



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:44 am BST

PDB ID : 4C2V  
Title : Aurora B kinase in complex with the specific inhibitor Barasertib  
Authors : Sessa, F.; Villa, F.  
Deposited on : 2013-08-20  
Resolution : 1.49 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.

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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 : 2.11  
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) : 2.11

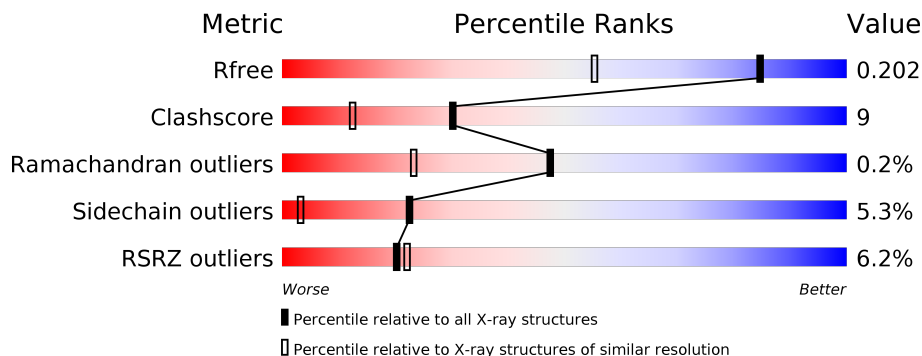
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.49 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on 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	285	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 78% 13% 5%</p>
1	B	285	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 75% 20% ...</p>
2	C	44	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5% 80% 7% 7% 7%</p>
2	D	44	<div style="display: flex; align-items: center;"> <div style="width: 25%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">25% 77% 18% ...</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5996 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.

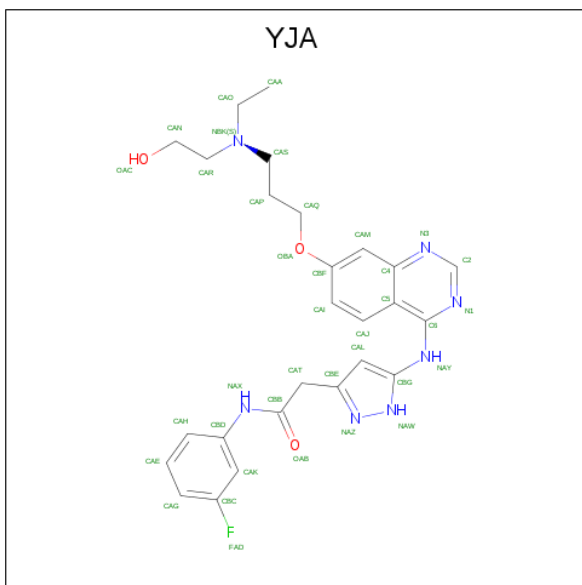
- Molecule 1 is a protein called AURORA KINASE B-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	271	Total	C	N	O	P	S	0	3	0
			2276	1458	408	396	1	13			
1	B	281	Total	C	N	O	P	S	0	4	0
			2366	1512	428	411	1	14			

- Molecule 2 is a protein called INNER CENTROMERE PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	41	Total	C	N	O	S	0	0	0
			334	217	54	62	1			
2	D	43	Total	C	N	O	S	0	0	0
			351	225	58	67	1			

- Molecule 3 is 2-[5-[[7-[3-[ethyl(2-hydroxyethyl)amino]propoxy]quinazolin-4-yl]amino]-1H-pyrazol-3-yl]-N-(3-fluorophenyl)ethanamide (three-letter code: YJA) (formula: C<sub>26</sub>H<sub>30</sub>FN<sub>7</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			37	26	1	7	3		
3	B	1	Total	C	F	N	O	0	0
			37	26	1	7	3		

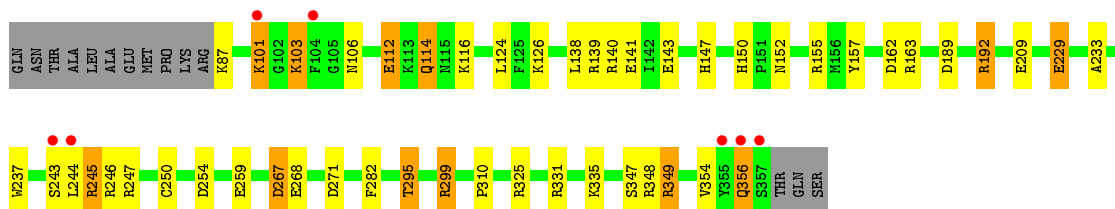
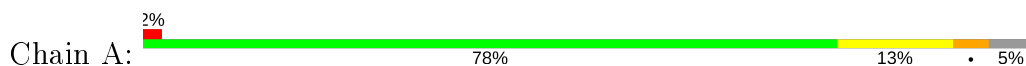
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	280	Total	O	0	0
			280	280		
4	B	282	Total	O	0	0
			282	282		
4	C	12	Total	O	0	0
			12	12		
4	D	21	Total	O	0	0
			21	21		

