



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:25 PM EDT

PDB ID : 7C61 / pdb_00007c61
Title : Crystal structure of 5-HT1B-BRIL and SRP2070_Fab complex
Authors : Suzuki, M.; Miyagi, H.; Asada, H.; Yasunaga, M.; Suno, C.; Takahashi, Y.;
Saito, J.; Iwata, S.
Deposited on : 2020-05-21
Resolution : 3.00 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:

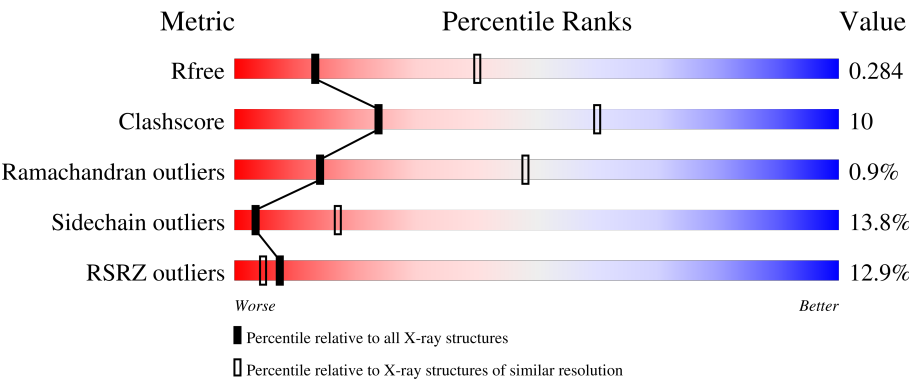
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	L	214	2% 63% 30% 7%
2	H	323	2% 49% 15% • 33%
3	A	399	23% 64% 23% • • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6186 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 IGG LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1657	1029	283	339	6			

- Molecule 2 is a protein called IGG HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1647	1054	264	322	7			

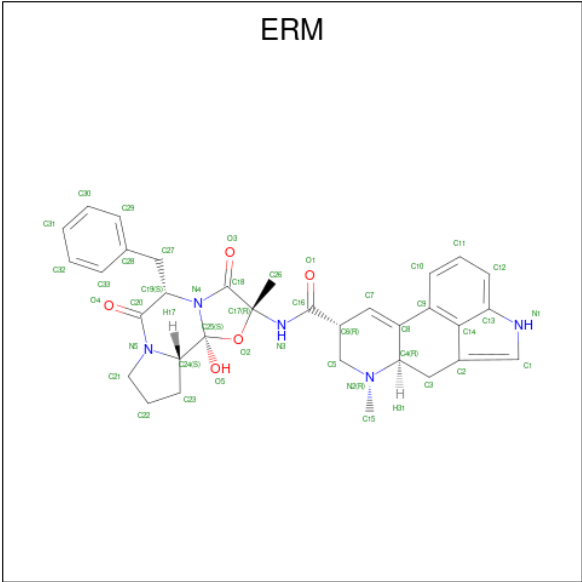
- Molecule 3 is a protein called 5-hydroxytryptamine receptor 1B,Soluble cytochrome b562,5-hydroxytryptamine receptor 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	362	Total	C	N	O	S	0	0	0
			2839	1870	448	505	16			

