



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:49 AM UTC

PDB ID : 6ME7 / pdb_00006me7
Title : XFEL crystal structure of human melatonin receptor MT2 (H208A) in complex with 2-phenylmelatonin
Authors : Johansson, L.C.; Stauch, B.; McCorvy, J.; Han, G.W.; Patel, N.; Batyuk, A.; Gati, C.; Li, C.; Grandner, J.; Hao, S.; Olsen, R.H.J.; Tribo, A.R.; Zaare, S.; Zhu, L.; Zatsepin, N.A.; Weierstall, U.; Liu, W.; Roth, B.L.; Katritch, V.; Cherezov, V.
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

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)

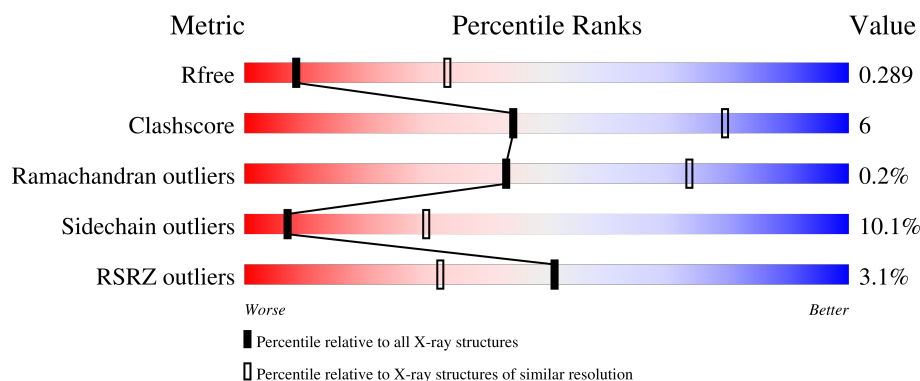
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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	460	% 74% 21% • •
1	B	460	5% 71% 12% • 15%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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:

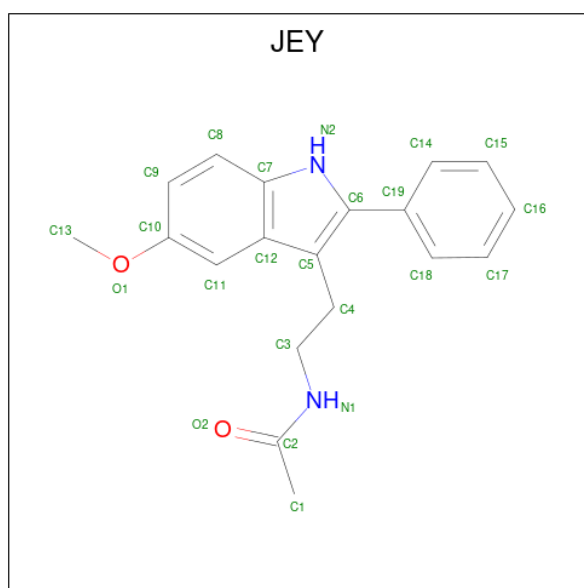
Chain	Residue	Modelled	Actual	Comment	Reference
A	2007	TRP	MET	engineered mutation	UNP P0ABE7
A	2102	ILE	HIS	engineered mutation	UNP P0ABE7
A	2106	LEU	ARG	engineered mutation	UNP P0ABE7
A	31	GLY	-	linker	UNP P0ABE7
A	32	ASP	-	linker	UNP P0ABE7
A	33	GLY	-	linker	UNP P0ABE7
A	34	ALA	-	linker	UNP P0ABE7
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 (CCD ID: JEY) (formula: C₁₉H₂₀N₂O₂).