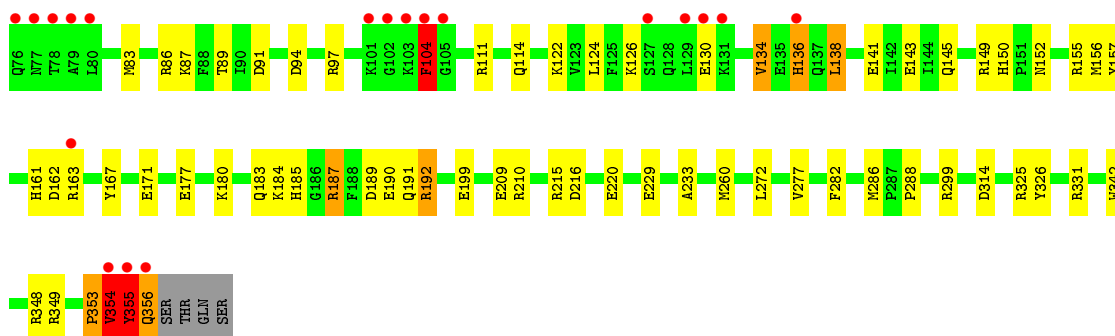
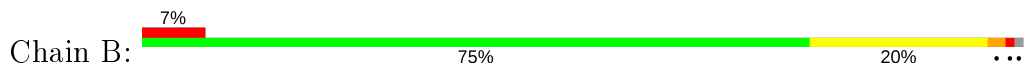
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

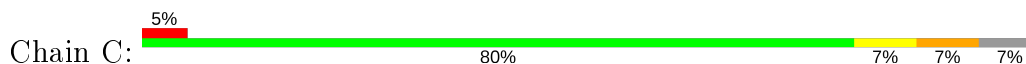
- Molecule 1: AURORA KINASE B-A



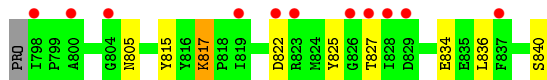
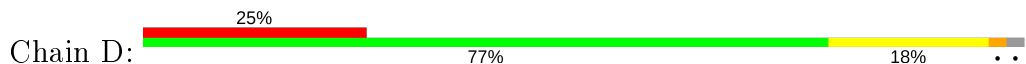
- Molecule 1: AURORA KINASE B-A



- Molecule 2: INNER CENTROMERE PROTEIN A



- Molecule 2: INNER CENTROMERE PROTEIN A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.06Å 68.10Å 117.09Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	38.77 – 1.49 44.22 – 1.49	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.77-1.49) 98.4 (44.22-1.49)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.49Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.167 , 0.197 0.174 , 0.202	Depositor DCC
$R_{free}$ test set	5766 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtrriage
Anisotropy	0.439	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: TPO, YJA

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	1.29	11/2326 (0.5%)	1.44	25/3130 (0.8%)
1	B	1.21	8/2417 (0.3%)	1.30	27/3252 (0.8%)
2	C	1.06	1/343 (0.3%)	1.22	1/466 (0.2%)
2	D	0.95	1/359 (0.3%)	1.04	0/485
All	All	1.22	21/5445 (0.4%)	1.35	53/7333 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	GLU	CD-OE1	11.23	1.38	1.25
1	B	143	GLU	CD-OE1	10.03	1.36	1.25
1	A	246	ARG	CD-NE	-9.78	1.29	1.46
1	B	220	GLU	CD-OE1	8.71	1.35	1.25
1	B	229	GLU	CD-OE1	-8.13	1.16	1.25
1	A	259	GLU	CD-OE1	7.66	1.34	1.25
1	B	199	GLU	CD-OE2	7.15	1.33	1.25
1	B	143	GLU	CG-CD	6.89	1.62	1.51
1	A	229	GLU	CD-OE1	-6.73	1.18	1.25
1	A	246	ARG	CZ-NH2	-5.58	1.25	1.33
1	B	342	TRP	CD1-NE1	-5.54	1.28	1.38
1	A	349	ARG	CG-CD	-5.51	1.38	1.51
1	B	326	TYR	CE2-CZ	-5.39	1.31	1.38
1	A	347	SER	CA-CB	-5.33	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	TYR	CE2-CZ	-5.25	1.31	1.38
2	C	815	TYR	CG-CD1	5.18	1.45	1.39
2	D	815	TYR	CG-CD1	5.11	1.45	1.39
1	B	190	GLU	CD-OE2	-5.10	1.20	1.25
1	A	141	GLU	CD-OE2	-5.06	1.20	1.25
1	A	163	ARG	CD-NE	-5.02	1.38	1.46
1	A	209	GLU	CG-CD	5.02	1.59	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH2	-22.15	109.22	120.30
1	B	325	ARG	NE-CZ-NH2	-14.63	112.98	120.30
1	A	163	ARG	NE-CZ-NH2	-13.89	113.36	120.30
1	A	246	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	A	245	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	192	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	B	260	MET	CG-SD-CE	-12.06	80.90	100.20
1	A	163	ARG	NE-CZ-NH1	10.55	125.57	120.30
1	A	325	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	A	245	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	A	247	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	B	331	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	B	210	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	325	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	162	ASP	CB-CG-OD1	7.25	124.83	118.30
2	C	815	TYR	CB-CG-CD1	7.21	125.33	121.00
1	A	192	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	83	MET	CG-SD-CE	6.82	111.11	100.20
1	A	282	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	A	271	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	140	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	215	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	189	ASP	CB-CG-OD1	6.47	124.13	118.30
1	B	187[A]	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	187[B]	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	229	GLU	CA-CB-CG	6.32	127.31	113.40
1	A	349	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	A	209	GLU	CG-CD-OE2	-6.16	105.97	118.30
1	A	267	ASP	CB-CG-OD1	5.97	123.68	118.30
1	B	192	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	282	PHE	CB-CG-CD2	-5.88	116.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	299	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	104	PHE	CA-C-N	5.62	127.43	116.20
1	A	209	GLU	CG-CD-OE1	5.61	129.52	118.30
1	A	189	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	272	LEU	CB-CG-CD1	5.55	120.43	111.00
1	B	111	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	157	TYR	CG-CD1-CE1	5.31	125.55	121.30
1	B	216	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	247	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	314	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	A	331	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	167	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	B	187[A]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	187[B]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	229	GLU	CG-CD-OE1	-5.09	108.12	118.30
1	A	140	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	143	GLU	CA-CB-CG	5.07	124.55	113.40
1	B	199	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	162	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	299	ARG	CG-CD-NE	-5.02	101.26	111.80
1	B	220	GLU	CG-CD-OE2	-5.01	108.28	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	89	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	PHE	Peptide
1	B	353	PRO	Peptide
1	B	354	VAL	Peptide
1	B	355	TYR	Peptide

