



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:50 AM UTC

PDB ID : 4C2V / pdb_00004c2v
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 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

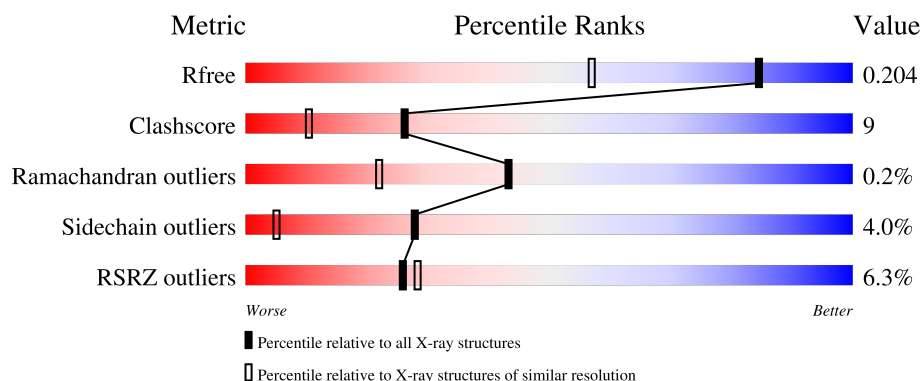
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	4% 76% 15% 5%
1	B	285	7% 79% 16% ...
2	C	44	7% 75% 14% 5% 7%
2	D	44	14% 77% 18% ...

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.

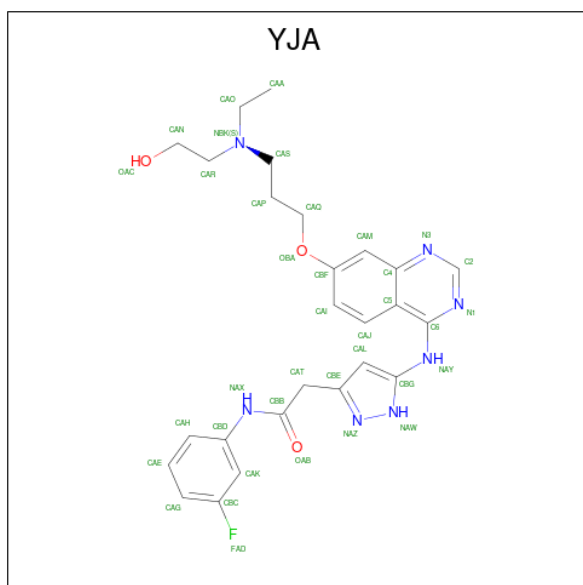
- Molecule 1 is a protein called AURORA KINASE B-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
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
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 (CCD ID: YJA) (formula: C₂₆H₃₀FN₇O₃).



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.

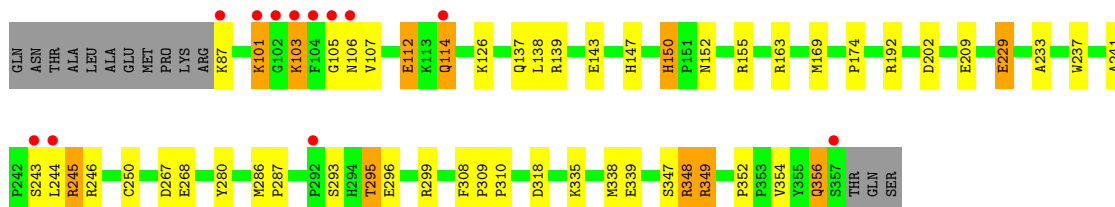
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	280	Total	O	0	0
			280	280		
4	B	282	Total	O	0	0
			282	282		
4	C	12	Total	O	0	0
			12	12		
4	D	21	Total	O	0	0
			21	21		

3 Residue-property plots

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.

