



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:44 PM UTC

PDB ID : 8ZMG / pdb_00008zmg
Title : Crystal structure of an inverse agonist antipsychotic drug pimavanserin-bound 5-HT2A
Authors : Oguma, T.; Asada, H.; Sekiguchi, Y.; Imono, M.; Iwata, S.; Kusakabe, K.
Deposited on : 2024-05-23
Resolution : 3.40 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

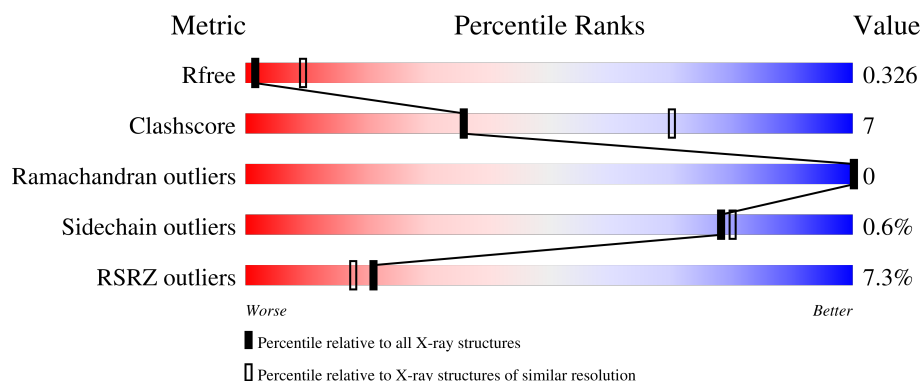
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	414	5% 71% 16% 12%
1	B	414	8% 70% 17% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5769 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 5-hydroxytryptamine receptor 2A, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2862	1878	456	510	18			
1	B	361	Total	C	N	O	S	0	0	0
			2845	1869	453	505	18			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP P28223
A	38	LYS	-	expression tag	UNP P28223
A	39	THR	-	expression tag	UNP P28223
A	40	ILE	-	expression tag	UNP P28223
A	41	ILE	-	expression tag	UNP P28223
A	42	ALA	-	expression tag	UNP P28223
A	43	LEU	-	expression tag	UNP P28223
A	44	SER	-	expression tag	UNP P28223
A	45	TYR	-	expression tag	UNP P28223
A	46	ILE	-	expression tag	UNP P28223
A	47	PHE	-	expression tag	UNP P28223
A	48	CYS	-	expression tag	UNP P28223
A	49	LEU	-	expression tag	UNP P28223
A	50	VAL	-	expression tag	UNP P28223
A	51	PHE	-	expression tag	UNP P28223
A	52	ALA	-	expression tag	UNP P28223
A	53	ASP	-	expression tag	UNP P28223
A	54	TYR	-	expression tag	UNP P28223
A	55	LYS	-	expression tag	UNP P28223
A	56	ASP	-	expression tag	UNP P28223
A	57	ASP	-	expression tag	UNP P28223
A	58	ASP	-	expression tag	UNP P28223
A	59	ASP	-	expression tag	UNP P28223
A	60	LYS	-	expression tag	UNP P28223
A	61	GLU	-	expression tag	UNP P28223

