



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:07 pm BST

PDB ID : 6ME7  
Title : XFEL crystal structure of human melatonin receptor MT2 (H208A) in complex with 2-phenylmelatonin  
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Deposited on : 2018-09-05  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

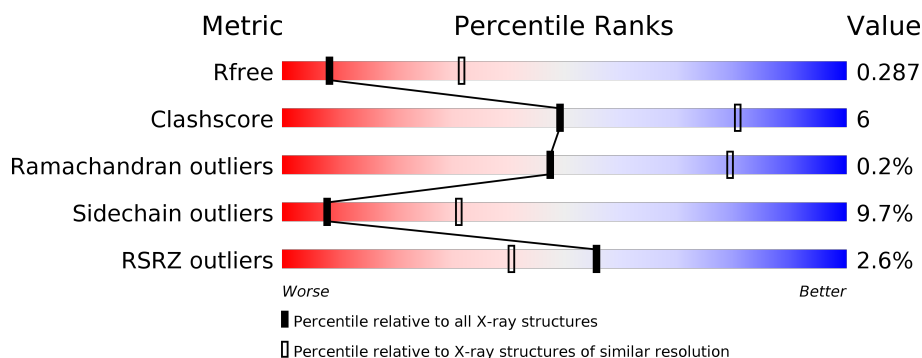
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	460	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 21%, green 75%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>75%</span> <span>21%</span> <span>• •</span> </div> </div>
1	B	460	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 12%, green 72%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>72%</span> <span>12%</span> <span>• 15%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6188 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 Soluble cytochrome b562,Melatonin receptor type 1B,Rubredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3343	2182	535	607	19			
1	B	393	Total	C	N	O	S	0	0	0
			2786	1829	453	494	10			

There are 34 discrepancies between the modelled and reference sequences:

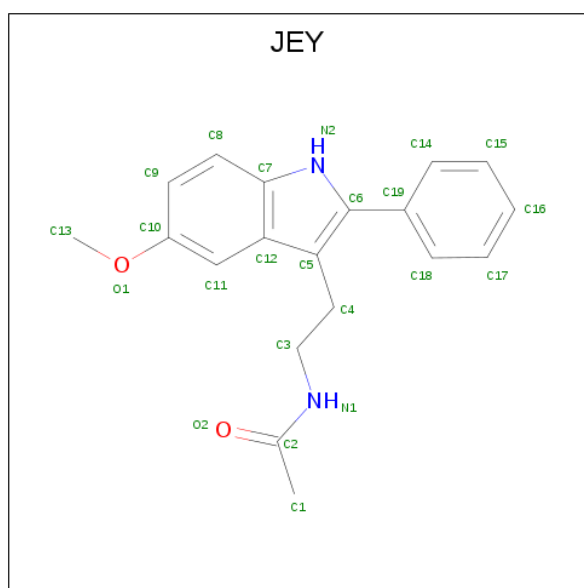
Chain	Residue	Modelled	Actual	Comment	Reference
A	2007	TRP	MET	engineered mutation	UNP P0ABE7
A	2102	ILE	HIS	engineered mutation	UNP P0ABE7
A	2106	LEU	ARG	engineered mutation	UNP P0ABE7
A	31	GLY	-	linker	UNP P0ABE7
A	32	ASP	-	linker	UNP P0ABE7
A	33	GLY	-	linker	UNP P0ABE7
A	34	ALA	-	linker	UNP P0ABE7
A	37	SER	PRO	engineered mutation	UNP P49286
A	86	ASN	ASP	engineered mutation	UNP P49286
A	108	PHE	LEU	engineered mutation	UNP P49286
A	129	TRP	PHE	engineered mutation	UNP P49286
A	137	ASP	ASN	engineered mutation	UNP P49286
A	140	LEU	CYS	engineered mutation	UNP P49286
A	208	ALA	HIS	engineered mutation	UNP P49286
A	264	PHE	TRP	engineered mutation	UNP P49286
A	305	PRO	ALA	engineered mutation	UNP P49286
A	312	ASP	ASN	engineered mutation	UNP P49286
B	2007	TRP	MET	engineered mutation	UNP P0ABE7
B	2102	ILE	HIS	engineered mutation	UNP P0ABE7
B	2106	LEU	ARG	engineered mutation	UNP P0ABE7
B	31	GLY	-	linker	UNP P0ABE7
B	32	ASP	-	linker	UNP P0ABE7
B	33	GLY	-	linker	UNP P0ABE7
B	34	ALA	-	linker	UNP P0ABE7
B	37	SER	PRO	engineered mutation	UNP P49286

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Chain	Residue	Modelled	Actual	Comment	Reference
B	86	ASN	ASP	engineered mutation	UNP P49286
B	108	PHE	LEU	engineered mutation	UNP P49286
B	129	TRP	PHE	engineered mutation	UNP P49286
B	137	ASP	ASN	engineered mutation	UNP P49286
B	140	LEU	CYS	engineered mutation	UNP P49286
B	208	ALA	HIS	engineered mutation	UNP P49286
B	264	PHE	TRP	engineered mutation	UNP P49286
B	305	PRO	ALA	engineered mutation	UNP P49286
B	312	ASP	ASN	engineered mutation	UNP P49286

- Molecule 2 is N-[2-(5-methoxy-2-phenyl-1H-indol-3-yl)ethyl]acetamide (three-letter code: JEY) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>).