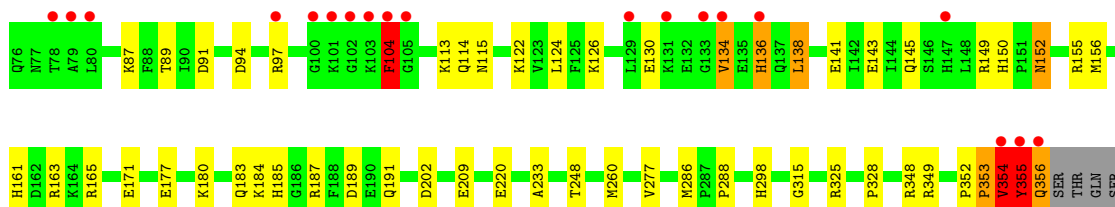
• Molecule 1: AURORA KINASE B-A

Chain A: 



• Molecule 1: AURORA KINASE B-A

Chain B: 



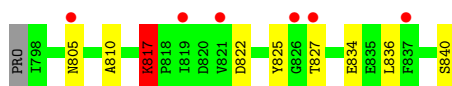
• Molecule 2: INNER CENTROMERE PROTEIN A

Chain C: 



• Molecule 2: INNER CENTROMERE PROTEIN A

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.06Å 68.10Å 117.09Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	38.77 – 1.49 38.77 – 1.49	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.77-1.49) 98.4 (38.77-1.49)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.167 , 0.197 (Not available) , 0.204	Depositor DCC
R_{free} test set	5766 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5996	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.58	18/2326 (0.8%)	1.48	21/3130 (0.7%)
1	B	1.47	9/2417 (0.4%)	1.32	8/3252 (0.2%)
2	C	1.29	2/343 (0.6%)	1.36	2/466 (0.4%)
2	D	1.14	0/359	1.28	2/485 (0.4%)
All	All	1.49	29/5445 (0.5%)	1.39	33/7333 (0.5%)