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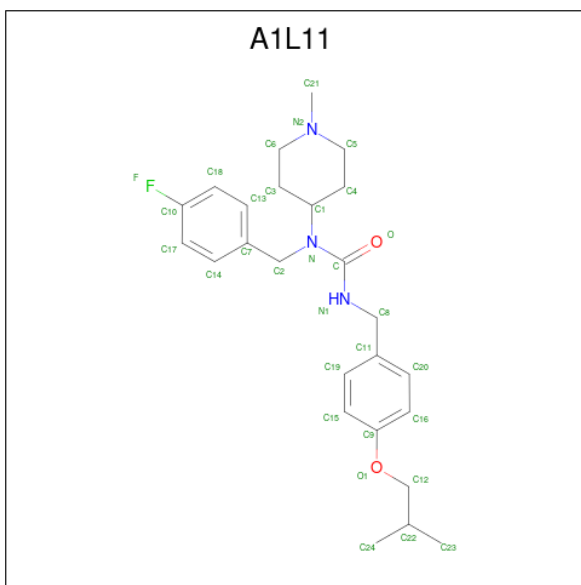
Chain	Residue	Modelled	Actual	Comment	Reference
A	62	ASN	-	expression tag	UNP P28223
A	63	LEU	-	expression tag	UNP P28223
A	64	TYR	-	expression tag	UNP P28223
A	65	PHE	-	expression tag	UNP P28223
A	66	GLN	-	expression tag	UNP P28223
A	67	GLY	-	expression tag	UNP P28223
A	68	THR	-	expression tag	UNP P28223
A	69	SER	-	expression tag	UNP P28223
A	162	LYS	SER	engineered mutation	UNP P28223
A	164	TRP	MET	engineered mutation	UNP P28223
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1041	GLY	-	linker	UNP P0ABE7
A	1042	SER	-	linker	UNP P0ABE7
A	1043	GLY	-	linker	UNP P0ABE7
A	1044	SER	-	linker	UNP P0ABE7
A	1045	GLY	-	linker	UNP P0ABE7
A	1078	ILE	ARG	engineered mutation	UNP P0ABE7
A	1082	ILE	HIS	engineered mutation	UNP P0ABE7
A	1086	GLY	ARG	engineered mutation	UNP P0ABE7
A	404	LEU	-	expression tag	UNP P28223
A	405	GLU	-	expression tag	UNP P28223
A	406	GLU	-	expression tag	UNP P28223
A	407	ASN	-	expression tag	UNP P28223
A	408	LEU	-	expression tag	UNP P28223
A	409	TYR	-	expression tag	UNP P28223
A	410	PHE	-	expression tag	UNP P28223
A	411	GLN	-	expression tag	UNP P28223
B	37	MET	-	initiating methionine	UNP P28223
B	38	LYS	-	expression tag	UNP P28223
B	39	THR	-	expression tag	UNP P28223
B	40	ILE	-	expression tag	UNP P28223
B	41	ILE	-	expression tag	UNP P28223
B	42	ALA	-	expression tag	UNP P28223
B	43	LEU	-	expression tag	UNP P28223
B	44	SER	-	expression tag	UNP P28223
B	45	TYR	-	expression tag	UNP P28223
B	46	ILE	-	expression tag	UNP P28223
B	47	PHE	-	expression tag	UNP P28223
B	48	CYS	-	expression tag	UNP P28223
B	49	LEU	-	expression tag	UNP P28223
B	50	VAL	-	expression tag	UNP P28223
B	51	PHE	-	expression tag	UNP P28223

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Chain	Residue	Modelled	Actual	Comment	Reference
B	52	ALA	-	expression tag	UNP P28223
B	53	ASP	-	expression tag	UNP P28223
B	54	TYR	-	expression tag	UNP P28223
B	55	LYS	-	expression tag	UNP P28223
B	56	ASP	-	expression tag	UNP P28223
B	57	ASP	-	expression tag	UNP P28223
B	58	ASP	-	expression tag	UNP P28223
B	59	ASP	-	expression tag	UNP P28223
B	60	LYS	-	expression tag	UNP P28223
B	61	GLU	-	expression tag	UNP P28223
B	62	ASN	-	expression tag	UNP P28223
B	63	LEU	-	expression tag	UNP P28223
B	64	TYR	-	expression tag	UNP P28223
B	65	PHE	-	expression tag	UNP P28223
B	66	GLN	-	expression tag	UNP P28223
B	67	GLY	-	expression tag	UNP P28223
B	68	THR	-	expression tag	UNP P28223
B	69	SER	-	expression tag	UNP P28223
B	162	LYS	SER	engineered mutation	UNP P28223
B	164	TRP	MET	engineered mutation	UNP P28223
B	1007	TRP	MET	engineered mutation	UNP P0ABE7
B	1041	GLY	-	linker	UNP P0ABE7
B	1042	SER	-	linker	UNP P0ABE7
B	1043	GLY	-	linker	UNP P0ABE7
B	1044	SER	-	linker	UNP P0ABE7
B	1045	GLY	-	linker	UNP P0ABE7
B	1078	ILE	ARG	engineered mutation	UNP P0ABE7
B	1082	ILE	HIS	engineered mutation	UNP P0ABE7
B	1086	GLY	ARG	engineered mutation	UNP P0ABE7
B	404	LEU	-	expression tag	UNP P28223
B	405	GLU	-	expression tag	UNP P28223
B	406	GLU	-	expression tag	UNP P28223
B	407	ASN	-	expression tag	UNP P28223
B	408	LEU	-	expression tag	UNP P28223
B	409	TYR	-	expression tag	UNP P28223
B	410	PHE	-	expression tag	UNP P28223
B	411	GLN	-	expression tag	UNP P28223

- Molecule 2 is Pimavanserin (CCD ID: A1L11) (formula: C₂₅H₃₄FN₃O₂) (labeled as "Ligand of Interest" by depositor).