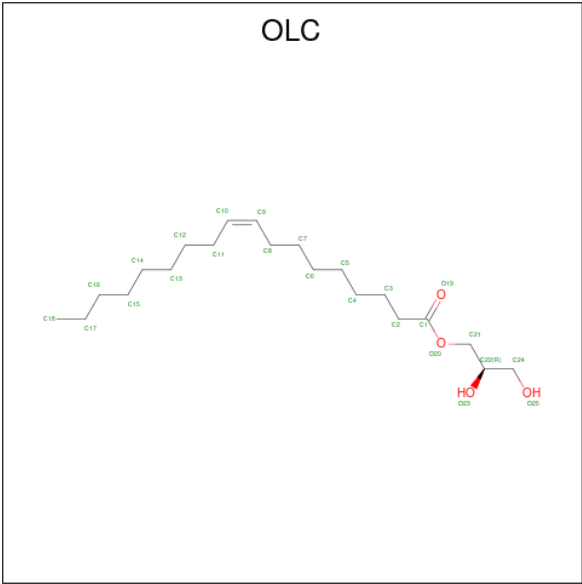
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	19	2	2		
2	B	1	Total	C	N	O	0	0
			23	19	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

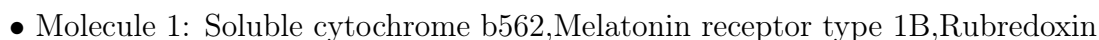
- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula:

C₂₁H₄₀O₄).



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

- 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, α , β , γ	69.23Å 146.19Å 77.34Å 90.00° 105.15° 90.00°	Depositor
Resolution (Å)	21.99 – 3.20 21.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (21.99-3.20) 99.6 (21.99-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.23Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.224 , 0.250 0.257 , 0.289	Depositor DCC
R_{free} test set	1218 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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 ²)	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.*

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: JEY, OLC, ZN

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	0.87	0/3429	1.46	14/4718 (0.3%)
1	B	0.89	1/2855 (0.0%)	1.47	14/3938 (0.4%)
All	All	0.88	1/6284 (0.0%)	1.46	28/8656 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	MET	SD-CE	-5.16	1.66	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2022	ASN	CA-CB-CG	6.09	118.69	112.60
1	B	54	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	70	LYS	CA-C-N	6.06	129.22	120.38
1	B	70	LYS	C-N-CA	6.06	129.22	120.38
1	B	206	VAL	CA-C-N	5.90	128.55	120.46
1	B	206	VAL	C-N-CA	5.90	128.55	120.46
1	B	128	VAL	N-CA-CB	5.90	117.45	110.55
1	A	54	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	1033	PRO	CA-C-N	5.73	129.86	120.63
1	A	1033	PRO	C-N-CA	5.73	129.86	120.63
1	A	39	VAL	N-CA-CB	5.67	116.80	110.62
1	A	312	ASP	CA-C-N	5.45	127.53	120.44
1	A	312	ASP	C-N-CA	5.45	127.53	120.44
1	A	150	ARG	CA-C-N	5.42	129.36	122.37
1	A	150	ARG	C-N-CA	5.42	129.36	122.37
1	B	316	ARG	CA-C-N	5.34	127.38	120.44
1	B	316	ARG	C-N-CA	5.34	127.38	120.44
1	A	244	PRO	CA-C-N	5.33	128.16	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	PRO	C-N-CA	5.33	128.16	120.38
1	A	128	VAL	N-CA-CB	5.27	116.71	110.55
1	A	119	VAL	CA-C-N	5.22	127.27	120.28
1	A	119	VAL	C-N-CA	5.22	127.27	120.28
1	B	295	LEU	CA-C-N	5.06	127.02	120.44
1	B	295	LEU	C-N-CA	5.06	127.02	120.44
1	B	315	PHE	CA-C-N	5.04	127.35	120.54
1	B	315	PHE	C-N-CA	5.04	127.35	120.54
1	B	248	ARG	CA-C-N	5.03	127.53	120.28
1	B	248	ARG	C-N-CA	5.03	127.53	120.28

There are no chirality outliers.

There are no planarity outliers.

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	3343	0	3167	45	0
1	B	2786	0	2543	26	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	71	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 (71) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:121:GLY:HA3	1:A:172:LEU:HD21	1.91	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:A:167:LEU:C	1:A:167:LEU:HD23	2.41	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:53:VAL:HB	1:A:302:CYS:HB2	1.97	0.45
1:A:97:ILE:HG12	1:A:189:SER:HB3	1.98	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:153:ARG:HA	1:A:156:HIS:HB2	1.98	0.44
1:A:1008:CYS:HB3	1:A:1041:CYS:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:ALA:O	1:A:119:VAL:HG23	2.19	0.43
1:A:1028:ASP:OD2	1:A:1030:LYS:HB2	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:256:VAL:HG13	1:B:304:ASN:ND2	2.34	0.42
1:B:299:PHE:CE2	1:B:303:LEU:HD21	2.54	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:H	1:B:71:LEU:HG	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:H	1:A:242:LEU:HG	1.79	0.41
1:B:155:TRP:C	1:B:158:PRO:HD2	2.45	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 [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	446/460 (97%)	415 (93%)	30 (7%)	1 (0%)	43	73
1	B	389/460 (85%)	361 (93%)	27 (7%)	1 (0%)	36	68
All	All	835/920 (91%)	776 (93%)	57 (7%)	2 (0%)	43	73