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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ARG	CD-NE	-11.73	1.29	1.46
1	B	352	PRO	CA-C	9.21	1.56	1.51
1	A	209	GLU	CD-OE1	6.66	1.38	1.25
1	A	348	ARG	N-CA	6.03	1.53	1.46
1	B	143	GLU	CD-OE1	5.96	1.36	1.25
1	A	163	ARG	CD-NE	-5.96	1.38	1.46
1	A	246	ARG	CZ-NH2	-5.89	1.25	1.33
1	B	355	TYR	N-CA	5.86	1.53	1.46
1	B	189	ASP	N-CA	-5.57	1.38	1.45
1	A	339	GLU	N-CA	5.53	1.53	1.46
1	A	202	ASP	CG-OD1	-5.46	1.15	1.25
1	A	169	MET	CA-C	5.46	1.59	1.52
1	A	318	ASP	N-CA	-5.39	1.40	1.46
1	A	280	TYR	N-CA	5.32	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	819	ILE	C-O	5.30	1.28	1.23
1	A	293	SER	N-CA	-5.21	1.39	1.46
1	B	165	ARG	N-CA	5.21	1.52	1.45
1	B	220	GLU	CD-OE1	5.20	1.35	1.25
1	B	152	ASN	C-O	5.19	1.30	1.24
1	B	298	HIS	N-CA	-5.17	1.40	1.46
1	A	296	GLU	N-CA	-5.15	1.40	1.46
1	A	241	ALA	C-O	-5.13	1.18	1.24
1	A	338	MET	SD-CE	-5.11	1.66	1.79
2	C	806	LEU	N-CA	5.10	1.52	1.46
1	A	107	VAL	N-CA	5.09	1.52	1.46
1	A	308	PHE	C-O	5.07	1.30	1.24
1	A	347	SER	CA-CB	-5.03	1.45	1.53
1	A	349	ARG	NE-CZ	-5.02	1.27	1.33
1	B	202	ASP	N-CA	5.02	1.52	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH2	-11.08	109.22	119.20
1	B	260	MET	CG-SD-CE	-9.09	80.90	100.90
1	A	105	GLY	N-CA-C	7.60	121.75	110.42
1	B	325	ARG	NE-CZ-NH2	-6.91	112.98	119.20
1	B	328	PRO	N-CA-C	6.74	118.93	110.70
1	A	229	GLU	CA-CB-CG	6.60	127.31	114.10
1	A	163	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	A	150	HIS	O-C-N	-6.21	117.50	121.85
1	A	309	PRO	N-CA-C	6.17	116.40	110.47
1	A	308	PHE	CA-C-N	-5.94	115.33	119.66
1	A	308	PHE	C-N-CA	-5.94	115.33	119.66
1	B	104	PHE	CB-CA-C	-5.85	100.67	110.56
2	C	819	ILE	CA-C-O	-5.79	117.11	121.68
1	A	137	GLN	N-CA-CB	-5.77	101.64	110.12
1	A	245	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	A	286	MET	CA-C-N	-5.55	114.66	120.38
1	A	286	MET	C-N-CA	-5.55	114.66	120.38
1	A	192	ARG	NE-CZ-NH2	-5.49	114.25	119.20
1	A	349	ARG	CD-NE-CZ	-5.48	116.72	124.40
1	A	246	ARG	CB-CG-CD	-5.45	98.78	111.30
1	B	113	LYS	N-CA-C	5.43	117.20	111.28
1	A	209	GLU	CG-CD-OE2	-5.40	105.97	118.40
1	A	246	ARG	NE-CZ-NH1	5.38	126.89	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	GLU	CA-CB-CG	5.22	124.55	114.10
1	A	352	PRO	O-C-N	5.22	123.71	121.31
1	A	174	PRO	N-CA-C	5.19	120.66	113.65
1	B	315	GLY	O-C-N	5.16	127.14	122.19
1	A	287	PRO	CA-C-N	5.15	124.65	119.19
1	A	287	PRO	C-N-CA	5.15	124.65	119.19
2	D	810	ALA	O-C-N	5.15	127.58	122.12
2	C	833	LEU	N-CA-C	5.09	117.49	111.33
2	D	817	LYS	CB-CG-CD	5.07	122.95	111.30
1	B	354	VAL	CB-CA-C	5.05	119.57	111.29

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

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	55	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	21	0	0	2	0
All	All	5996	0	5387	101	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 (101) 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:HAK	3:B:1357:YJA:OAB	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ3	1:A:101:LYS:HA	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:B:126:LYS:HZ3	1:B:161:HIS:HD2	1.55	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
3:B:1357:YJA:N1	3:B:1357:YJA:HAL	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
1:B:136:HIS:CD2	1:B:136:HIS:C	2.90	0.49
3:A:1357:YJA:HAH	4:A:2043:HOH:O	2.10	0.49
1:B:115:ASN:HD21	2:C:824:MET:HE2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:NZ	1:A:101:LYS:HA	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:104:PHE:HE1	1:B:177:GLU:CD	2.23	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: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:HA	1:A:101:LYS:CE	2.49	0.43
1:B:156:MET:CE	3:B:1357:YJA:HAH	2.48	0.43
1:A:139:ARG:CZ	1:A:139:ARG:HB2	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:B:286:MET:HE3	4:B:2214:HOH:O	2.18	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:233:ALA:O	3:B:1357:YJA:HAT1	2.20	0.41
3:B:1357:YJA:N1	3:B:1357:YJA:CAL	2.80	0.41
1:B:180:LYS:HA	1:B:183:GLN:HG2	2.03	0.40
1:B:355:TYR:HD1	1:B:355:TYR:HA	1.74	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:A:2008:HOH:O	4:A:2212:HOH:O[2_555]	1.21	0.99
4:B:2223:HOH:O	4:C:2001:HOH:O[2_756]	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/285 (95%)	262 (97%)	9 (3%)	0	100	100
1	B	282/285 (99%)	271 (96%)	10 (4%)	1 (0%)	30	12
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%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/256 (96%)	238 (96%)	9 (4%)	31	6
1	B	256/256 (100%)	249 (97%)	7 (3%)	39	12
2	C	36/39 (92%)	33 (92%)	3 (8%)	10	1
2	D	38/39 (97%)	34 (90%)	4 (10%)	6	0
All	All	577/590 (98%)	554 (96%)	23 (4%)	28	5