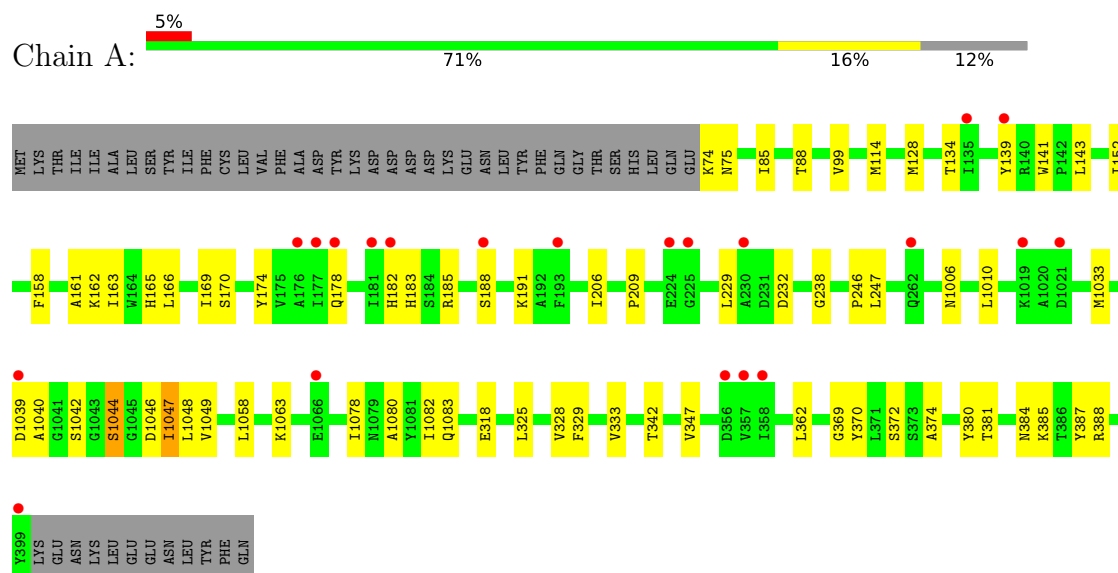


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 25	F 1	N 3	O 2	0	0
2	B	1	Total 31	C 25	F 1	N 3	O 2	0	0

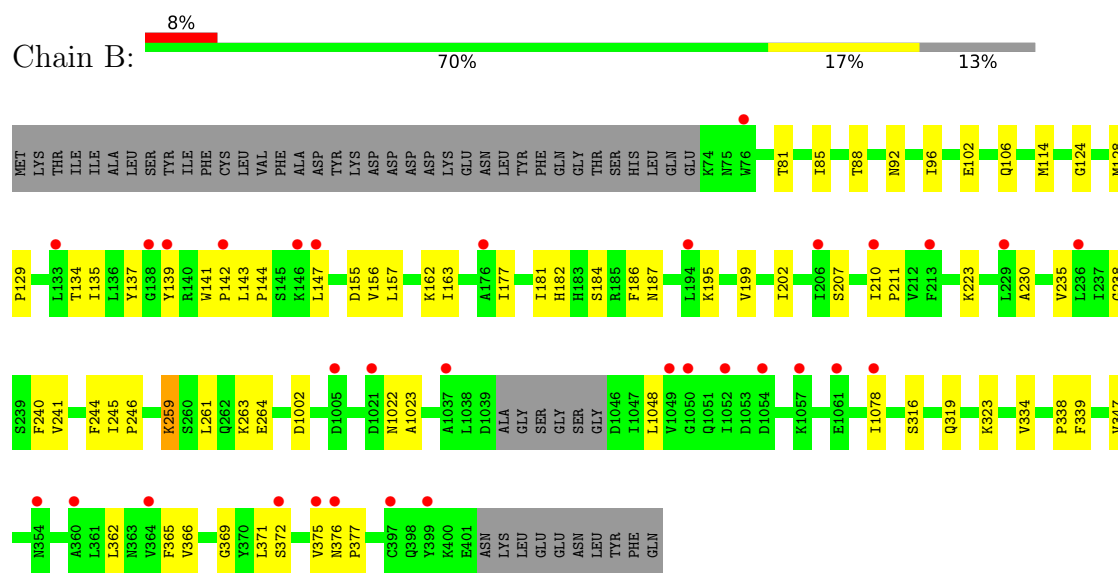
3 Residue-property plots

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: 5-hydroxytryptamine receptor 2A,Soluble cytochrome b562



