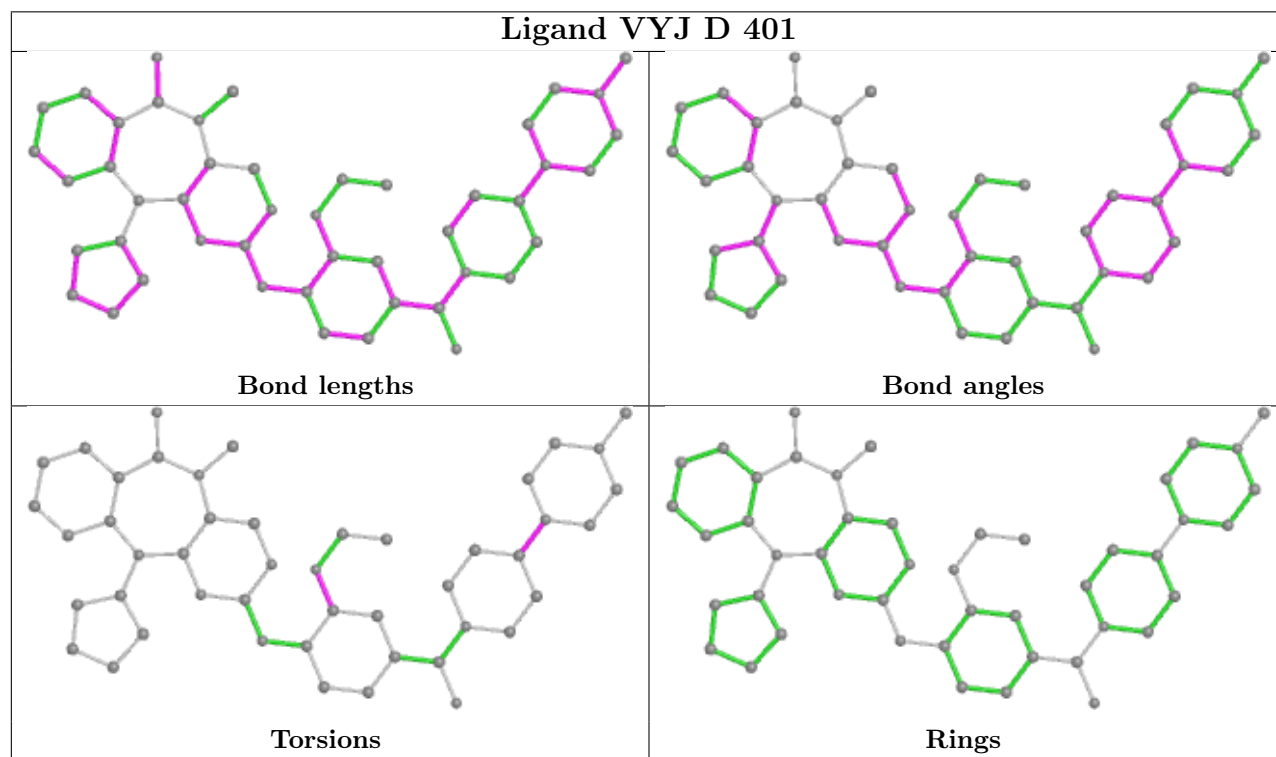
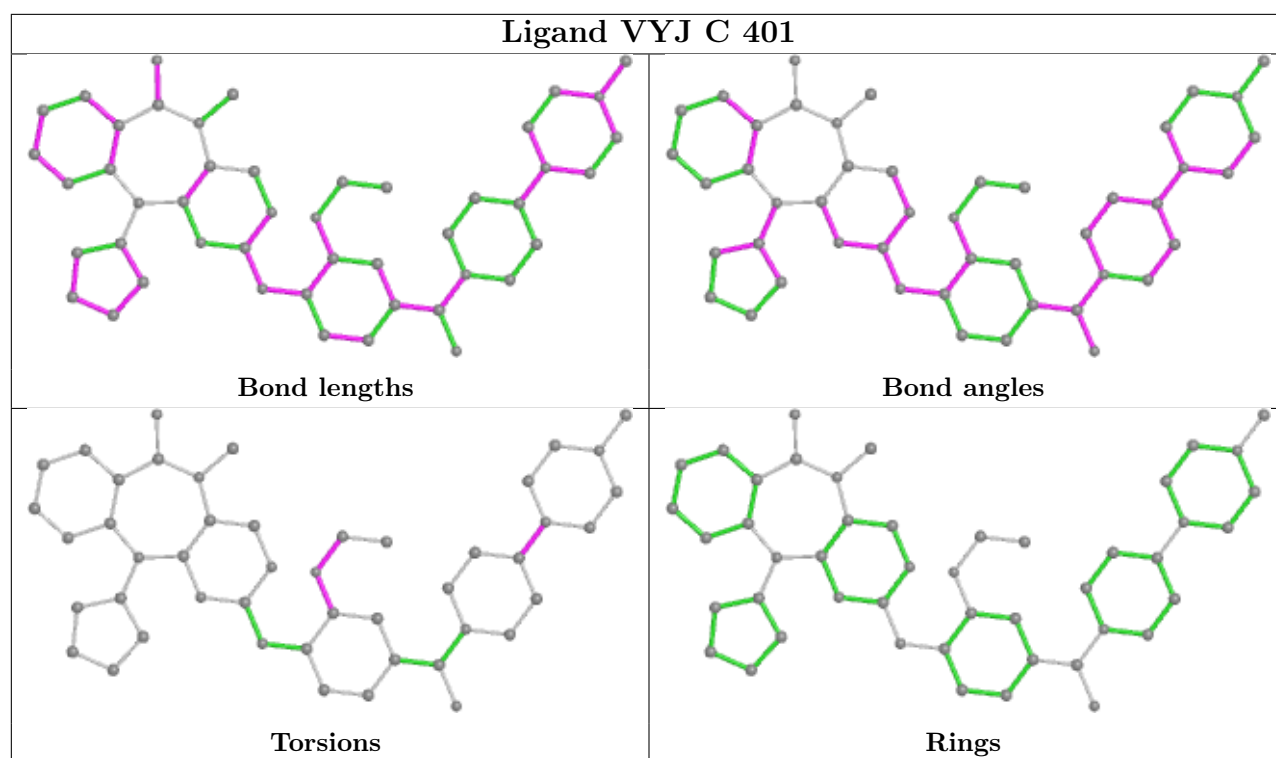
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	VYJ	1	0
2	C	401	VYJ	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 ⓘ