All (23) 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	229	GLU
1	A	295	THR
1	A	299	ARG
1	A	335	LYS
1	A	356	GLN
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	356	GLN
2	C	806	LEU
2	C	829	ASP
2	C	834	GLU
2	D	805	ASN
2	D	817	LYS
2	D	827	THR
2	D	840	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	128	GLN
1	A	147	HIS
1	A	150	HIS
1	A	152	ASN
1	A	191	GLN
1	A	298	HIS
1	A	303	ASN
1	A	330	GLN
1	B	137	GLN
1	B	150	HIS
1	B	152	ASN
1	B	161	HIS
1	B	183	GLN
2	D	805	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	248	1	8,10,11	0.59	0	10,14,16	0.75	0
1	TPO	B	248	1	8,10,11	0.96	0	10,14,16	1.28	1 (10%)

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	A	248	1	-	0/9/11/13	-
1	TPO	B	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	-2.43	100.68	109.33

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 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	$\# Z > 2$
3	YJA	A	1357	-	38,40,40	1.73	7 (18%)	46,53,53	2.26	13 (28%)
3	YJA	B	1357	-	38,40,40	2.67	8 (21%)	46,53,53	2.91	17 (36%)

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	-	-	5/24/24/24	0/4/4/4
3	YJA	B	1357	-	-	12/24/24/24	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1357	YJA	FAD-CBC	11.58	1.64	1.36
3	A	1357	YJA	FAD-CBC	5.36	1.49	1.36
3	B	1357	YJA	CAT-CBE	5.12	1.60	1.50
3	B	1357	YJA	CAT-CBB	4.88	1.58	1.51
3	A	1357	YJA	CAT-CBB	4.85	1.58	1.51
3	B	1357	YJA	CBD-NAX	-4.59	1.32	1.41
3	B	1357	YJA	C2-N3	4.48	1.39	1.32
3	A	1357	YJA	NAW-NAZ	-3.26	1.29	1.36
3	A	1357	YJA	C6-N1	3.22	1.38	1.34
3	A	1357	YJA	CAT-CBE	3.06	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1357	YJA	CAM-C4	2.61	1.45	1.41
3	A	1357	YJA	CAJ-CAI	2.46	1.42	1.36
3	B	1357	YJA	CAL-CBE	-2.40	1.35	1.40
3	A	1357	YJA	CAL-CBG	-2.23	1.35	1.38
3	B	1357	YJA	CAL-CBG	-2.18	1.36	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1357	YJA	CBG-CAL-CBE	9.64	110.95	105.25
3	A	1357	YJA	C6-C5-C4	7.12	120.07	115.86
3	B	1357	YJA	C5-C4-N3	-6.90	115.51	122.82
3	B	1357	YJA	C6-C5-C4	6.42	119.65	115.86
3	B	1357	YJA	CBD-CAK-CBC	5.61	123.53	117.96
3	A	1357	YJA	C5-C6-N1	-5.52	117.27	121.35
3	B	1357	YJA	C2-N3-C4	5.19	121.33	115.43
3	B	1357	YJA	CAG-CBC-CAK	-5.17	116.41	123.23
3	A	1357	YJA	CAJ-C5-C4	-4.42	113.43	118.36
3	A	1357	YJA	CAT-CBB-NAX	-3.91	110.60	115.06
3	A	1357	YJA	CAR-NBK-CAS	3.90	120.73	111.44
3	B	1357	YJA	CBD-NAX-CBB	-3.59	121.17	127.52
3	B	1357	YJA	FAD-CBC-CAG	3.57	124.27	118.55
3	B	1357	YJA	CAM-C4-C5	3.44	123.42	119.58
3	A	1357	YJA	C5-C4-N3	-3.43	119.18	122.82
3	B	1357	YJA	CAQ-OBA-CBF	3.38	126.71	117.93
3	A	1357	YJA	CAI-CBF-CAM	-3.28	116.56	120.83
3	A	1357	YJA	CAM-C4-C5	3.26	123.22	119.58
3	B	1357	YJA	CAJ-C5-C4	-3.12	114.88	118.36
3	B	1357	YJA	CAP-CAS-NBK	-2.86	105.90	113.93
3	A	1357	YJA	OAB-CBB-NAX	2.71	128.51	123.64
3	A	1357	YJA	OAC-CAN-CAR	-2.68	100.17	111.22
3	B	1357	YJA	CAM-C4-N3	2.56	120.96	118.01
3	B	1357	YJA	OBA-CAQ-CAP	-2.44	99.33	108.30
3	B	1357	YJA	CAL-CBE-NAZ	-2.40	106.84	110.57
3	A	1357	YJA	FAD-CBC-CAG	2.40	122.40	118.55
3	B	1357	YJA	N3-C2-N1	-2.32	125.52	128.67
3	B	1357	YJA	CAJ-CAI-CBF	2.32	123.13	120.13
3	A	1357	YJA	C5-C6-NAY	2.09	121.87	119.78
3	A	1357	YJA	CBD-CAK-CBC	2.07	120.02	117.96