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

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2276	0	2277	34	1
1	B	2366	0	2372	53	0
2	C	334	0	331	4	0
2	D	351	0	347	5	0
3	A	37	0	30	6	0
3	B	37	0	30	12	0
4	A	280	0	0	11	5
4	B	282	0	0	21	2
4	C	12	0	0	2	1
4	D	21	0	0	2	0
All	All	5996	0	5387	100	6

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 9.

All (100) 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)
3:B:1357:YJA:FAD	3:B:1357:YJA:CBC	1.64	1.36
1:B:185:HIS:CE1	4:B:2119:HOH:O	1.73	1.29
1:B:348:ARG:CZ	4:B:2277:HOH:O	1.89	1.21
1:B:348:ARG:NH2	4:B:2277:HOH:O	1.73	1.19
1:B:94:ASP:OD2	4:B:2024:HOH:O	1.70	1.07
1:B:286:MET:HG2	4:B:2214:HOH:O	1.55	1.04
1:B:355:TYR:HB3	1:B:356:GLN:HA	1.45	0.98
1:A:101:LYS:NZ	1:A:106:ASN:OD1	2.08	0.86
3:B:1357:YJA:OAB	3:B:1357:YJA:HAK	1.81	0.81
1:B:150:HIS:HD2	1:B:152:ASN:H	1.26	0.80
1:A:150:HIS:HD2	1:A:152:ASN:H	1.26	0.80
1:B:354:VAL:HG12	1:B:355:TYR:H	1.46	0.79
1:B:185:HIS:ND1	4:B:2119:HOH:O	1.95	0.78
1:B:114:GLN:NE2	4:B:2013:HOH:O	2.17	0.77
1:B:134:VAL:HG13	4:B:2044:HOH:O	1.84	0.77
1:A:143:GLU:OE1	4:A:2047:HOH:O	2.02	0.75
1:A:268:GLU:HG3	4:A:2137:HOH:O	1.89	0.73
1:A:139:ARG:NH2	4:A:2039:HOH:O	2.10	0.73
1:B:191:GLN:HG2	4:B:2277:HOH:O	1.88	0.72
1:B:353:PRO:HB3	1:B:354:VAL:HB	1.71	0.72
1:A:356:GLN:HA	1:A:356:GLN:OE1	1.89	0.71
1:B:355:TYR:CB	1:B:356:GLN:HA	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:HIS:CD2	1:B:152:ASN:H	2.09	0.70
1:B:138:LEU:HD23	3:B:1357:YJA:HAG	1.74	0.70
1:A:150:HIS:CD2	1:A:152:ASN:H	2.08	0.70
1:B:191:GLN:CG	4:B:2277:HOH:O	2.38	0.70
3:A:1357:YJA:CAH	4:A:2043:HOH:O	2.42	0.65
1:B:355:TYR:HB3	1:B:356:GLN:CA	2.23	0.63
2:D:834:GLU:HB3	4:D:2018:HOH:O	1.98	0.63
1:A:237:TRP:CD2	1:A:250:CYS:HB2	2.34	0.62
1:A:138:LEU:HD12	3:A:1357:YJA:HAG	1.82	0.62
1:B:138:LEU:CD2	3:B:1357:YJA:HAG	2.30	0.61
1:A:112:GLU:HG2	2:D:825:TYR:OH	2.00	0.61
1:A:310:PRO:HG2	4:A:2226:HOH:O	2.00	0.61
3:A:1357:YJA:HAP2	3:A:1357:YJA:HAN1	1.85	0.59
1:A:101:LYS:HA	1:A:101:LYS:HZ3	1.66	0.59
2:D:817:LYS:HG2	4:D:2014:HOH:O	2.03	0.58
1:B:353:PRO:CB	1:B:354:VAL:HB	2.33	0.58
1:A:143:GLU:O	1:A:147:HIS:HD2	1.86	0.58
1:B:354:VAL:HG12	1:B:355:TYR:N	2.18	0.58
1:B:126:LYS:NZ	1:B:161:HIS:HD2	2.03	0.56
1:B:134:VAL:CG1	4:B:2044:HOH:O	2.49	0.56
1:A:152:ASN:HD21	1:A:349:ARG:HH21	1.53	0.56
1:B:353:PRO:CA	1:B:354:VAL:HB	2.36	0.56
1:A:103:LYS:HE3	1:A:103:LYS:H	1.70	0.55
1:B:122:LYS:HE2	1:B:124:LEU:HD21	1.87	0.55
1:B:89:THR:HG23	1:B:91:ASP:H	1.72	0.54
1:A:233:ALA:O	3:A:1357:YJA:HAT1	2.07	0.54
1:B:354:VAL:CG1	1:B:355:TYR:H	2.19	0.54