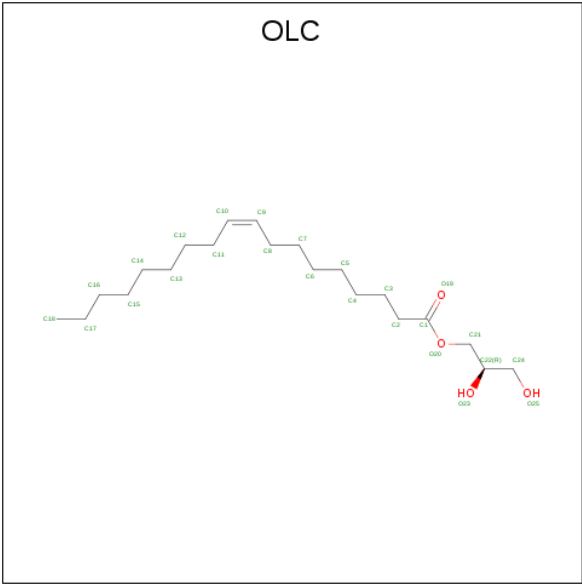
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	19	2	2		
2	B	1	Total	C	N	O	0	0
			23	19	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC)

(formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).

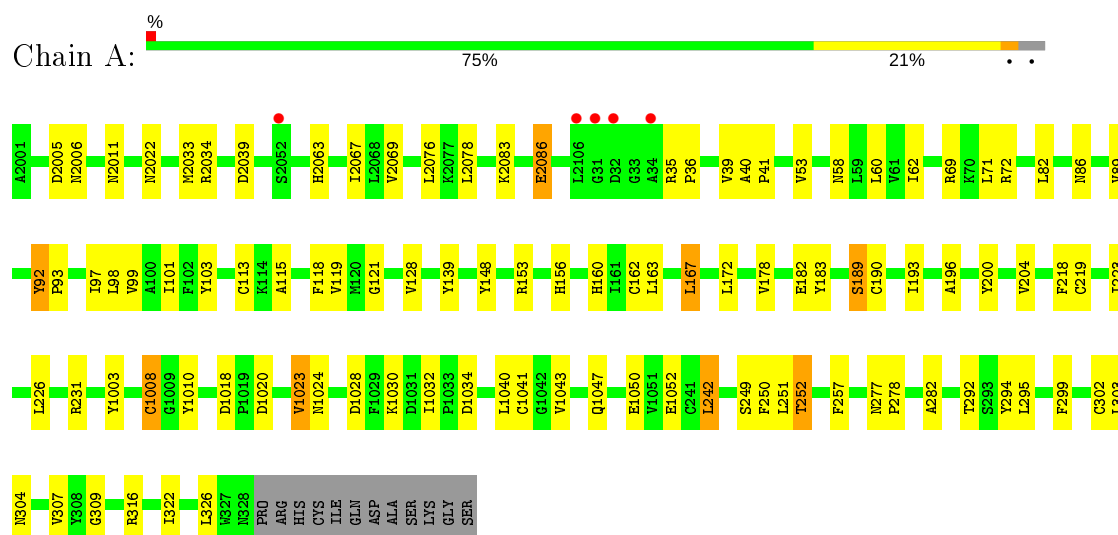


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	8	4		

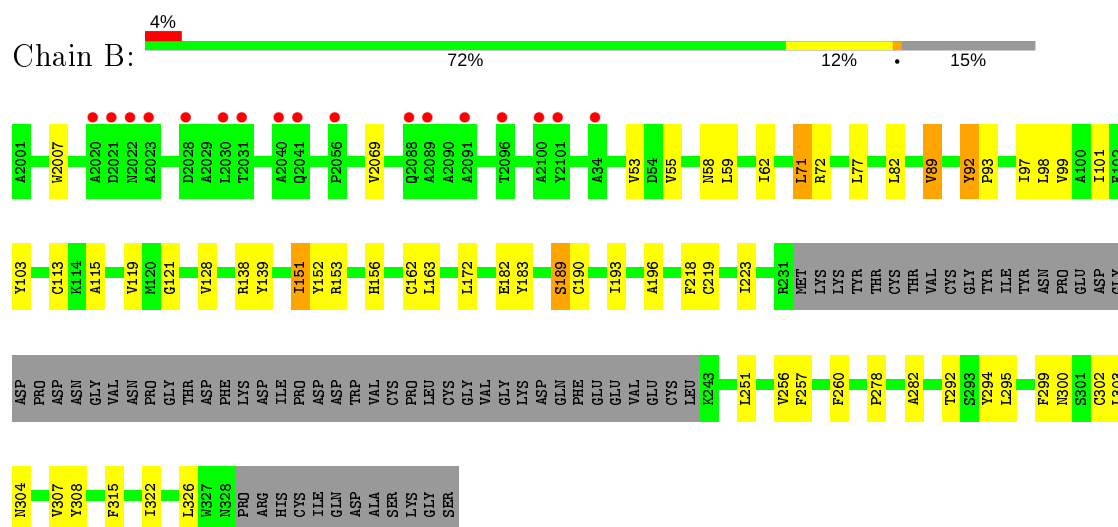
### 3 Residue-property plots

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: Soluble cytochrome b562,Melatonin receptor type 1B,Rubredoxin



- Molecule 1: Soluble cytochrome b562,Melatonin receptor type 1B,Rubredoxin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.23 Å 146.19 Å 77.34 Å 90.00° 105.15° 90.00°	Depositor
Resolution (Å)	21.99 – 3.20 21.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (21.99-3.20) 99.9 (21.98-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 3.23 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.224 , 0.250 0.257 , 0.287	Depositor DCC
$R_{free}$ test set	1218 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 98.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6188	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.47% 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: JEY, ZN, OLC

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	0.49	0/3429	0.65	0/4718
1	B	0.50	0/2855	0.64	0/3938
All	All	0.49	0/6284	0.64	0/8656

There are no bond length outliers.

There are no bond angle outliers.

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	3343	0	3167	45	0
1	B	2786	0	2543	25	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
3	A	1	0	0	0	0
4	B	12	0	13	0	0
All	All	6188	0	5723	70	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 6.

All (70) 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:B:139:TYR:HA	1:B:223:ILE:HD11	1.51	0.92
1:A:139:TYR:HA	1:A:223:ILE:HD11	1.49	0.92
1:A:1018:ASP:HB3	1:A:1023:VAL:HG13	1.63	0.81
1:B:183:TYR:HA	1:B:190:CYS:HA	1.69	0.74
1:A:86:ASN:HD21	1:A:304:ASN:HD22	1.35	0.73
1:A:183:TYR:HA	1:A:190:CYS:HA	1.69	0.73
1:B:138:ARG:HH11	1:B:138:ARG:HA	1.57	0.70
1:A:226:LEU:HG	1:A:231:ARG:HB2	1.77	0.66
1:A:1018:ASP:HB3	1:A:1023:VAL:CG1	2.28	0.63
1:A:2006:ASN:HD21	1:A:2039:ASP:HB3	1.66	0.60
1:A:2078:LEU:HD22	1:A:2086:GLU:HB3	1.83	0.60
1:B:92:TYR:HB3	1:B:93:PRO:HD3	1.85	0.58
1:A:92:TYR:HB3	1:A:93:PRO:HD3	1.87	0.57
1:A:1010:TYR:HB2	1:A:1040:LEU:HD12	1.88	0.55
1:B:55:VAL:O	1:B:59:LEU:HB2	2.09	0.53
1:A:148:TYR:OH	1:A:153:ARG:HD3	2.09	0.53