There are no chirality outliers.

All (17) torsion outliers are listed below:

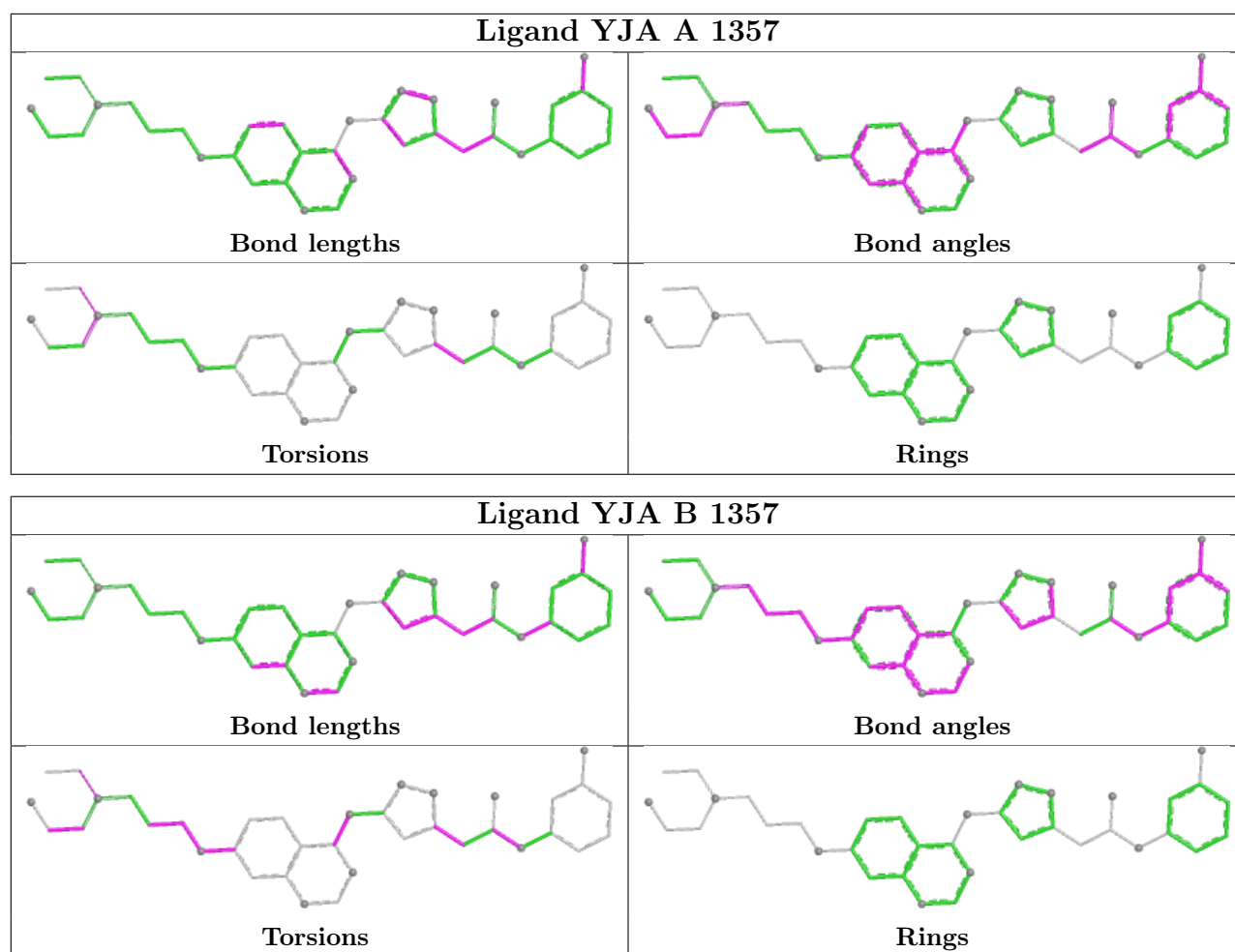
Mol	Chain	Res	Type	Atoms
3	A	1357	YJA	CBB-CAT-CBE-NAZ
3	A	1357	YJA	CAN-CAR-NBK-CAS
3	B	1357	YJA	CBB-CAT-CBE-NAZ
3	B	1357	YJA	OAC-CAN-CAR-NBK
3	B	1357	YJA	CAS-CAP-CAQ-OBA
3	A	1357	YJA	CAA-CAO-NBK-CAR
3	B	1357	YJA	CAP-CAQ-OBA-CBF
3	A	1357	YJA	CBB-CAT-CBE-CAL
3	B	1357	YJA	CBB-CAT-CBE-CAL
3	A	1357	YJA	CAA-CAO-NBK-CAS
3	B	1357	YJA	C5-C6-NAY-CBG
3	B	1357	YJA	N1-C6-NAY-CBG
3	B	1357	YJA	CAA-CAO-NBK-CAS
3	B	1357	YJA	CAM-CBF-OBA-CAQ
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	270/285 (94%)	0.01	12 (4%)	39 43	5, 17, 37, 66	3 (1%)
1	B	280/285 (98%)	0.06	19 (6%)	23 25	5, 17, 48, 91	4 (1%)
2	C	41/44 (93%)	0.88	3 (7%)	21 23	19, 28, 44, 57	0
2	D	43/44 (97%)	1.19	6 (13%)	6 6	17, 36, 52, 67	0