1:B:171:GLU:O	3:B:1357:YJA:H2	2.08	0.53
1:B:354:VAL:CG1	1:B:355:TYR:N	2.71	0.53
1:A:245:ARG:NH2	1:A:267:ASP:OD2	2.42	0.52
3:B:1357:YJA:OAB	3:B:1357:YJA:CAK	2.50	0.52
1:B:191:GLN:HG3	4:B:2277:HOH:O	2.06	0.52
1:B:155:ARG:NE	4:B:2069:HOH:O	2.42	0.52
2:C:834:GLU:HG3	4:C:2012:HOH:O	2.10	0.52
1:A:237:TRP:CE3	1:A:250:CYS:HB2	2.45	0.52
1:B:348:ARG:NE	4:B:2277:HOH:O	2.25	0.52
1:A:295:THR:HG23	4:A:2214:HOH:O	2.09	0.51
1:B:141:GLU:HG2	3:B:1357:YJA:CAE	2.40	0.51
1:A:354:VAL:HG22	4:A:2274:HOH:O	2.10	0.51
2:C:823:ARG:NH1	4:C:2010:HOH:O	2.25	0.51
1:B:87:LYS:HE3	4:B:2007:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1357:YJA:HAL	3:B:1357:YJA:N1	2.27	0.50
1:B:209:GLU:HG2	4:B:2153:HOH:O	2.12	0.49
1:A:112:GLU:OE2	1:A:114:GLN:HB2	2.12	0.49
3:A:1357:YJA:HAH	4:A:2043:HOH:O	2.10	0.49
1:A:155:ARG:NH2	2:D:822:ASP:OD2	2.46	0.48
1:B:184:LYS:HE2	4:B:2119:HOH:O	2.14	0.48
1:B:155:ARG:HD2	4:B:2066:HOH:O	2.13	0.48
1:A:101:LYS:HA	1:A:101:LYS:NZ	2.29	0.47
1:B:145:GLN:OE1	3:B:1357:YJA:HAH	2.14	0.47
1:B:353:PRO:HA	1:B:354:VAL:HB	1.96	0.47
1:B:353:PRO:HD3	2:C:815:TYR:CZ	2.50	0.47
1:B:152:ASN:HD21	1:B:349:ARG:HH21	1.63	0.46
1:B:354:VAL:O	1:B:355:TYR:CG	2.70	0.45
1:A:87:LYS:HD2	4:A:2002:HOH:O	2.17	0.45
1:B:136:HIS:C	1:B:136:HIS:CD2	2.90	0.44
1:B:286:MET:HE3	4:B:2214:HOH:O	2.16	0.44
1:A:237:TRP:CE3	1:A:250:CYS:CB	3.01	0.44
1:A:152:ASN:ND2	1:A:349:ARG:HH21	2.16	0.43
1:B:277:VAL:HG13	1:B:288:PRO:HD2	2.00	0.43
1:A:101:LYS:CE	1:A:101:LYS:HA	2.49	0.43
1:B:156:MET:CE	3:B:1357:YJA:HAH	2.48	0.43
1:A:139:ARG:HB2	1:A:139:ARG:CZ	2.48	0.43
1:A:126:LYS:HE2	2:D:836:LEU:O	2.19	0.43
1:A:354:VAL:HG13	4:A:2274:HOH:O	2.17	0.43
1:A:101:LYS:CE	1:A:106:ASN:OD1	2.67	0.42
1:B:161:HIS:HE1	4:B:2095:HOH:O	2.02	0.42
1:B:187[B]:ARG:HH11	1:B:187[B]:ARG:HD3	1.72	0.42
1:A:243:SER:OG	1:A:244:LEU:HD13	2.19	0.42
1:A:138:LEU:CD1	3:A:1357:YJA:HAG	2.48	0.42
1:A:155:ARG:NH1	4:A:2063:HOH:O	2.49	0.42
1:B:104:PHE:HE1	1:B:177:GLU:CD	2.23	0.41
3:B:1357:YJA:CAL	3:B:1357:YJA:N1	2.80	0.41
1:B:233:ALA:O	3:B:1357:YJA:HAT1	2.20	0.41
1:B:180:LYS:HA	1:B:183:GLN:HG2	2.03	0.40
1:B:355:TYR:HA	1:B:355:TYR:HD1	1.74	0.40
2:C:824:MET:HE3	2:C:824:MET:HB3	1.79	0.40
1:B:149:ARG:HD2	4:B:2052:HOH:O	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2032:HOH:O	4:A:2098:HOH:O[2_555]	1.16	1.04
4:B:2223:HOH:O	4:C:2001:HOH:O[2_756]	1.21	0.99
4:A:2008:HOH:O	4:A:2212:HOH:O[2_555]	1.21	0.99
4:A:2007:HOH:O	4:A:2214:HOH:O[2_555]	1.43	0.77
1:A:348:ARG:NH1	4:A:2197:HOH:O[1_655]	1.99	0.21
4:A:2258:HOH:O	4:B:2229:HOH:O[1_545]	2.12	0.08