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	112/117 (95%)	0.20	2 (1%) 68 76	26, 37, 70, 95	0
1	B	116/117 (99%)	0.23	3 (2%) 56 65	28, 41, 61, 94	0
1	C	112/117 (95%)	0.96	13 (11%) 4 5	28, 58, 97, 118	0
1	D	114/117 (97%)	0.38	8 (7%) 16 19	29, 52, 84, 100	0
All	All	454/468 (97%)	0.44	26 (5%) 23 28	26, 46, 84, 118	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	VAL	4.6
1	C	378	ILE	4.6
1	C	335	TYR	4.5
1	C	268	LYS	3.7
1	A	267	VAL	3.5
1	D	269	VAL	3.4
1	C	271	GLU	3.3
1	C	267	VAL	3.3
1	C	338	ALA	3.2
1	D	307	HIS	3.2
1	C	373	PHE	3.2
1	C	275	HIS	2.5
1	D	377	PRO	2.5
1	D	273	LEU	2.4
1	B	307	HIS	2.3
1	D	276	CYS	2.3
1	C	307	HIS	2.3
1	C	376	ILE	2.2
1	C	285	ALA	2.2
1	B	289	PHE	2.2
1	C	377	PRO	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	267	VAL	2.1
1	D	334	ALA	2.1
1	B	263	ALA	2.1
1	A	269	VAL	2.1
1	D	331	TYR	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](#)