All	All	634/658 (96%)	0.17	40 (6%)	26 28	5, 18, 48, 91	7 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	PHE	6.8
1	B	102	GLY	6.3
1	B	354	VAL	5.2
2	C	837	PHE	5.0
1	B	355	TYR	4.7
1	B	103	LYS	4.6
2	C	797	PRO	4.0
2	D	837	PHE	3.7
1	B	104	PHE	3.6
1	A	103	LYS	3.6
1	A	102	GLY	3.3
1	B	101	LYS	3.3
1	A	101	LYS	3.2
1	B	134	VAL	3.1
1	A	357	SER	2.9
1	B	129	LEU	2.8
2	C	836	LEU	2.8
1	A	243	SER	2.7
1	A	105	GLY	2.7
1	B	79	ALA	2.7
1	B	105	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	136	HIS	2.6
1	B	356	GLN	2.5
1	B	78	THR	2.4
1	A	87	LYS	2.4
1	B	133	GLY	2.3
2	D	826	GLY	2.3
1	A	244	LEU	2.3
1	B	80	LEU	2.3
1	A	106	ASN	2.2
1	A	292	PRO	2.2
2	D	821	VAL	2.2
2	D	805	ASN	2.2
2	D	819	ILE	2.2
1	B	100	GLY	2.2
1	B	97	ARG	2.2
1	A	114	GLN	2.2
1	B	131	LYS	2.1
2	D	827	THR	2.1
1	B	147	HIS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	A	248	11/12	0.99	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](#)