1:B:308:TYR:HB3	1:B:315:PHE:CD2	2.45	0.51
1:A:121:GLY:HA3	1:A:172:LEU:HD21	1.91	0.51
1:A:2083:LYS:HB3	1:A:2086:GLU:HB2	1.92	0.51
1:A:36:PRO:O	1:A:39:VAL:HG12	2.10	0.51
1:A:2063:HIS:O	1:A:2067:ILE:HG12	2.11	0.51
1:A:2034:ARG:HG3	1:A:2069:VAL:HG13	1.93	0.49
1:B:121:GLY:HA3	1:B:172:LEU:HD21	1.92	0.49
1:A:86:ASN:O	1:A:89:VAL:HG12	2.13	0.49
1:B:322:ILE:O	1:B:326:LEU:HG	2.13	0.49
1:A:98:LEU:HA	1:A:101:ILE:HD12	1.95	0.49
1:A:219:CYS:O	1:A:223:ILE:HG12	2.12	0.49
1:B:219:CYS:O	1:B:223:ILE:HG12	2.13	0.49
1:A:322:ILE:O	1:A:326:LEU:HG	2.13	0.48
1:B:98:LEU:HA	1:B:101:ILE:HD12	1.96	0.48
1:A:89:VAL:HA	1:A:93:PRO:HD2	1.96	0.47
1:A:1003:TYR:CZ	1:A:1050:GLU:HB3	2.49	0.47
1:A:193:ILE:HG22	1:A:196:ALA:H	1.80	0.46
1:B:97:ILE:HG12	1:B:189:SER:HB3	1.98	0.46
1:B:193:ILE:HG22	1:B:196:ALA:H	1.81	0.46
1:A:97:ILE:HG12	1:A:189:SER:HB3	1.98	0.45
1:A:53:VAL:HB	1:A:302:CYS:HB2	1.97	0.45
1:A:1003:TYR:CE2	1:A:1050:GLU:HB3	2.51	0.45
1:B:260:PHE:HA	1:B:300:ASN:HD21	1.82	0.45
1:B:89:VAL:HA	1:B:93:PRO:HD2	1.99	0.45
1:A:1008:CYS:HB3	1:A:1041:CYS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:HA	1:A:156:HIS:HB2	1.98	0.44
1:A:40:ALA:HB3	1:A:41:PRO:HD3	2.00	0.44
1:A:58:ASN:O	1:A:62:ILE:HG13	2.17	0.44
1:B:292:THR:HA	1:B:295:LEU:HD12	1.99	0.44
1:A:99:VAL:O	1:A:103:TYR:HD1	2.01	0.43
1:B:53:VAL:HB	1:B:302:CYS:HB2	1.99	0.43
1:A:309:GLY:O	1:A:316:ARG:HD3	2.18	0.43
1:A:249:SER:HB3	1:A:252:THR:HG23	2.00	0.43
1:A:292:THR:HA	1:A:295:LEU:HD12	1.99	0.43
1:A:1028:ASP:OD2	1:A:1030:LYS:HB2	2.19	0.43
1:A:115:ALA:O	1:A:119:VAL:HG23	2.19	0.43
1:A:1043:VAL:HG11	1:A:1047:GLN:HB2	2.01	0.43
1:B:115:ALA:O	1:B:119:VAL:HG23	2.19	0.42
1:B:99:VAL:O	1:B:103:TYR:HD1	2.02	0.42
1:B:299:PHE:CE2	1:B:303:LEU:HD21	2.54	0.42
1:B:256:VAL:HG13	1:B:304:ASN:ND2	2.34	0.42
1:A:278:PRO:O	1:A:282:ALA:HB3	2.19	0.42
1:A:299:PHE:CE2	1:A:303:LEU:HD21	2.54	0.42
1:A:69:ARG:HA	1:A:72:ARG:HH21	1.85	0.41
1:B:71:LEU:HG	1:B:71:LEU:H	1.39	0.41
1:B:278:PRO:O	1:B:282:ALA:HB3	2.20	0.41
1:B:58:ASN:O	1:B:62:ILE:HG13	2.21	0.41
1:A:242:LEU:HG	1:A:242:LEU:H	1.79	0.41
1:A:167:LEU:HD23	1:A:167:LEU:C	2.41	0.41
1:A:58:ASN:HD21	1:A:86:ASN:HD22	1.68	0.41
1:B:151:ILE:O	1:B:151:ILE:HG12	2.20	0.41
1:B:153:ARG:CD	1:B:153:ARG:H	2.34	0.41
1:A:200:TYR:O	1:A:204:VAL:HG23	2.21	0.40
1:A:118:PHE:CE1	1:A:172:LEU:HB3	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/460 (97%)	415 (93%)	30 (7%)	1 (0%)	47	79
1	B	389/460 (85%)	361 (93%)	27 (7%)	1 (0%)	41	74
All	All	835/920 (91%)	776 (93%)	57 (7%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	TYR
1	B	92	TYR