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%)	296 (89%)	36 (11%)	6	27
1	B	245/390 (63%)	223 (91%)	22 (9%)	9	34
All	All	577/780 (74%)	519 (90%)	58 (10%)	7	30

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2005	ASP
1	A	2017	ILE
1	A	2022	ASN
1	A	2033	MET
1	A	2076	LEU
1	A	2084	VAL
1	A	2086	GLU
1	A	35	ARG
1	A	60	LEU
1	A	62	ILE
1	A	71	LEU
1	A	82	LEU
1	A	113	CYS
1	A	128	VAL

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Mol	Chain	Res	Type
1	A	160	HIS
1	A	162	CYS
1	A	163	LEU
1	A	167	LEU
1	A	178	VAL
1	A	180	SER
1	A	182	GLU
1	A	189	SER
1	A	207	ILE
1	A	226	LEU
1	A	1020	ASP
1	A	1023	VAL
1	A	1024	ASN
1	A	1032	ILE
1	A	1052	GLU
1	A	242	LEU
1	A	248	ARG
1	A	250	PHE
1	A	251	LEU
1	A	252	THR
1	A	277	ASN
1	A	307	VAL
1	B	2007	TRP
1	B	2069	VAL
1	B	2072	ILE
1	B	59	LEU
1	B	62	ILE
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	138	ARG
1	B	151	ILE
1	B	152	TYR
1	B	162	CYS
1	B	163	LEU
1	B	182	GLU
1	B	189	SER
1	B	207	ILE

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Mol	Chain	Res	Type
1	B	251	LEU
1	B	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2006	ASN
1	A	2013	ASN
1	A	86	ASN
1	A	156	HIS
1	A	1013	ASN
1	A	1047	GLN
1	A	279	GLN
1	B	2006	ASN
1	B	73	ASN
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 oligosaccharides 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	-	25,25,25	0.82	1 (4%)	34,34,34	1.09	2 (5%)
2	JEY	B	2201	-	25,25,25	0.92	1 (4%)	34,34,34	1.04	3 (8%)
4	OLC	B	2202	-	11,11,24	0.72	1 (9%)	12,12,25	1.16	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201	JEY	C6-C5	2.61	1.40	1.38
2	A	2201	JEY	C6-C5	2.52	1.40	1.38
4	B	2202	OLC	O20-C1	2.01	1.39	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2201	JEY	C19-C6-N2	2.90	123.39	119.74
4	B	2202	OLC	O20-C1-C2	2.73	120.15	111.83
2	A	2201	JEY	C8-C7-C12	-2.66	119.61	122.19
2	A	2201	JEY	C19-C6-N2	2.65	123.08	119.74
2	B	2201	JEY	C8-C7-C12	-2.29	119.97	122.19
2	B	2201	JEY	C5-C6-N2	-2.16	108.06	109.61

There are no chirality outliers.