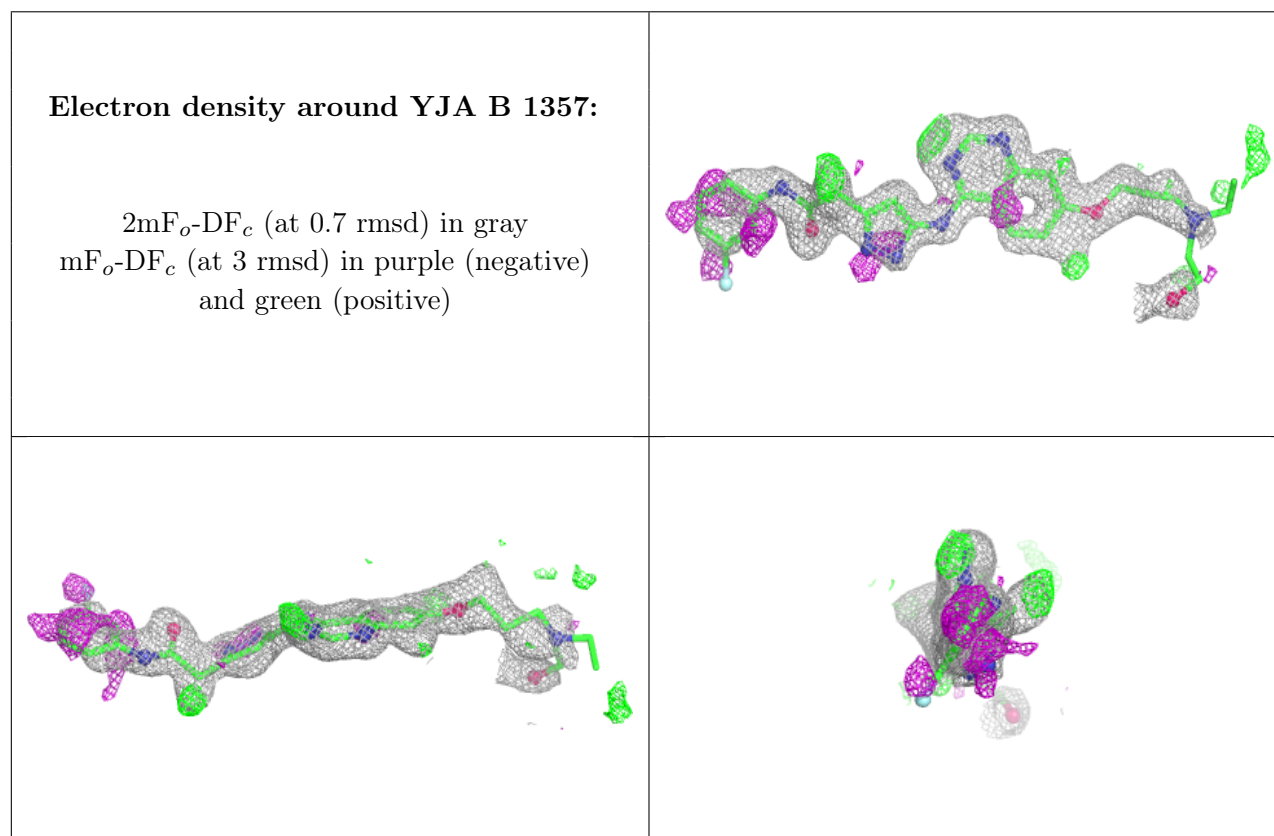
There are no oligosaccharides in this entry.