### 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	332/390 (85%)	297 (90%)	35 (10%)	7	28
1	B	245/390 (63%)	224 (91%)	21 (9%)	10	38
All	All	577/780 (74%)	521 (90%)	56 (10%)	8	31

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2005	ASP
1	A	2011	ASN
1	A	2022	ASN
1	A	2033	MET
1	A	2076	LEU
1	A	2086	GLU
1	A	35	ARG
1	A	60	LEU
1	A	71	LEU
1	A	82	LEU
1	A	113	CYS
1	A	128	VAL
1	A	160	HIS
1	A	162	CYS

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Mol	Chain	Res	Type
1	A	163	LEU
1	A	167	LEU
1	A	178	VAL
1	A	182	GLU
1	A	189	SER
1	A	218	PHE
1	A	1008	CYS
1	A	1020	ASP
1	A	1023	VAL
1	A	1024	ASN
1	A	1032	ILE
1	A	1034	ASP
1	A	1052	GLU
1	A	242	LEU
1	A	250	PHE
1	A	251	LEU
1	A	252	THR
1	A	257	PHE
1	A	277	ASN
1	A	294	TYR
1	A	307	VAL
1	B	2007	TRP
1	B	2069	VAL
1	B	71	LEU
1	B	72	ARG
1	B	77	LEU
1	B	82	LEU
1	B	89	VAL
1	B	113	CYS
1	B	128	VAL
1	B	151	ILE
1	B	152	TYR
1	B	156	HIS
1	B	162	CYS
1	B	163	LEU
1	B	182	GLU
1	B	189	SER
1	B	218	PHE
1	B	251	LEU
1	B	257	PHE
1	B	294	TYR
1	B	307	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2006	ASN
1	A	86	ASN
1	A	156	HIS
1	B	86	ASN
1	B	160	HIS
1	B	300	ASN
1	B	304	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	JEY	A	2201	-	23,25,25	0.78	0	29,34,34	0.98	1 (3%)
2	JEY	B	2201	-	23,25,25	0.83	0	29,34,34	1.00	2 (6%)
4	OLC	B	2202	-	11,11,24	0.72	1 (9%)	12,12,25	1.13	1 (8%)