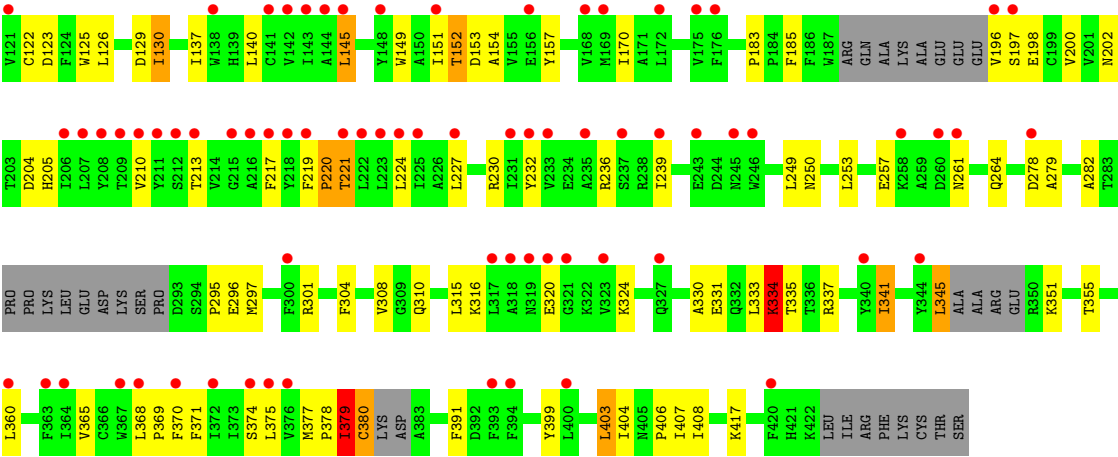
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	expression tag	UNP P28222
A	138	TRP	LEU	engineered mutation	UNP P28222
A	246	TRP	MET	engineered mutation	UNP P0ABE7
A	341	ILE	HIS	engineered mutation	UNP P0ABE7
A	345	LEU	ARG	engineered mutation	UNP P0ABE7

- Molecule 4 is Ergotamine (CCD ID: ERM) (formula: C₃₃H₃₅N₅O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			43	33	5	5		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.80Å 65.70Å 79.73Å 90.00° 98.79° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-3.00) 99.9 (40.00-3.00)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.252 , 0.290 0.249 , 0.284	Depositor DCC
R_{free} test set	1247 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 90.1	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	0.90	EDS
Total number of atoms	6186	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: ERM

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	L	1.06	0/1695	1.45	7/2302 (0.3%)
2	H	1.04	0/1694	1.40	5/2314 (0.2%)
3	A	1.05	0/2907	1.58	8/3972 (0.2%)
All	All	1.05	0/6296	1.50	20/8588 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	183	PRO	N-CA-C	7.55	119.92	110.70
1	L	5	THR	CA-CB-OG1	-6.39	100.02	109.60
1	L	105	GLU	CB-CA-C	6.14	120.94	109.71
2	H	82	GLN	CB-CA-C	6.07	120.14	110.19
1	L	80	THR	CA-CB-OG1	-5.72	101.01	109.60
2	H	61	ASN	CA-CB-CG	5.66	118.26	112.60
3	A	334	LYS	CB-CA-C	-5.66	101.07	110.68
3	A	334	LYS	N-CA-CB	5.57	118.41	110.06
1	L	165	ASP	N-CA-C	-5.52	103.62	110.41
1	L	5	THR	CA-C-O	-5.50	115.04	120.98
2	H	13	LYS	CB-CA-C	5.47	117.30	109.26
3	A	296	GLU	CA-C-N	5.45	127.58	120.28
3	A	296	GLU	C-N-CA	5.45	127.58	120.28
3	A	310	GLN	N-CA-C	-5.33	105.55	111.36
2	H	58	THR	CA-CB-OG1	-5.33	101.61	109.60
1	L	167	ASP	CA-C-N	5.23	127.24	120.44
1	L	167	ASP	C-N-CA	5.23	127.24	120.44
2	H	38	LYS	CA-C-O	-5.22	115.18	120.71
3	A	335	THR	CA-C-N	5.01	127.26	120.44
3	A	335	THR	C-N-CA	5.01	127.26	120.44

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	L	1657	0	1581	47	0
2	H	1647	0	1599	23	0
3	A	2839	0	2833	59	0
4	A	43	0	35	2	0
All	All	6186	0	6048	123	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 10.