- Molecule 1: 5-hydroxytryptamine receptor 2A,Soluble cytochrome b562



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.26Å 42.04Å 90.41Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	45.14 – 3.40 45.14 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.14-3.40) 99.6 (45.14-3.40)	Depositor EDS
R_{merge}	1.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, R_{free}	0.291 , 0.328 0.291 , 0.326	Depositor DCC
R_{free} test set	1475 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5769	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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: A1L11

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	0.11	0/2922	0.27	0/3970
1	B	0.13	0/2903	0.30	0/3942
All	All	0.12	0/5825	0.28	0/7912

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

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	2862	0	2947	41	0
1	B	2845	0	2936	44	0
2	A	31	0	0	1	0
2	B	31	0	0	1	0
All	All	5769	0	5883	85	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 7.

All (85) 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:177:ILE:HD13	1:B:261:LEU:HD21	1.74	0.69
1:A:1006:ASN:ND2	1:A:1039:ASP:OD1	2.27	0.67
1:B:372:SER:HA	1:B:375:VAL:HG22	1.77	0.65
1:B:88:THR:O	1:B:92:ASN:ND2	2.35	0.60
1:A:163:ILE:HG13	1:A:246:PRO:HB2	1.84	0.59
1:B:1048:LEU:HD11	1:B:1078:ILE:HG13	1.85	0.58
1:A:183:HIS:NE2	1:A:318:GLU:OE1	2.35	0.58
1:A:384:ASN:O	1:A:388:ARG:HG3	2.04	0.58
1:A:188:SER:HB2	1:A:191:LYS:HB2	1.86	0.57
1:A:381:THR:O	1:A:388:ARG:HG2	2.05	0.57
1:B:238:GLY:HA3	2:B:1201:A1L11:C9	2.36	0.56
1:B:263:LYS:NZ	1:B:1002:ASP:OD2	2.37	0.56
1:B:339:PHE:HB2	1:B:365:PHE:HB3	1.87	0.56
1:A:85:ILE:HG12	1:A:128:MET:HB3	1.88	0.55
1:B:241:VAL:HG23	1:B:245:ILE:HD12	1.88	0.55
1:A:99:VAL:HG11	1:A:114:MET:HB2	1.89	0.55
1:B:369:GLY:O	1:B:372:SER:OG	2.21	0.55
1:B:319:GLN:O	1:B:323:LYS:HG2	2.07	0.54
1:B:207:SER:O	1:B:211:PRO:HD2	2.08	0.54
1:A:1044:SER:O	1:A:1047:ILE:HG22	2.08	0.54
1:A:161:ALA:O	1:A:165:HIS:N	2.35	0.54
1:B:235:VAL:HG11	1:B:347:VAL:HG21	1.91	0.53
1:B:102:GLU:O	1:B:106:GLN:NE2	2.42	0.53
1:B:181:ILE:HG22	1:B:184:SER:H	1.74	0.52
1:A:1010:LEU:HD12	1:A:1082:ILE:HD11	1.90	0.52
1:B:199:VAL:HA	1:B:202:ILE:HG12	1.93	0.51
1:A:185:ARG:NH1	1:A:1042:SER:O	2.43	0.51
1:A:342:THR:HB	1:A:362:LEU:HD21	1.93	0.51
1:B:182:HIS:NE2	1:B:264:GLU:OE2	2.44	0.50
1:B:240:PHE:HA	1:B:244:PHE:HD2	1.75	0.50
1:B:207:SER:HA	1:B:210:ILE:HD12	1.93	0.50
1:B:362:LEU:O	1:B:366:VAL:HG23	2.12	0.49
1:A:128:MET:HE3	1:A:370:TYR:HB3	1.94	0.49
1:B:334:VAL:O	1:B:338:PRO:HD3	2.11	0.49
1:A:380:TYR:HB3	1:A:387:TYR:CD2	2.47	0.49
1:B:371:LEU:O	1:B:375:VAL:HG13	2.13	0.48
1:B:134:THR:HG22	1:B:139:TYR:HA	1.95	0.48
1:A:134:THR:HG22	1:A:139:TYR:HA	1.96	0.48