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	JEY	A	2201	-	-	2/12/12/12	0/3/3/3
2	JEY	B	2201	-	-	2/12/12/12	0/3/3/3
4	OLC	B	2202	-	-	4/11/11/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2202	OLC	O20-C1	2.01	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2202	OLC	O20-C1-C2	2.63	120.15	111.91
2	B	2201	JEY	C6-N2-C7	2.47	108.97	103.90
2	B	2201	JEY	C3-C4-C5	-2.37	107.99	113.07
2	A	2201	JEY	C6-N2-C7	2.21	108.44	103.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

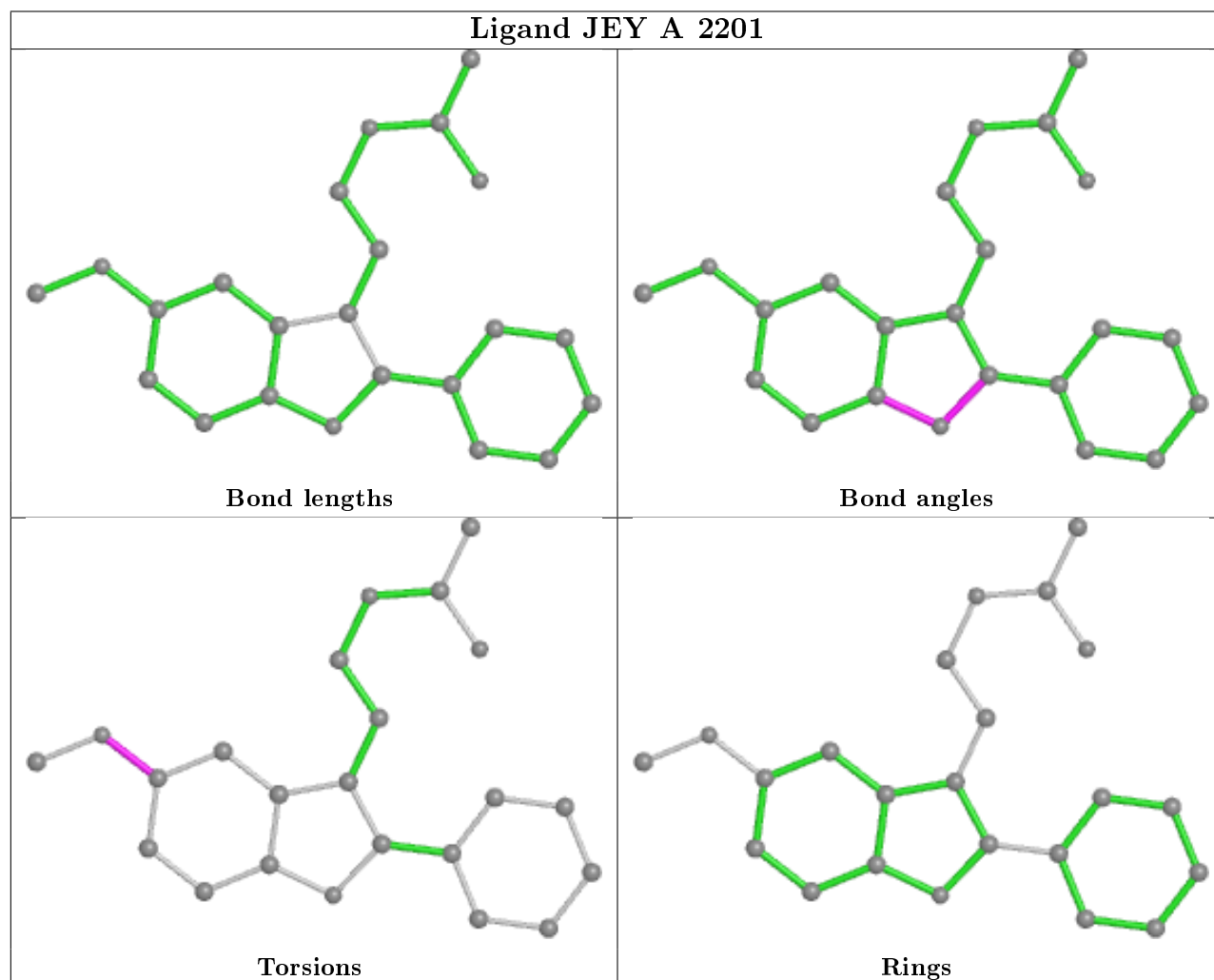
Mol	Chain	Res	Type	Atoms
4	B	2202	OLC	O20-C21-C22-C24
2	B	2201	JEY	C9-C10-O1-C13
2	B	2201	JEY	C11-C10-O1-C13
2	A	2201	JEY	C11-C10-O1-C13
2	A	2201	JEY	C9-C10-O1-C13
4	B	2202	OLC	O20-C21-C22-O23
4	B	2202	OLC	O20-C1-C2-C3
4	B	2202	OLC	O19-C1-C2-C3