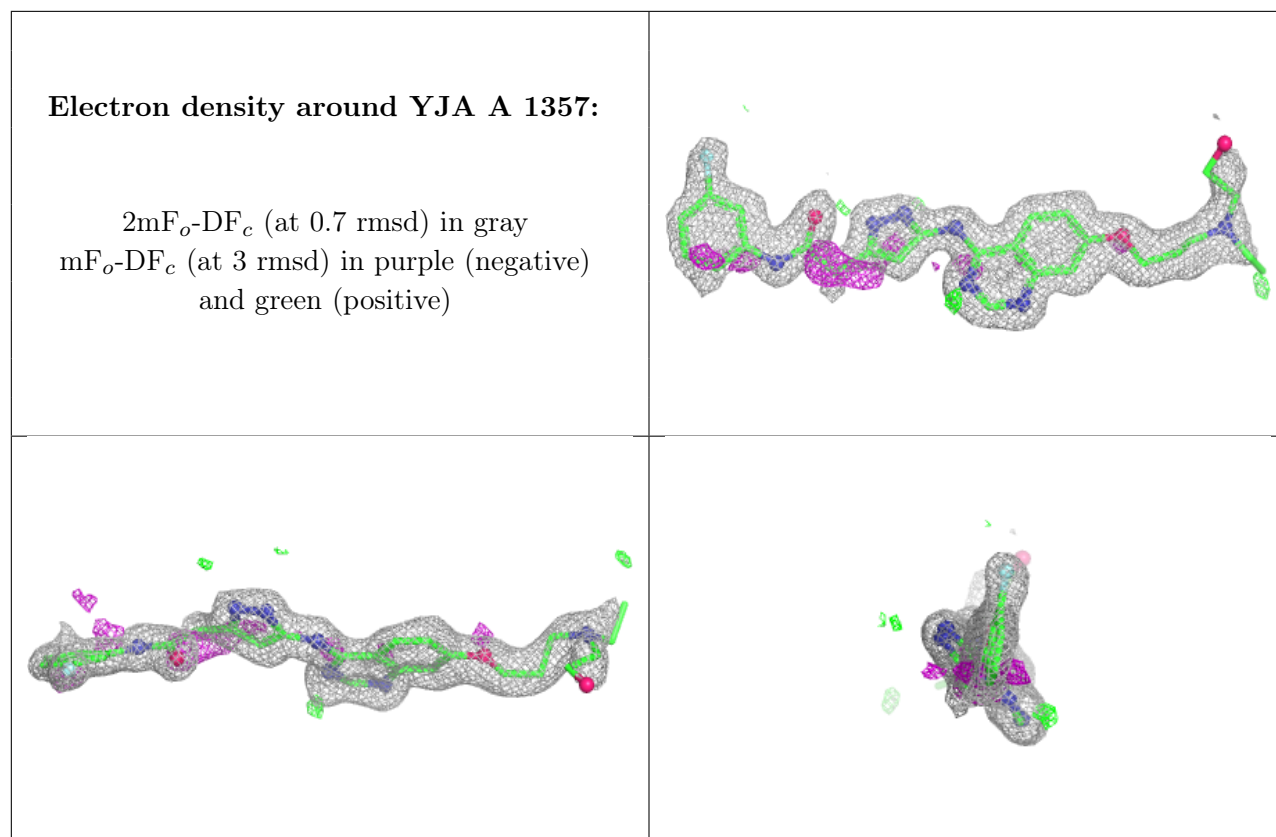
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	YJA	B	1357	37/37	0.79	0.17	19,38,63,65	0
3	YJA	A	1357	37/37	0.87	0.14	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.