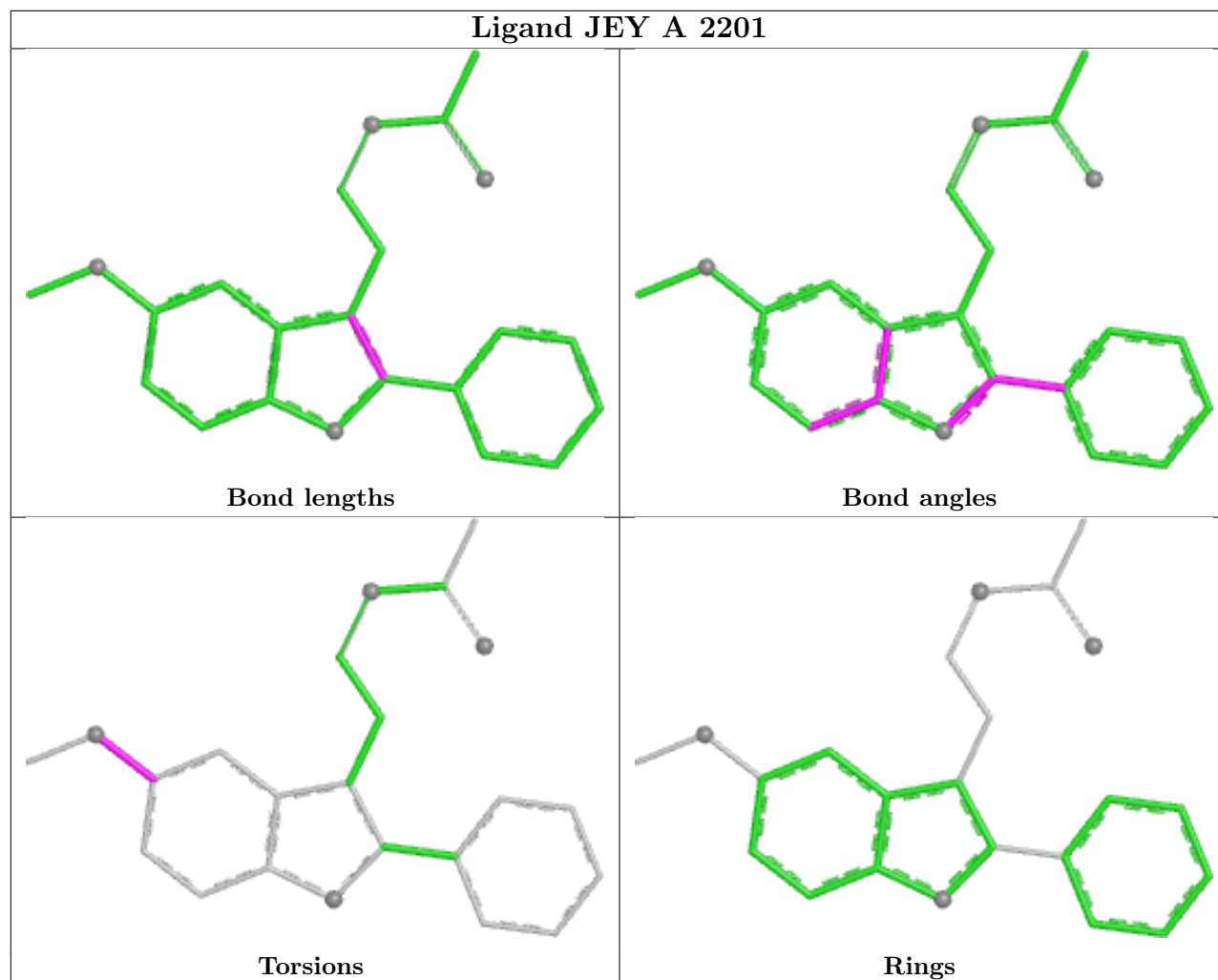
All (8) torsion outliers are listed below:

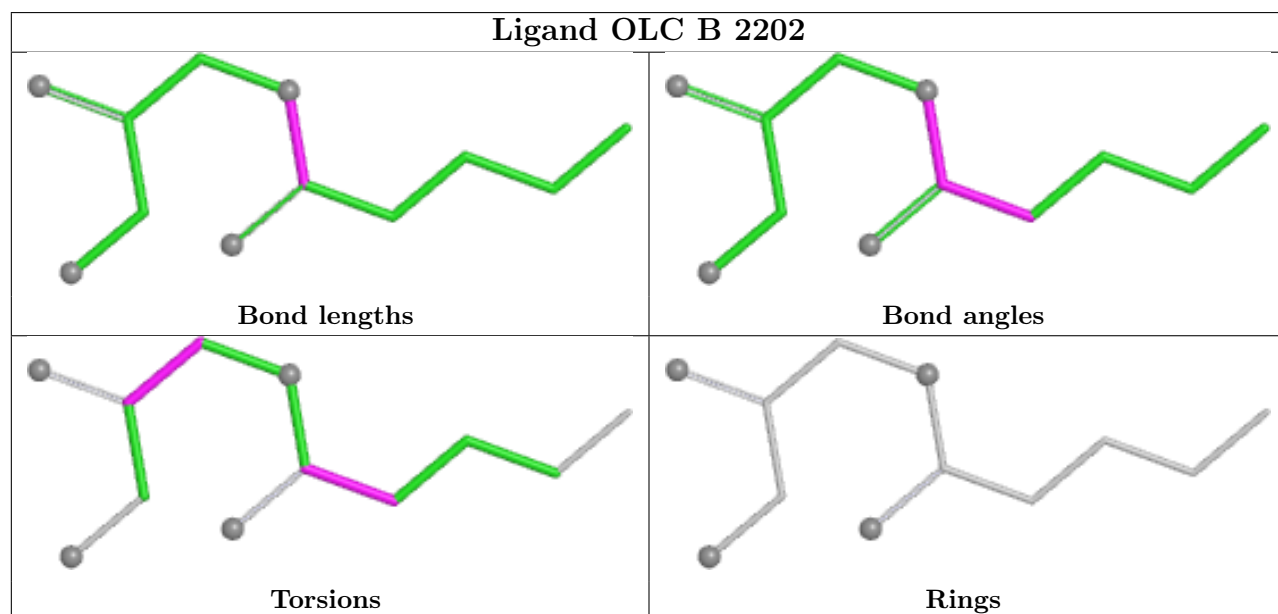
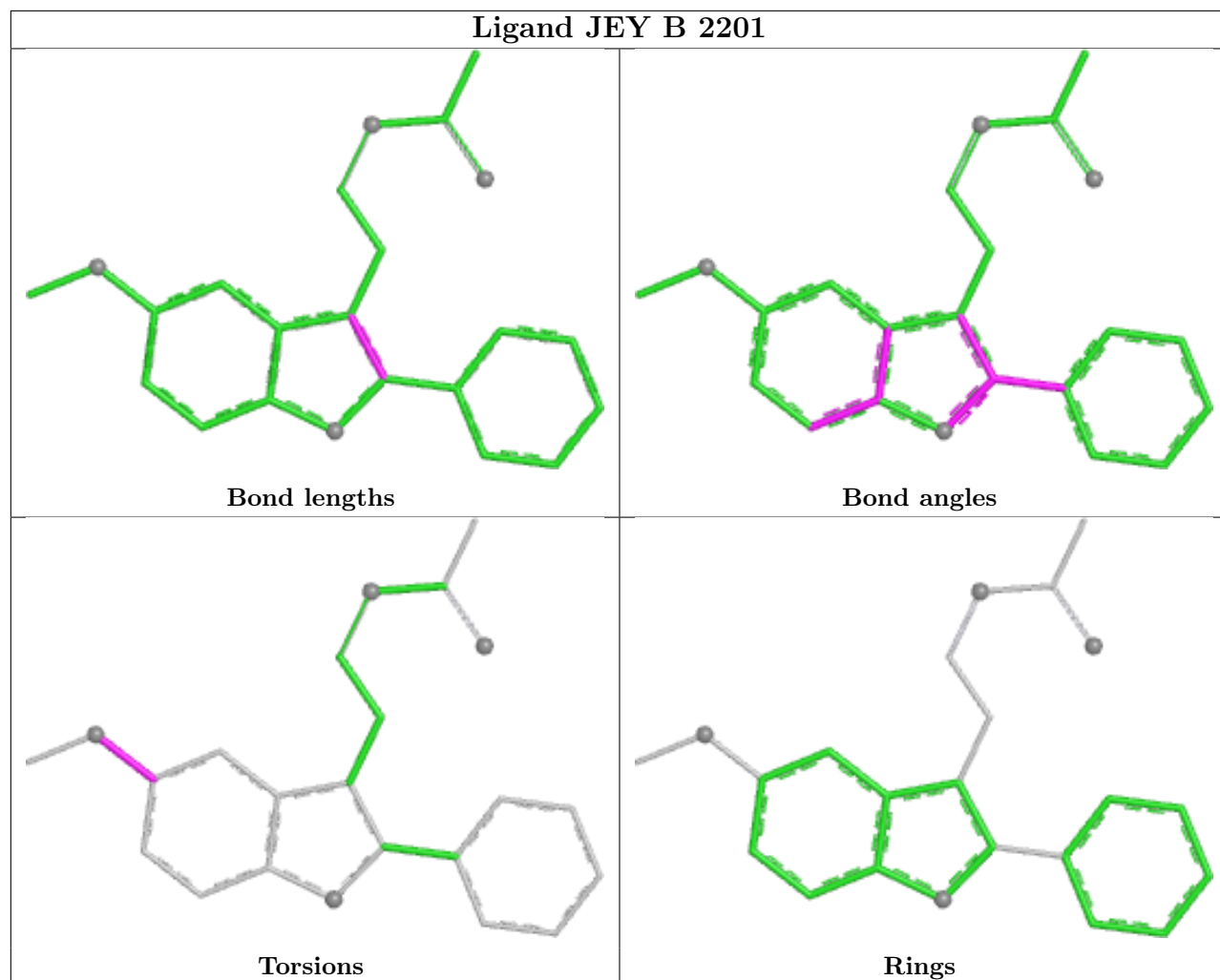
Mol	Chain	Res	Type	Atoms
4	B	2202	OLC	O20-C21-C22-C24
2	B	2201	JEY	C11-C10-O1-C13
2	B	2201	JEY	C9-C10-O1-C13
2	A	2201	JEY	C11-C10-O1-C13
2	A	2201	JEY	C9-C10-O1-C13
4	B	2202	OLC	O20-C21-C22-O23
4	B	2202	OLC	O20-C1-C2-C3
4	B	2202	OLC	O19-C1-C2-C3