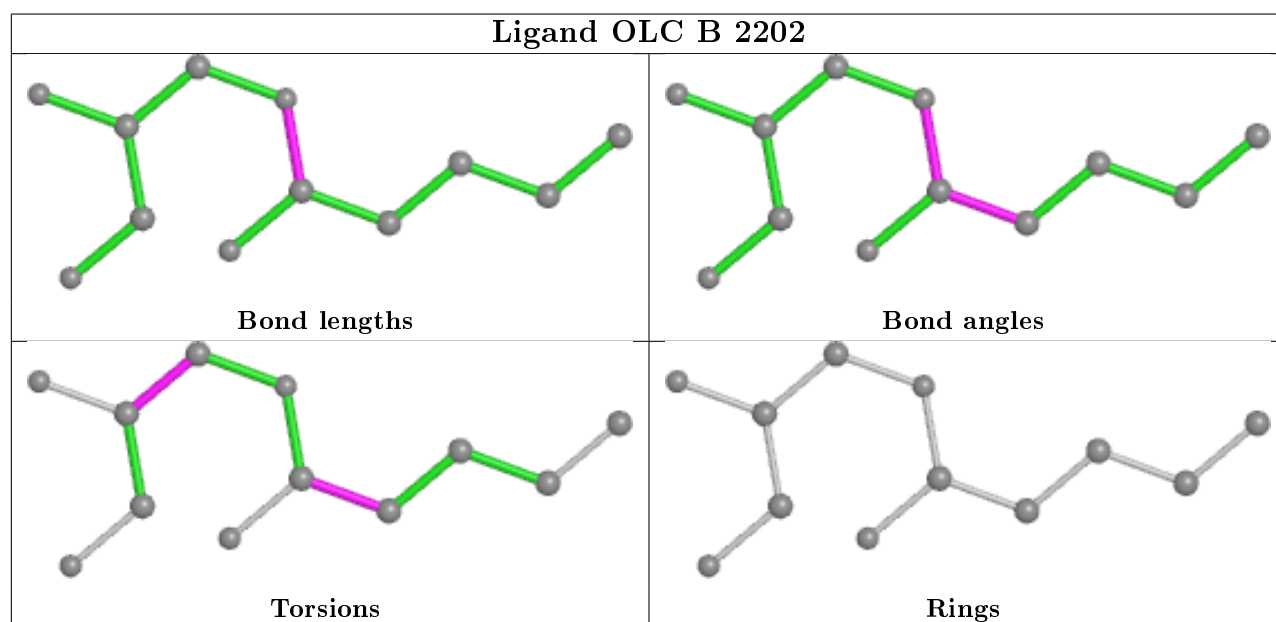
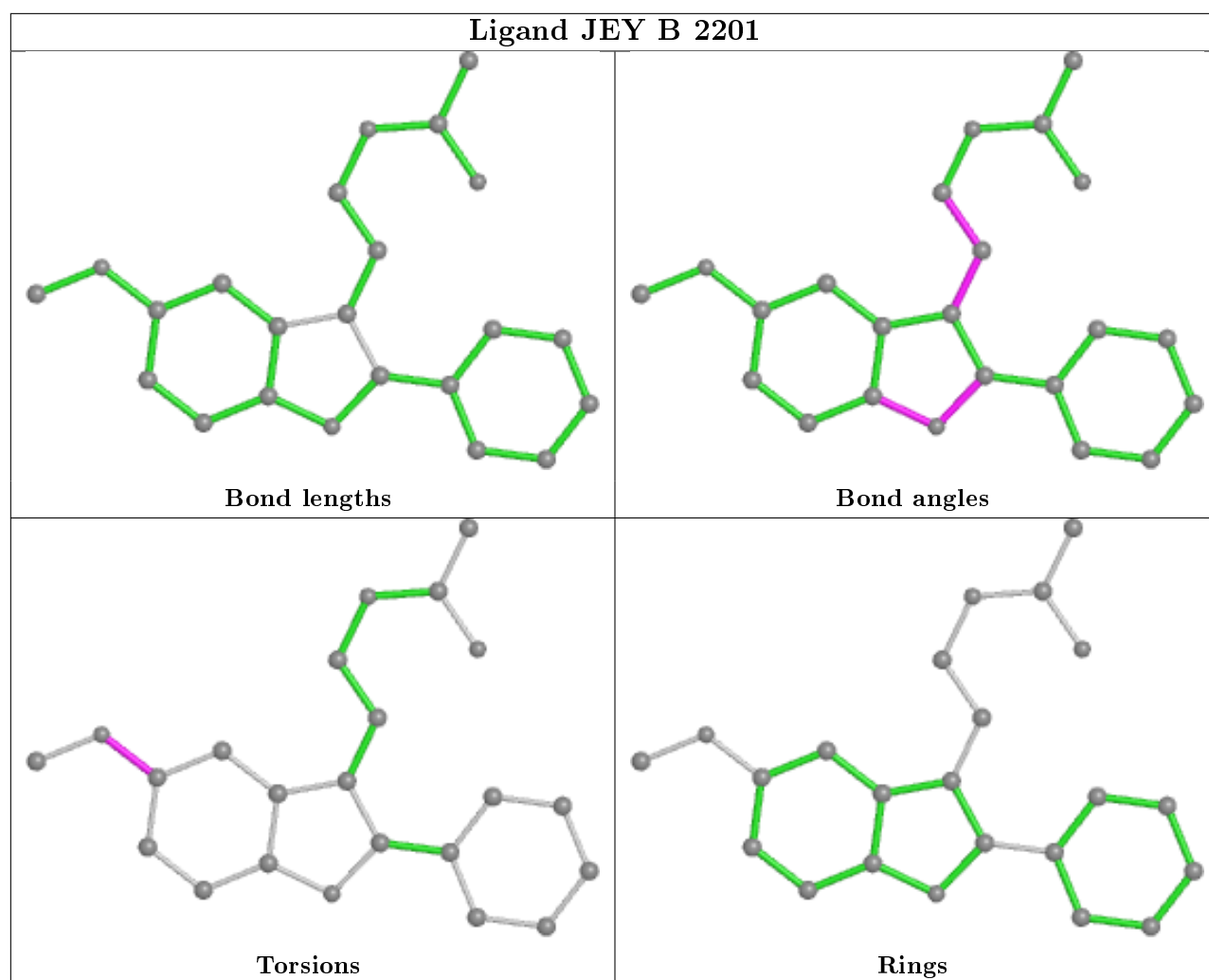
There are no ring outliers.