1:A:247:LEU:HD13	1:A:333:VAL:HG21	1.96	0.48
1:A:1046:ASP:HA	1:A:1049:VAL:HB	1.96	0.47
1:B:143:LEU:HB3	1:B:147:LEU:HD12	1.97	0.47
1:A:141:TRP:CE2	1:A:143:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:HIS:NE2	1:A:318:GLU:OE2	2.48	0.46
1:B:144:PRO:HD2	1:B:147:LEU:HD12	1.97	0.46
1:B:85:ILE:HG12	1:B:128:MET:HE2	1.98	0.46
1:B:124:GLY:HA2	1:B:128:MET:SD	2.55	0.46
1:A:1010:LEU:HD23	1:A:1033:MET:HG2	1.98	0.46
1:B:1048:LEU:HD21	1:B:1078:ILE:HG12	1.97	0.46
1:A:170:SER:O	1:A:174:TYR:N	2.46	0.45
1:A:1058:LEU:HD22	1:A:1063:LYS:HE3	1.99	0.45
1:B:163:ILE:HG13	1:B:246:PRO:HB2	1.99	0.45
1:B:81:THR:O	1:B:85:ILE:HG13	2.17	0.45
1:B:223:LYS:HE3	1:B:230:ALA:HA	1.99	0.45
1:A:1048:LEU:HD21	1:A:1078:ILE:HG12	1.98	0.45
1:A:247:LEU:HD13	1:A:333:VAL:HG11	1.98	0.45
1:A:1039:ASP:HB3	1:A:1040:ALA:H	1.51	0.44
1:B:1022:ASN:OD1	1:B:1023:ALA:N	2.49	0.44
1:B:141:TRP:CE2	1:B:143:LEU:HB2	2.53	0.44
1:A:141:TRP:CZ2	1:A:143:LEU:HB2	2.53	0.44
1:A:369:GLY:O	1:A:372:SER:OG	2.19	0.44
1:A:232:ASP:HB3	1:A:347:VAL:HG13	2.00	0.43
1:A:238:GLY:HA3	2:A:1201:A1L11:C19	2.48	0.43
1:B:156:VAL:O	1:B:157:LEU:C	2.62	0.43
1:A:325:LEU:O	1:A:328:VAL:HG22	2.19	0.42
1:B:135:ILE:HG12	1:B:139:TYR:CE1	2.54	0.42
1:B:259:LYS:HE2	1:B:259:LYS:HB3	1.68	0.42
1:A:152:ILE:HG21	1:A:229:LEU:HG	2.02	0.42
1:A:206:ILE:O	1:A:209:PRO:HD2	2.19	0.42
1:A:1080:ALA:O	1:A:1083:GLN:HG3	2.20	0.41
1:B:137:TYR:CE2	1:B:142:PRO:HB3	2.55	0.41
1:B:162:LYS:HE2	1:B:162:LYS:HB3	1.92	0.41
1:B:155:ASP:O	1:B:156:VAL:C	2.64	0.41
1:A:166:LEU:HB3	1:A:329:PHE:CE1	2.56	0.41
1:A:88:THR:OG1	1:A:374:ALA:HB2	2.21	0.41
1:A:165:HIS:O	1:A:169:ILE:HG13	2.21	0.41
1:A:385:LYS:HD2	1:A:388:ARG:HD3	2.03	0.41
1:B:96:ILE:HA	1:B:114:MET:HG3	2.03	0.41
1:B:186:PHE:CG	1:B:187:ASN:N	2.82	0.41
1:A:74:LYS:HG3	1:A:75:ASN:H	1.85	0.41
1:B:124:GLY:O	1:B:129:PRO:HD3	2.21	0.41
1:B:195:LYS:O	1:B:199:VAL:HG23	2.22	0.40
1:B:316:SER:O	1:B:319:GLN:HG2	2.22	0.40
1:A:158:PHE:O	1:A:161:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASN:HB2	1:B:377:PRO:HD3	2.03	0.40
1:A:162:LYS:HE2	1:A:162:LYS:HB3	1.78	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	363/414 (88%)	352 (97%)	11 (3%)	0	100	100
1	B	357/414 (86%)	344 (96%)	13 (4%)	0	100	100
All	All	720/828 (87%)	696 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/359 (87%)	310 (99%)	3 (1%)	68	75
1	B	312/359 (87%)	311 (100%)	1 (0%)	86	84
All	All	625/718 (87%)	621 (99%)	4 (1%)	78	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	1044	SER
1	A	1047	ILE
1	B	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	398	GLN
1	B	398	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	A1L11	A	1201	-	33,33,33	0.49	0	43,44,44	1.34	4 (9%)
2	A1L11	B	1201	-	33,33,33	0.48	0	43,44,44	1.41	6 (13%)