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 [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	448/460 (97%)	-0.18	3 (0%) 84 69	68, 98, 173, 203	0
1	B	393/460 (85%)	0.14	23 (5%) 28 18	62, 108, 197, 206	0
All	All	841/920 (91%)	-0.03	26 (3%) 51 32	62, 101, 190, 206	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2030	LEU	7.3
1	B	2040	ALA	6.9
1	B	2033	MET	5.0
1	B	2101	TYR	3.9
1	B	2037	ALA	3.5
1	B	2031	THR	3.5
1	A	154	ARG	3.0
1	B	2032	LYS	2.9
1	B	2009	THR	2.8
1	B	2017	ILE	2.8
1	B	2072	ILE	2.5
1	B	255	VAL	2.4
1	B	2034	ARG	2.4
1	B	2038	LEU	2.2
1	B	2012	ASP	2.2
1	B	2104	LYS	2.2
1	B	2068	LEU	2.2
1	A	1045	LYS	2.1
1	B	2069	VAL	2.1
1	B	2094	LEU	2.1
1	B	2075	ALA	2.1
1	B	2071	GLN	2.1
1	A	275	ALA	2.0
1	B	2035	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	2021	ASP	2.0
1	B	2010	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

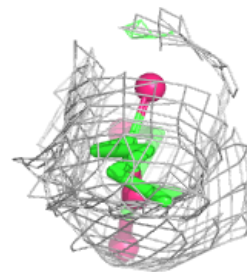
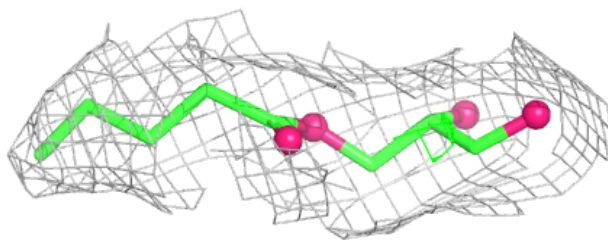
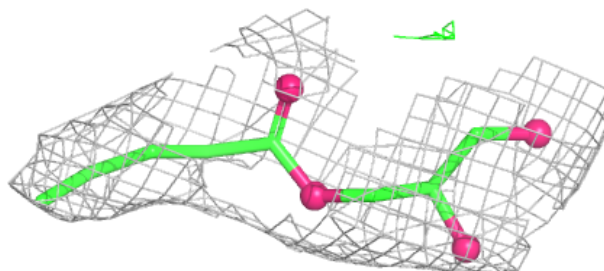
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
4	OLC	B	2202	12/25	0.89	0.10	100,113,114,116	0
2	JEY	B	2201	23/23	0.94	0.12	86,88,90,92	0
2	JEY	A	2201	23/23	0.96	0.08	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.