All (123) 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)
2:H:23:LYS:HG2	2:H:78:THR:HG22	1.65	0.77
3:A:145:LEU:HD22	3:A:227:LEU:HD21	1.68	0.75
3:A:217:PHE:O	3:A:221:THR:HG23	1.89	0.73
1:L:39:LYS:HE2	1:L:83:PHE:O	1.90	0.72
2:H:12:VAL:HG21	2:H:18:VAL:CG1	2.22	0.70
2:H:131:ALA:O	2:H:219:ARG:NH1	2.27	0.68
3:A:129:ASP:OD2	3:A:399:TYR:OH	2.12	0.67
1:L:150:ILE:HG23	1:L:192:TYR:CE1	2.30	0.66
2:H:177:GLN:HG2	2:H:177:GLN:O	1.97	0.65
1:L:145:ASN:HB2	1:L:197:THR:HG22	1.78	0.65
3:A:145:LEU:HD12	3:A:149:TRP:CH2	2.35	0.62
1:L:39:LYS:NZ	1:L:81:GLU:O	2.34	0.61
3:A:217:PHE:CD1	3:A:371:PHE:CD2	2.89	0.61
3:A:370:PHE:O	3:A:374:SER:HB2	2.02	0.59
3:A:126:LEU:O	3:A:130:ILE:HG22	2.03	0.59
3:A:46:LEU:HD22	3:A:46:LEU:O	2.04	0.57
1:L:115:VAL:HG12	1:L:207:LYS:HG3	1.86	0.57
1:L:149:LYS:HB2	1:L:193:THR:HB	1.86	0.57
3:A:250:ASN:OD1	3:A:337:ARG:HD3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:257:GLU:OE2	3:A:334:LYS:CE	2.52	0.57
2:H:12:VAL:HG21	2:H:18:VAL:HG11	1.87	0.56
3:A:77:THR:HB	3:A:80:LEU:HB2	1.86	0.56
3:A:250:ASN:OD1	3:A:337:ARG:CD	2.55	0.55
1:L:136:LEU:HD13	1:L:136:LEU:N	2.21	0.55
1:L:198:HIS:CE1	1:L:200:THR:HG23	2.42	0.54
3:A:46:LEU:HD13	3:A:47:PRO:HD3	1.89	0.54
1:L:39:LYS:CE	1:L:83:PHE:O	2.56	0.54
1:L:108:ARG:HD3	1:L:109:ALA:O	2.08	0.54
3:A:219:PHE:HB3	3:A:220:PRO:HD3	1.90	0.53
3:A:261:ASN:ND2	3:A:264:GLN:HE21	2.05	0.53
2:H:36:TRP:CD1	2:H:70:LEU:HD22	2.43	0.53
1:L:145:ASN:HB2	1:L:197:THR:CG2	2.38	0.53
3:A:46:LEU:N	3:A:47:PRO:CD	2.72	0.53
1:L:49:LYS:NZ	2:H:104:TYR:O	2.42	0.52
3:A:56:LEU:HB3	3:A:107:THR:CG2	2.40	0.52
3:A:105:ILE:HD11	3:A:117:LEU:HD12	1.91	0.52
1:L:142:LYS:HB3	1:L:173:TYR:CE2	2.45	0.52
3:A:202:ASN:HD21	3:A:204:ASP:HB2	1.75	0.52
1:L:61:ARG:O	1:L:75:ILE:HA	2.11	0.50
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.92	0.50
1:L:80:THR:HA	1:L:106:LEU:HD13	1.94	0.49
1:L:124:GLN:HE22	1:L:131:SER:CB	2.24	0.49
3:A:210:VAL:HA	3:A:213:THR:HG22	1.93	0.49
3:A:391:PHE:CE1	4:A:2001:ERM:H22	2.46	0.49
2:H:18:VAL:O	2:H:82:GLN:HA	2.12	0.49
3:A:220:PRO:O	3:A:224:LEU:HD23	2.13	0.49
1:L:108:ARG:HG2	1:L:171:SER:HB2	1.95	0.48
3:A:217:PHE:CZ	3:A:368:LEU:HA	2.49	0.48
3:A:351:LYS:O	3:A:355:THR:HG23	2.13	0.48
2:H:194:TRP:CG	2:H:195:PRO:HA	2.49	0.47
3:A:316:LYS:O	3:A:320:GLU:HG3	2.13	0.47
3:A:330:ALA:O	3:A:333:LEU:HB2	2.14	0.47
3:A:399:TYR:CE1	4:A:2001:ERM:H6	2.49	0.47
3:A:119:GLN:NE2	3:A:123:ASP:OD2	2.47	0.47
1:L:118:PHE:CD2	2:H:130:LEU:HB3	2.50	0.47
3:A:404:ILE:HG22	3:A:408:ILE:HD11	1.96	0.46
1:L:85:MET:HE1	1:L:101:GLY:HA3	1.97	0.46
1:L:167:ASP:OD1	1:L:168:SER:N	2.48	0.46
3:A:377:MET:HB3	3:A:378:PRO:HD3	1.98	0.46
3:A:219:PHE:HB3	3:A:220:PRO:CD	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:122:SER:O	1:L:126:THR:HG23	2.16	0.45
2:H:156:VAL:CG2	2:H:183:LEU:HD13	2.46	0.45
1:L:49:LYS:HB2	2:H:100:VAL:HG21	1.98	0.45
2:H:6:GLN:OE1	2:H:95:PHE:HA	2.16	0.45