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	A1L11	A	1201	-	-	5/22/32/32	0/3/3/3
2	A1L11	B	1201	-	-	6/22/32/32	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	A1L11	C2-N-C1	-4.50	113.89	118.34
2	A	1201	A1L11	C3-C1-N	-3.95	106.33	111.83
2	A	1201	A1L11	C2-N-C1	-3.25	115.13	118.34
2	B	1201	A1L11	C3-C1-N	-3.20	107.38	111.83
2	B	1201	A1L11	C4-C1-N	-2.90	107.79	111.83
2	B	1201	A1L11	C2-N-C	2.88	127.28	118.83
2	A	1201	A1L11	C2-N-C	2.86	127.23	118.83
2	B	1201	A1L11	C11-C8-N1	-2.26	108.31	113.07
2	A	1201	A1L11	C18-C10-C17	-2.17	119.95	122.80
2	B	1201	A1L11	C18-C10-C17	-2.13	120.01	122.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

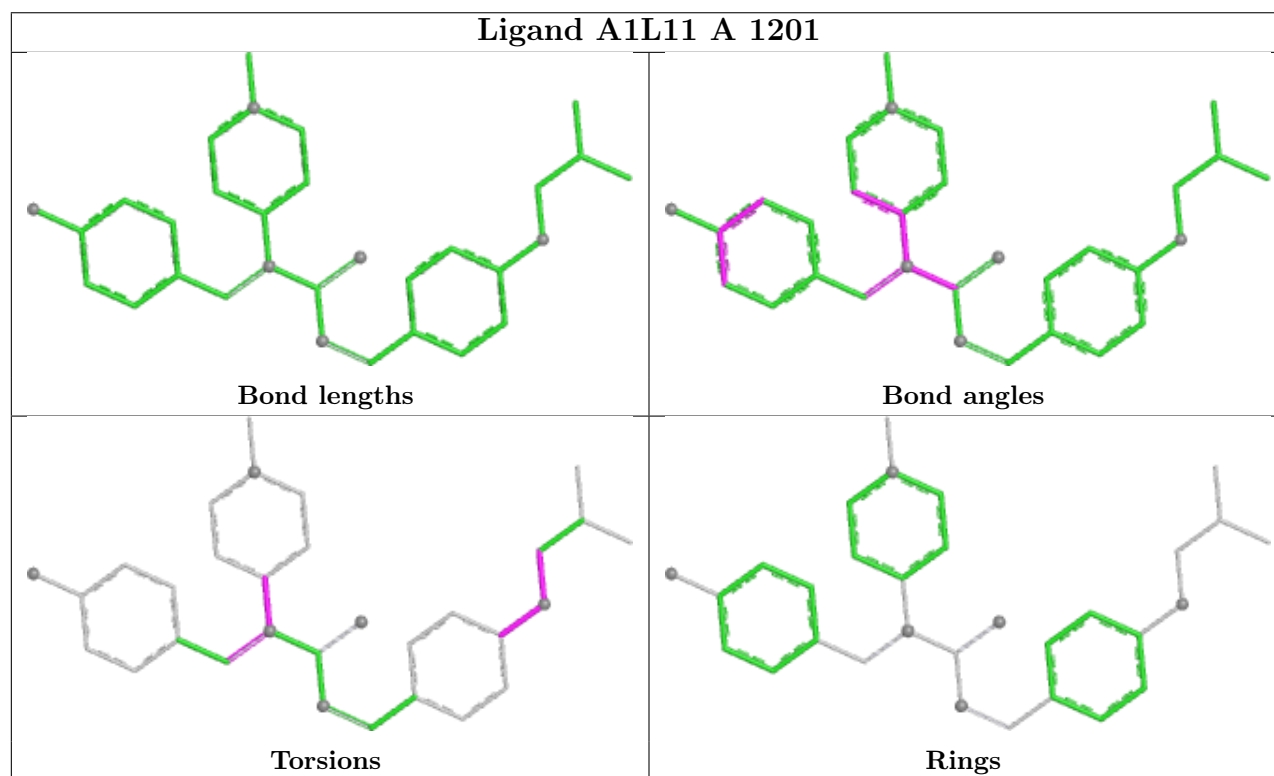
Mol	Chain	Res	Type	Atoms
2	A	1201	A1L11	C4-C1-N-C2
2	B	1201	A1L11	O1-C12-C22-C24
2	B	1201	A1L11	O1-C12-C22-C23
2	A	1201	A1L11	C16-C9-O1-C12
2	A	1201	A1L11	C15-C9-O1-C12
2	B	1201	A1L11	C15-C9-O1-C12
2	B	1201	A1L11	C16-C9-O1-C12
2	B	1201	A1L11	C7-C2-N-C
2	A	1201	A1L11	C22-C12-O1-C9
2	A	1201	A1L11	C7-C2-N-C
2	B	1201	A1L11	C7-C2-N-C1