No monomer is involved in short contacts.

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

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	448/460 (97%)	-0.42	5 (1%) 80 69	68, 98, 173, 203	0
1	B	393/460 (85%)	-0.21	17 (4%) 35 22	62, 108, 197, 206	0
All	All	841/920 (91%)	-0.32	22 (2%) 56 40	62, 101, 190, 206	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2031	THR	4.3
1	B	2100	ALA	3.8
1	B	2101	TYR	3.4
1	B	2020	ALA	3.3
1	A	31	GLY	3.2
1	B	2023	ALA	3.1
1	B	2040	ALA	3.0
1	B	2028	ASP	3.0
1	B	2021	ASP	2.8
1	B	2030	LEU	2.7
1	B	2096	THR	2.7
1	B	2089	ALA	2.7
1	A	32	ASP	2.6
1	B	2091	ALA	2.6
1	B	34	ALA	2.3
1	A	2106	LEU	2.2
1	B	2041	GLN	2.2
1	B	2056	PRO	2.2
1	A	2052	SER	2.1
1	B	2022	ASN	2.1
1	B	2088	GLN	2.0
1	A	34	ALA	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

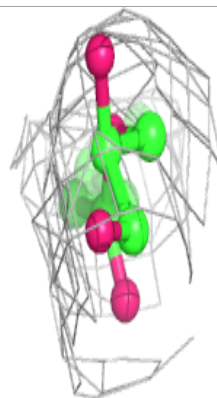
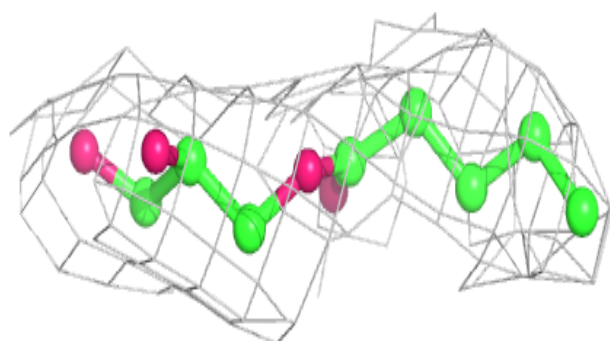
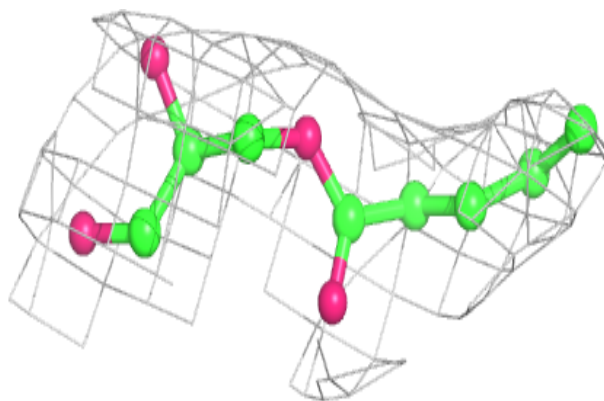
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	OLC	B	2202	12/25	0.90	0.25	100,113,114,116	0
2	JEY	B	2201	23/23	0.93	0.24	86,88,90,92	0
2	JEY	A	2201	23/23	0.97	0.20	69,72,77,78	0
3	ZN	A	2202	1/1	0.99	0.04	91,91,91,91	0