## 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	271/285 (95%)	262 (97%)	9 (3%)	0	100	100
1	B	282/285 (99%)	271 (96%)	10 (4%)	1 (0%)	34	13
2	C	39/44 (89%)	39 (100%)	0	0	100	100
2	D	41/44 (93%)	40 (98%)	1 (2%)	0	100	100
All	All	633/658 (96%)	612 (97%)	20 (3%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	VAL

### 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	247/256 (96%)	235 (95%)	12 (5%)	25	4
1	B	256/256 (100%)	246 (96%)	10 (4%)	32	7
2	C	36/39 (92%)	32 (89%)	4 (11%)	6	0
2	D	38/39 (97%)	34 (90%)	4 (10%)	7	0
All	All	577/590 (98%)	547 (95%)	30 (5%)	22	3

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	103	LYS
1	A	112	GLU
1	A	114	GLN
1	A	116	LYS
1	A	124	LEU
1	A	192	ARG
1	A	229	GLU
1	A	295	THR
1	A	299	ARG
1	A	335	LYS
1	A	356	GLN
1	B	86	ARG
1	B	97	ARG
1	B	130	GLU
1	B	134	VAL
1	B	136	HIS
1	B	138	LEU
1	B	163	ARG
1	B	192	ARG
1	B	355	TYR
1	B	356	GLN
2	C	806	LEU
2	C	823	ARG
2	C	829	ASP
2	C	834	GLU
2	D	805	ASN
2	D	817	LYS
2	D	827	THR
2	D	840	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	136	HIS
1	A	147	HIS
1	A	150	HIS
1	A	152	ASN
1	A	298	HIS
1	B	115	ASN
1	B	150	HIS
1	B	152	ASN
1	B	161	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](#)

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPO	B	248	1	8,10,11	0.90	0	10,14,16	1.23	1 (10%)
1	TPO	A	248	1	8,10,11	0.57	0	10,14,16	0.76	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
1	TPO	B	248	1	-	0/9/11/13	-
1	TPO	A	248	1	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	TPO	OG1-P-O1P	-2.26	100.68	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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
3	YJA	A	1357	-	39,40,40	1.76	6 (15%)	46,53,53	2.18	14 (30%)
3	YJA	B	1357	-	39,40,40	2.81	7 (17%)	46,53,53	2.67	18 (39%)

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
3	YJA	A	1357	-	-	3/20/24/24	0/4/4/4
3	YJA	B	1357	-	-	9/20/24/24	0/4/4/4

All (13) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1357	YJA	FAD-CBC	11.42	1.64	1.36
3	B	1357	YJA	CAT-CBE	9.33	1.60	1.51
3	A	1357	YJA	FAD-CBC	5.27	1.49	1.36
3	A	1357	YJA	CAT-CBE	5.20	1.56	1.51
3	B	1357	YJA	CBD-NAX	-4.57	1.32	1.41
3	B	1357	YJA	C2-N3	4.30	1.39	1.32
3	A	1357	YJA	NAW-NAZ	-4.00	1.29	1.37
3	A	1357	YJA	C6-N1	3.04	1.38	1.34
3	B	1357	YJA	CAT-CBB	3.00	1.58	1.51
3	A	1357	YJA	CAT-CBB	2.97	1.58	1.51
3	B	1357	YJA	CAL-CBE	-2.87	1.35	1.39
3	B	1357	YJA	CAM-C4	2.56	1.45	1.41
3	A	1357	YJA	CAJ-CAI	2.56	1.42	1.36