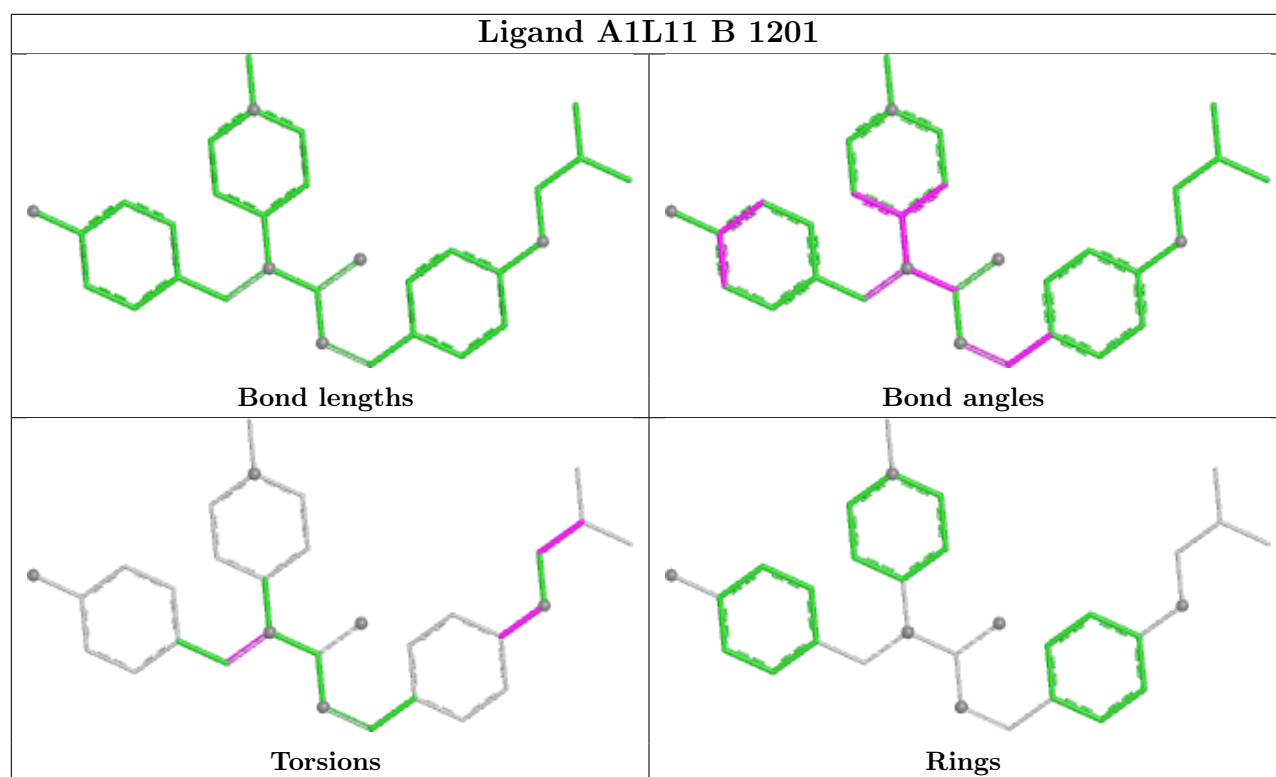
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	A1L11	1	0
2	B	1201	A1L11	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	365/414 (88%)	0.55	21 (5%) 29 22	48, 89, 157, 229	0
1	B	361/414 (87%)	0.78	32 (8%) 15 14	65, 107, 158, 251	0
All	All	726/828 (87%)	0.66	53 (7%) 21 18	48, 100, 158, 251	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1005	ASP	5.7
1	A	224	GLU	4.5
1	B	1049	VAL	4.2
1	A	358	ILE	3.7
1	A	181	ILE	3.6
1	A	1066	GLU	3.5
1	A	193	PHE	3.3
1	B	76	TRP	3.3
1	A	399	TYR	3.2
1	A	357	VAL	3.2
1	A	225	GLY	3.1
1	A	1019	LYS	3.0
1	B	397	CYS	3.0
1	B	142	PRO	3.0
1	B	133	LEU	2.9
1	B	1078	ILE	2.9
1	B	139	TYR	2.8
1	A	176	ALA	2.8
1	B	147	LEU	2.8
1	A	177	ILE	2.7
1	B	1054	ASP	2.7
1	B	1037	ALA	2.7
1	B	364	VAL	2.7
1	B	176	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1057	LYS	2.6
1	B	213	PHE	2.6
1	B	138	GLY	2.6
1	B	229	LEU	2.6
1	B	360	ALA	2.5
1	B	372	SER	2.5
1	B	1061	GLU	2.5
1	A	262	GLN	2.5
1	A	230	ALA	2.5
1	A	178	GLN	2.4
1	B	1050	GLY	2.4
1	B	376	ASN	2.4
1	B	1052	ILE	2.3
1	B	206	ILE	2.3
1	B	236	LEU	2.3
1	B	354	ASN	2.3
1	A	356	ASP	2.3
1	B	1021	ASP	2.3
1	B	375	VAL	2.3
1	A	182	HIS	2.2
1	A	139	TYR	2.2
1	A	1021	ASP	2.2
1	A	1039	ASP	2.2
1	B	399	TYR	2.2
1	A	135	ILE	2.2
1	B	146	LYS	2.2
1	A	188	SER	2.1
1	B	210	ILE	2.1
1	B	194	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