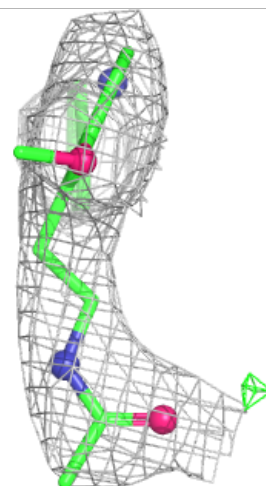
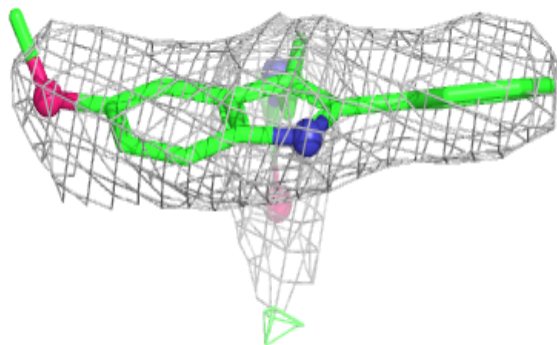
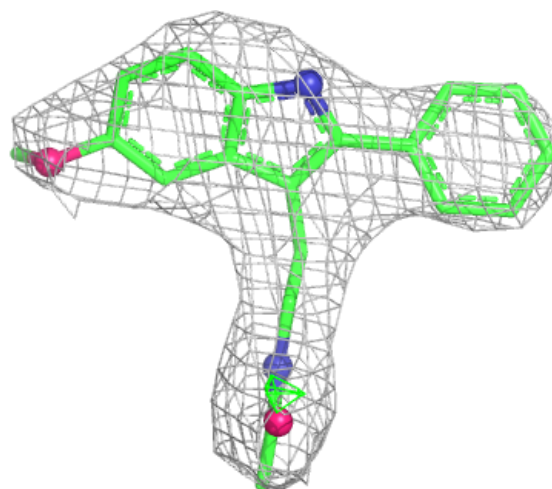
Electron density around OLC B 2202:

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



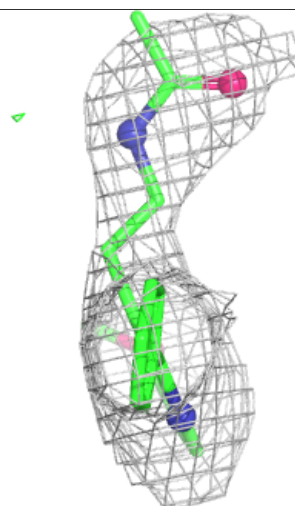
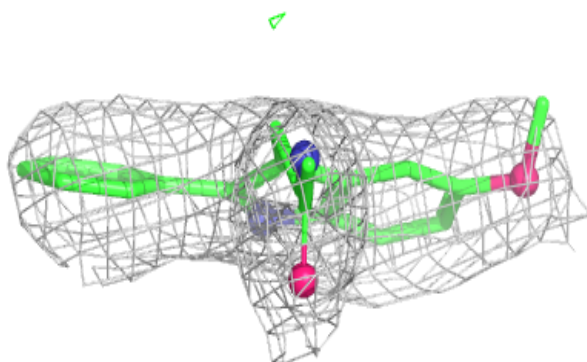
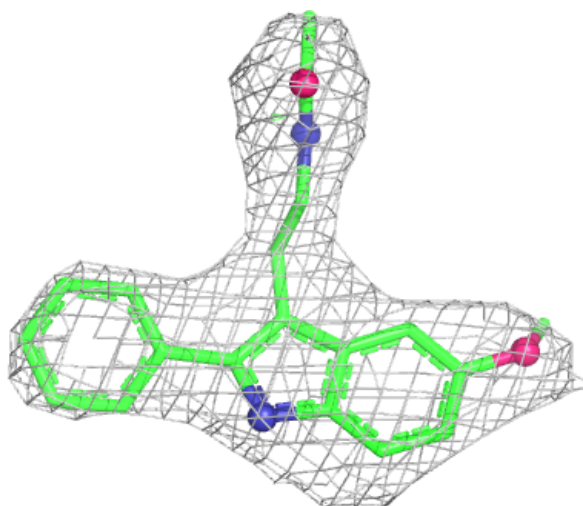
Electron density around JEY B 2201:

$2mF_o-DF_c$ (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.