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1357	YJA	C5-C4-N3	-6.87	115.51	122.83
3	A	1357	YJA	C6-C5-C4	6.66	120.07	115.88
3	B	1357	YJA	CBD-CAK-CBC	6.26	123.53	117.95
3	B	1357	YJA	C6-C5-C4	5.99	119.65	115.88
3	B	1357	YJA	CAG-CBC-CAK	-5.29	116.41	123.29
3	B	1357	YJA	CBG-CAL-CBE	5.10	110.95	105.95
3	A	1357	YJA	C5-C6-N1	-4.96	117.27	121.35
3	A	1357	YJA	CAJ-C5-C4	-4.38	113.43	118.33
3	B	1357	YJA	C2-N3-C4	4.30	121.33	115.40
3	A	1357	YJA	CAR-NBK-CAS	3.91	120.73	111.44
3	B	1357	YJA	CBD-NAX-CBB	-3.62	121.17	127.50
3	A	1357	YJA	C5-C4-N3	-3.43	119.18	122.83
3	B	1357	YJA	FAD-CBC-CAG	3.37	124.27	118.54
3	B	1357	YJA	CAQ-OBA-CBF	3.36	126.71	117.93
3	B	1357	YJA	CAM-C4-C5	3.27	123.42	119.65
3	B	1357	YJA	CAL-CBE-NAZ	-3.26	106.84	111.44
3	A	1357	YJA	CAL-CBG-NAW	-3.20	105.90	110.47
3	B	1357	YJA	CAL-CBG-NAW	-3.19	105.90	110.47
3	A	1357	YJA	CAI-CBF-CAM	-3.16	116.56	120.81
3	B	1357	YJA	CAP-CAS-NBK	-3.15	105.90	113.84
3	A	1357	YJA	CAM-C4-C5	3.10	123.22	119.65
3	B	1357	YJA	CAJ-C5-C4	-3.08	114.88	118.33
3	A	1357	YJA	OAB-CBB-NAX	2.68	128.51	123.63
3	A	1357	YJA	OAC-CAN-CAR	-2.66	100.17	111.19
3	B	1357	YJA	CAM-C4-N3	2.62	120.96	117.97
3	B	1357	YJA	OBA-CAQ-CAP	-2.42	99.33	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1357	YJA	CBD-CAK-CBC	2.31	120.02	117.95
3	A	1357	YJA	CBF-CAM-C4	2.29	121.67	119.27
3	A	1357	YJA	FAD-CBC-CAG	2.27	122.40	118.54
3	B	1357	YJA	CAJ-CAI-CBF	2.21	123.13	120.17
3	B	1357	YJA	N3-C2-N1	-2.02	125.52	128.68
3	A	1357	YJA	CAT-CBB-NAX	-2.02	110.60	114.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1357	YJA	CAN-CAR-NBK-CAS
3	B	1357	YJA	OAC-CAN-CAR-NBK
3	B	1357	YJA	CAS-CAP-CAQ-OBA
3	A	1357	YJA	CAA-CAO-NBK-CAR
3	B	1357	YJA	CAP-CAQ-OBA-CBF
3	B	1357	YJA	C5-C6-NAY-CBG
3	A	1357	YJA	CAA-CAO-NBK-CAS
3	B	1357	YJA	CAM-CBF-OBA-CAQ
3	B	1357	YJA	CAA-CAO-NBK-CAS
3	B	1357	YJA	CAA-CAO-NBK-CAR
3	B	1357	YJA	CAI-CBF-OBA-CAQ
3	B	1357	YJA	OAB-CBB-NAX-CBD