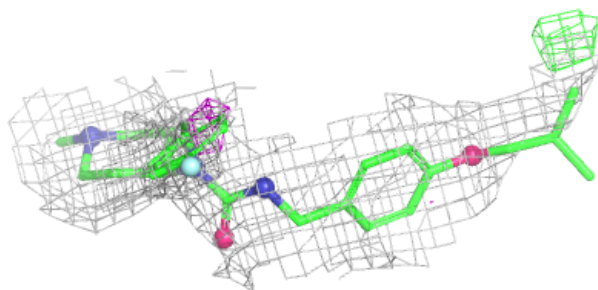
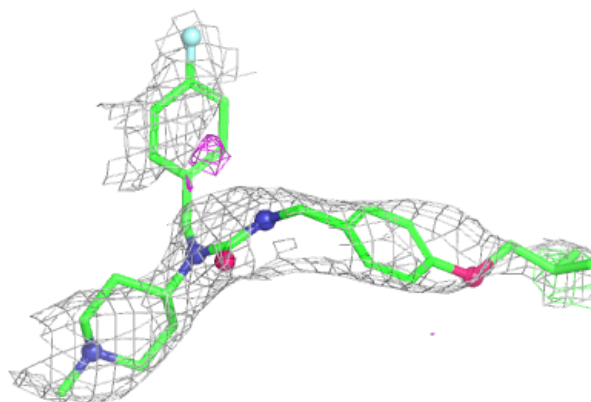
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
2	A1L11	B	1201	31/31	0.64	0.22	111,121,135,142	0
2	A1L11	A	1201	31/31	0.88	0.13	59,76,93,100	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.

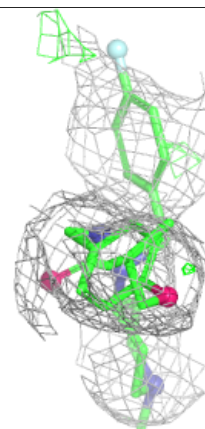
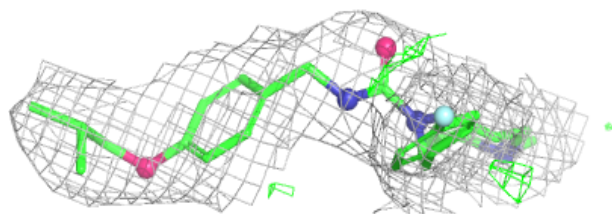
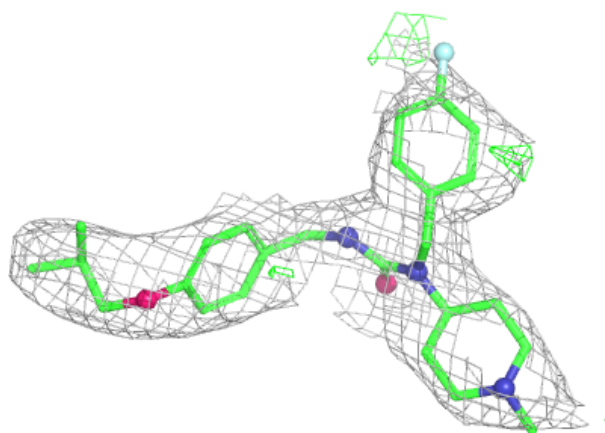
Electron density around A1L11 B 1201:

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 A1L11 A 1201:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.