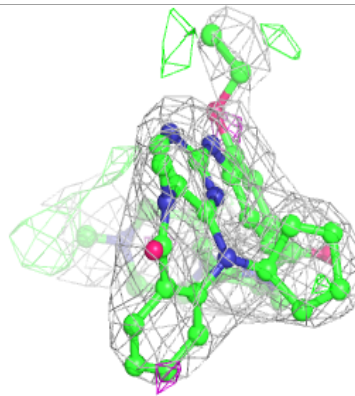
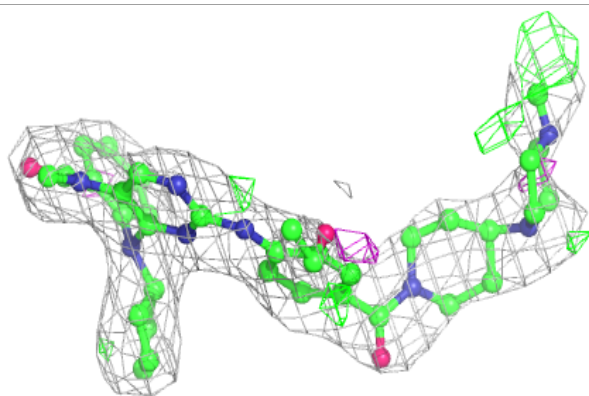
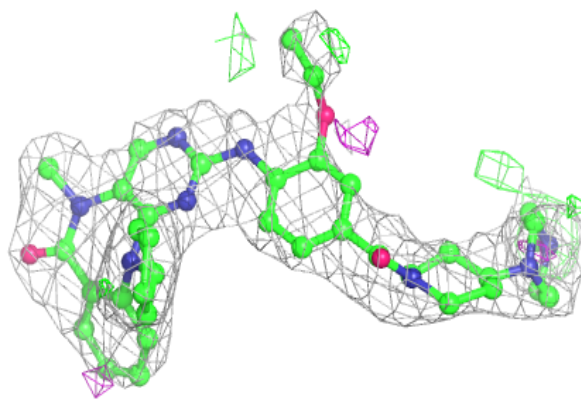
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	VYJ	A	401	47/47	0.90	0.26	16,36,77,93	0
2	VYJ	D	401	47/47	0.94	0.20	25,34,64,71	0
4	EDO	C	402	4/4	0.94	0.13	26,28,32,44	0
2	VYJ	B	401	47/47	0.95	0.20	23,39,64,74	0
2	VYJ	C	401	47/47	0.95	0.22	27,39,58,62	0
3	CL	B	402	1/1	0.96	0.21	46,46,46,46	1

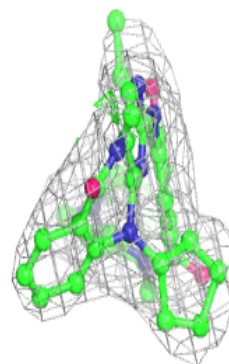
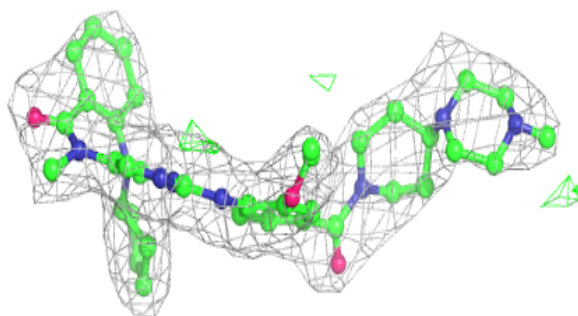
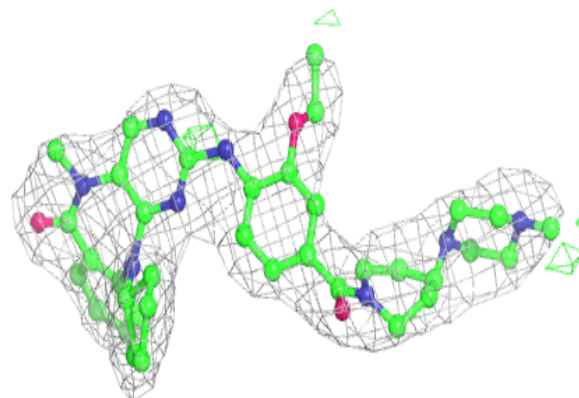
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around VYJ A 401:**