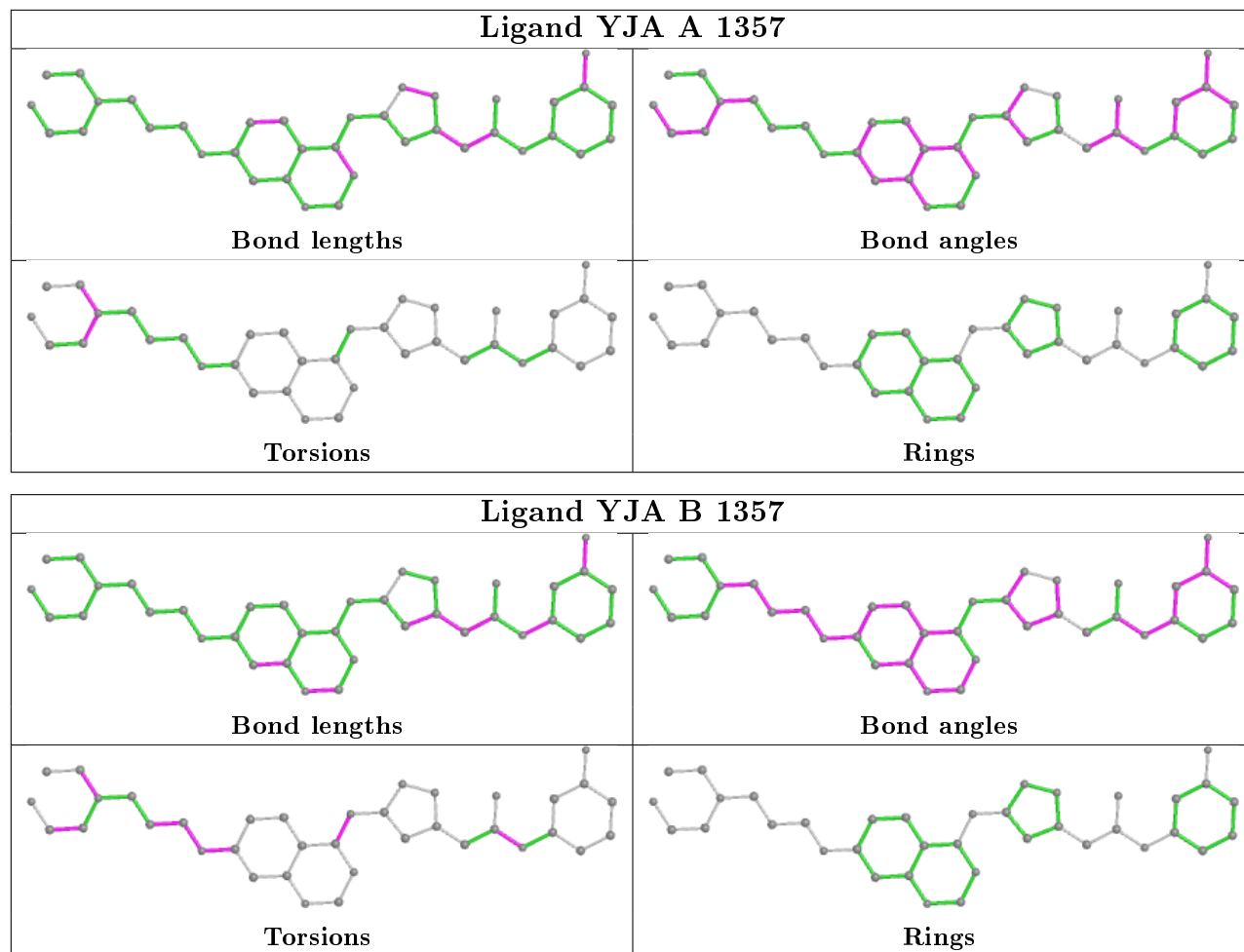
There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1357	YJA	6	0
3	B	1357	YJA	12	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	270/285 (94%)	-0.06	7 (2%) 56 61	9, 17, 37, 66	0
1	B	280/285 (98%)	-0.01	19 (6%) 17 18	9, 17, 48, 91	0
2	C	41/44 (93%)	0.25	2 (4%) 29 32	19, 28, 44, 57	0
2	D	43/44 (97%)	1.12	11 (25%) 0 0	17, 36, 52, 67	0
All	All	634/658 (96%)	0.06	39 (6%) 20 22	9, 18, 48, 91	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	PHE	6.3
1	B	76	GLN	5.7
2	C	837	PHE	5.7
1	B	103	LYS	5.6
1	B	102	GLY	5.3
1	B	101	LYS	4.4
2	D	826	GLY	4.3
1	B	78	THR	4.1
2	D	827	THR	4.1
1	B	355	TYR	3.6
1	B	354	VAL	3.6
1	B	80	LEU	3.6
1	B	77	ASN	3.6
1	A	357	SER	3.6
1	B	129	LEU	3.4
2	D	798	ILE	3.4
2	D	837	PHE	3.3
1	B	79	ALA	3.3
1	B	131	LYS	3.2
1	B	104	PHE	3.1
2	D	823	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	828	ILE	3.0
2	D	819	ILE	2.9
2	D	800	ALA	2.8
1	B	105	GLY	2.8
1	B	163	ARG	2.8
2	D	829	ASP	2.7
1	A	101	LYS	2.7
1	B	136	HIS	2.7
2	C	834	GLU	2.6
1	A	244	LEU	2.6
1	A	355	TYR	2.5
1	A	243	SER	2.5
2	D	822	ASP	2.3
1	B	130	GLU	2.3
1	B	127	SER	2.3
2	D	804	GLY	2.1
1	B	356	GLN	2.1
1	A	356	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	TPO	A	248	11/12	0.98	0.05	15,16,17,18	0
1	TPO	B	248	11/12	0.99	0.05	14,16,17,18	0

## 6.3 Carbohydrates [i](#)

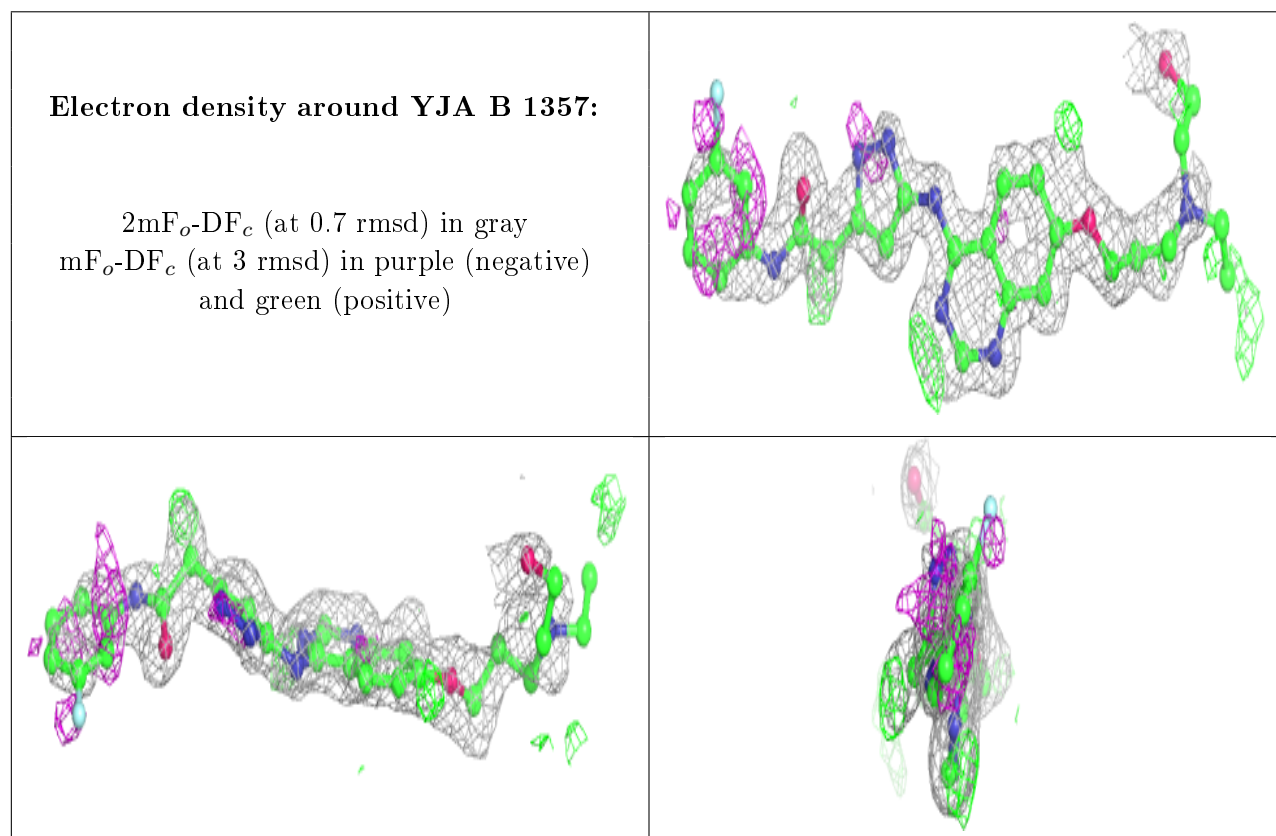
There are no carbohydrates in this entry.