3:A:149:TRP:HA	3:A:152:THR:HG22	1.97	0.45
3:A:198:GLU:O	3:A:198:GLU:HG2	2.16	0.45
1:L:85:MET:SD	1:L:103:LYS:HG2	2.56	0.45
1:L:112:ALA:N	1:L:200:THR:HG21	2.31	0.45
3:A:145:LEU:HD12	3:A:149:TRP:CZ3	2.52	0.45
1:L:135:PHE:C	1:L:136:LEU:HD13	2.42	0.44
3:A:375:LEU:O	3:A:379:ILE:HD13	2.16	0.44
3:A:377:MET:HB3	3:A:378:PRO:CD	2.47	0.44
1:L:212:ASN:O	1:L:212:ASN:ND2	2.51	0.44
2:H:125:PRO:HD2	2:H:210:THR:HG21	1.99	0.44
3:A:261:ASN:HD21	3:A:264:GLN:HE21	1.65	0.44
1:L:115:VAL:HG22	1:L:136:LEU:HD12	1.99	0.44
3:A:103:MET:HE2	3:A:399:TYR:HB3	1.99	0.43
1:L:19:VAL:CG1	1:L:75:ILE:HB	2.47	0.43
1:L:96:LEU:HD12	2:H:47:TRP:CD1	2.54	0.43
3:A:102:VAL:HG21	3:A:129:ASP:HA	2.00	0.43
3:A:145:LEU:CD2	3:A:227:LEU:HD21	2.43	0.43
3:A:278:ASP:O	3:A:279:ALA:C	2.59	0.43
2:H:30:THR:HA	2:H:53:PRO:HB2	2.00	0.43
3:A:82:THR:HB	3:A:83:PRO:HD2	2.01	0.43
1:L:50:TYR:OH	3:A:331:GLU:OE1	2.20	0.43
3:A:341:ILE:HD13	3:A:345:LEU:HD13	2.01	0.43
3:A:232:TYR:O	3:A:236:ARG:HB2	2.19	0.43
1:L:24:ARG:HA	1:L:69:THR:O	2.19	0.42
1:L:186:TYR:O	1:L:192:TYR:OH	2.37	0.42
3:A:103:MET:N	3:A:104:PRO:HD2	2.34	0.42
1:L:85:MET:HE3	1:L:85:MET:HB3	1.95	0.42
1:L:8:PRO:O	1:L:102:THR:HG23	2.18	0.42
3:A:56:LEU:HB3	3:A:107:THR:HG21	2.01	0.42
1:L:34:HIS:O	1:L:88:CYS:HA	2.19	0.42
1:L:140:TYR:CG	1:L:141:PRO:HA	2.54	0.42
3:A:137:ILE:O	3:A:140:LEU:HB2	2.18	0.42
1:L:49:LYS:HE2	1:L:53:GLN:NE2	2.35	0.42
1:L:108:ARG:O	1:L:109:ALA:C	2.62	0.42
1:L:160:LEU:HD11	2:H:175:VAL:HG12	2.01	0.42
1:L:21:LEU:O	1:L:72:THR:HA	2.20	0.42
2:H:194:TRP:CD1	2:H:195:PRO:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:LEU:O	3:A:406:PRO:HG2	2.20	0.42
3:A:304:PHE:O	3:A:308:VAL:HG23	2.20	0.42
3:A:379:ILE:HG22	3:A:380:CYS:N	2.35	0.42
3:A:56:LEU:HB3	3:A:107:THR:HG22	2.02	0.41
1:L:89:GLN:HG2	1:L:90:GLN:N	2.35	0.41
1:L:90:GLN:OE1	1:L:92:ASN:N	2.51	0.41
1:L:49:LYS:O	1:L:53:GLN:HB2	2.20	0.41
3:A:368:LEU:N	3:A:369:PRO:CD	2.84	0.41
3:A:105:ILE:HG23	3:A:125:TRP:HE1	1.86	0.41
1:L:155:ARG:HD2	1:L:156:GLN:N	2.36	0.41
3:A:153:ASP:O	3:A:154:ALA:C	2.64	0.41
3:A:250:ASN:OD1	3:A:337:ARG:HD2	2.20	0.41
1:L:207:LYS:HE3	1:L:207:LYS:HA	2.03	0.40
3:A:46:LEU:HD13	3:A:47:PRO:CD	2.51	0.40
1:L:95:PRO:O	1:L:97:THR:HG23	2.22	0.40
1:L:108:ARG:C	1:L:109:ALA:O	2.64	0.40
2:H:65:LYS:HA	2:H:65:LYS:HD2	1.83	0.40
2:H:11:LEU:C	2:H:12:VAL:HG23	2.46	0.40
2:H:20:ILE:O	2:H:80:PHE:HA	2.20	0.40
2:H:61:ASN:O	2:H:62:GLU:C	2.64	0.40
3:A:257:GLU:OE2	3:A:334:LYS:HE3	2.21	0.40
3:A:41:GLN:HE21	3:A:41:GLN:HB2	1.61	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	L	211/214 (99%)	194 (92%)	16 (8%)	1 (0%)	24	60
2	H	211/323 (65%)	191 (90%)	18 (8%)	2 (1%)	14	48
3	A	352/399 (88%)	311 (88%)	37 (10%)	4 (1%)	11	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	774/936 (83%)	696 (90%)	71 (9%)	7 (1%)	14	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	109	ALA
3	A	282	ALA
2	H	28	THR
2	H	162	SER
3	A	220	PRO
3	A	295	PRO
3	A	379	ILE