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

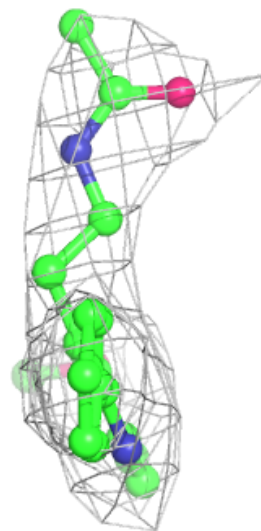
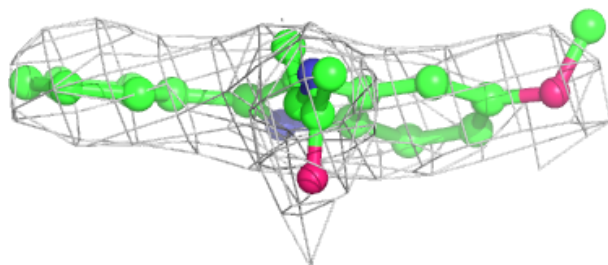
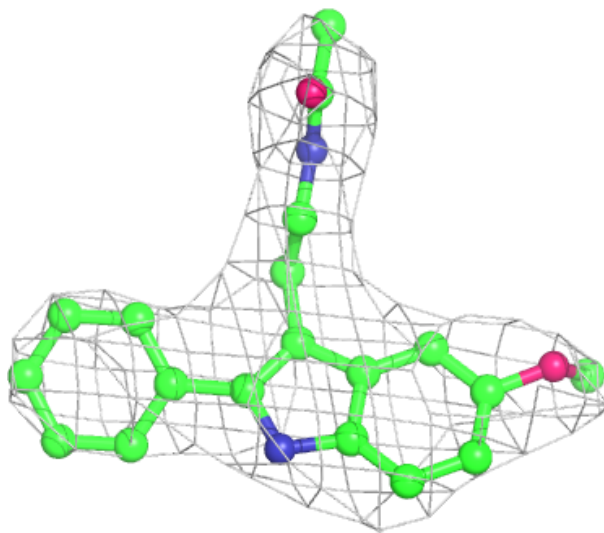
**Electron density around OLC B 2202:**

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



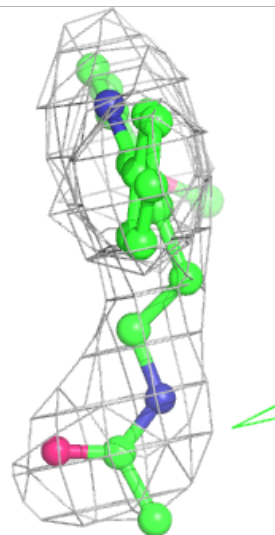
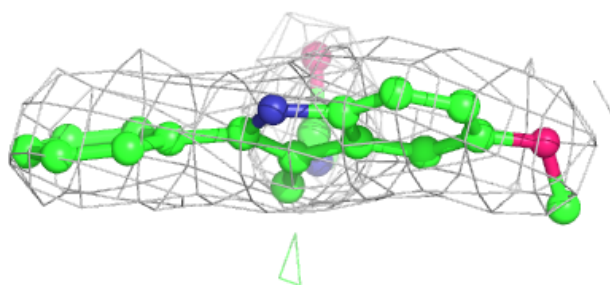
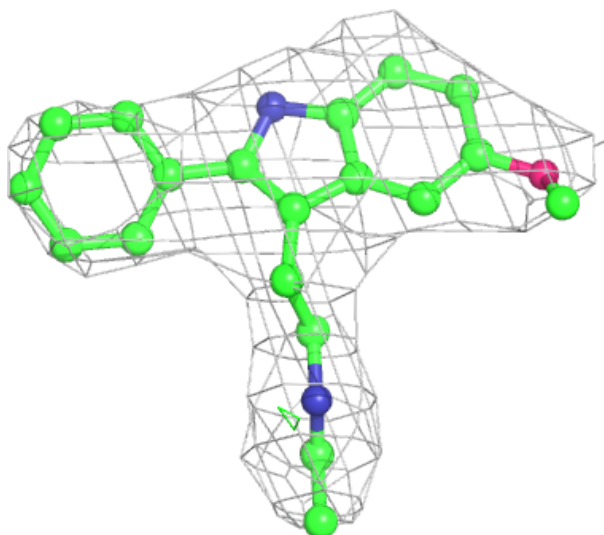
**Electron density around JEY B 2201:**

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



**Electron density around JEY A 2201:**

$2mF_o-DF_c$  (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.