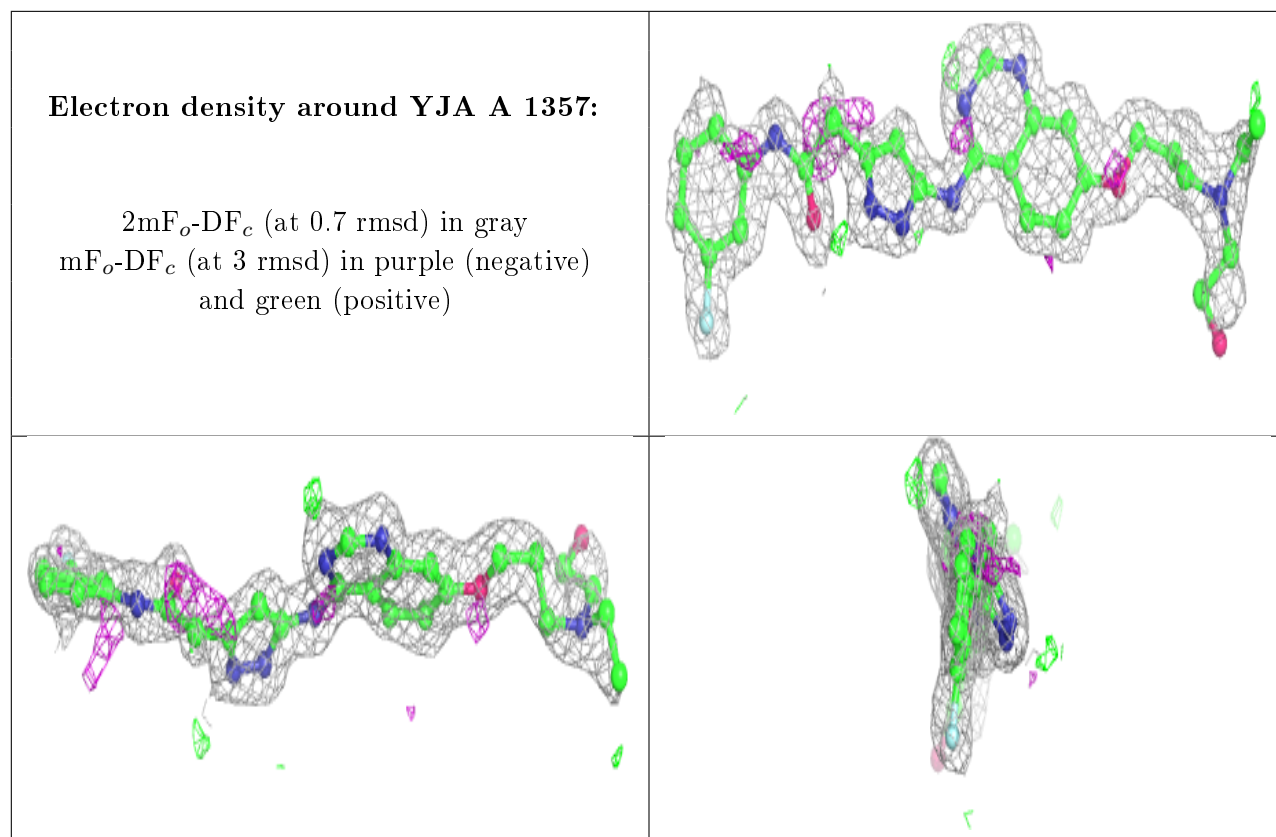
## 6.4 Ligands [i](#)

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
3	YJA	B	1357	37/37	0.79	0.26	19,38,63,65	0
3	YJA	A	1357	37/37	0.89	0.18	18,28,61,70	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.