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

**Electron density around VYJ D 401:**

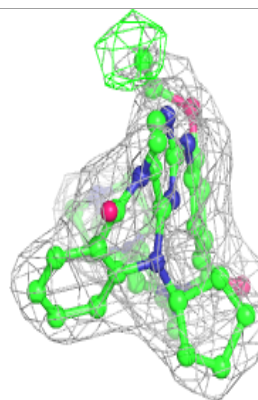
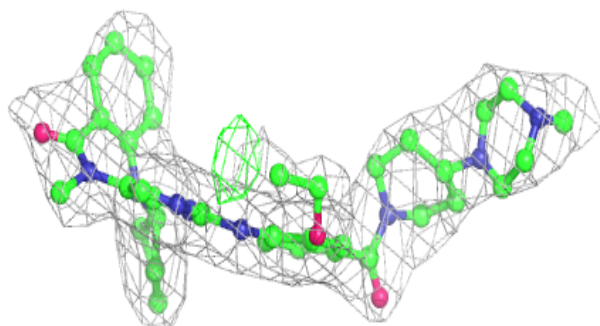
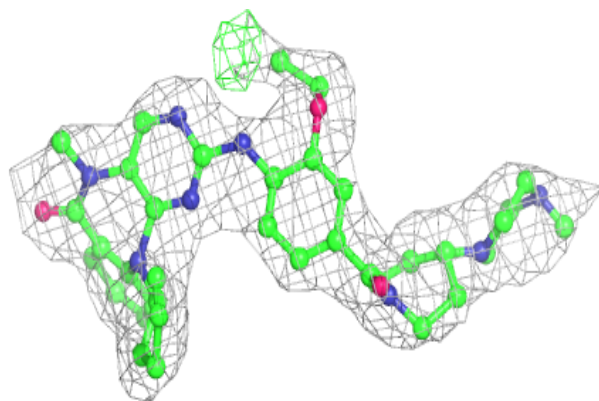
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



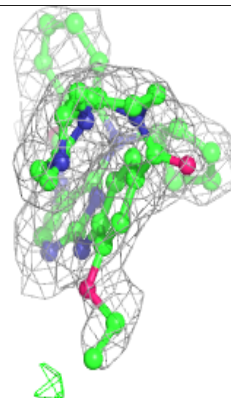
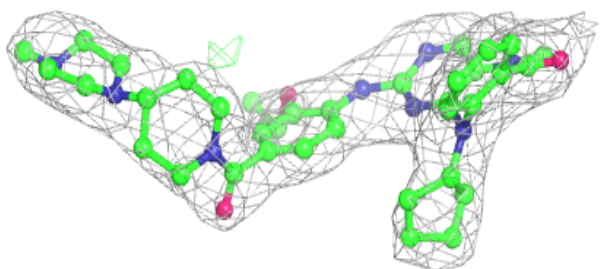
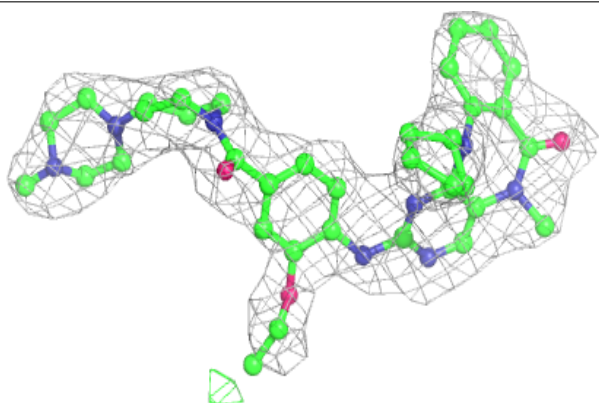


**Electron density around VYJ B 401:**

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

**Electron density around VYJ C 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.