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	L	192/193 (100%)	163 (85%)	29 (15%)	3	14
2	H	188/288 (65%)	162 (86%)	26 (14%)	3	17
3	A	300/343 (88%)	261 (87%)	39 (13%)	4	19
All	All	680/824 (82%)	586 (86%)	94 (14%)	3	17

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	THR
1	L	19	VAL
1	L	21	LEU
1	L	33	LEU
1	L	34	HIS
1	L	39	LYS
1	L	42	GLU
1	L	48	ILE
1	L	52	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	60	SER
1	L	65	SER
1	L	74	SER
1	L	78	VAL
1	L	80	THR
1	L	103	LYS
1	L	105	GLU
1	L	108	ARG
1	L	114	THR
1	L	136	LEU
1	L	143	ASP
1	L	147	LYS
1	L	168	SER
1	L	195	GLU
1	L	197	THR
1	L	201	SER
1	L	207	LYS
1	L	208	SER
1	L	210	ASN
1	L	212	ASN
2	H	18	VAL
2	H	19	LYS
2	H	34	ILE
2	H	41	PRO
2	H	63	LYS
2	H	65	LYS
2	H	72	VAL
2	H	74	THR
2	H	78	THR
2	H	82	GLN
2	H	84	ASN
2	H	85	SER
2	H	88	SER
2	H	91	SER
2	H	98	ARG
2	H	116	THR
2	H	121	LYS
2	H	126	SER
2	H	143	THR
2	H	157	THR
2	H	166	SER
2	H	176	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	177	GLN
2	H	183	LEU
2	H	184	SER
2	H	197	GLN
3	A	41	GLN
3	A	46	LEU
3	A	56	LEU
3	A	69	PHE
3	A	77	THR
3	A	93	VAL
3	A	94	THR
3	A	116	THR
3	A	122	CYS
3	A	130	ILE
3	A	145	LEU
3	A	151	ILE
3	A	152	THR
3	A	157	TYR
3	A	170	ILE
3	A	185	PHE
3	A	196	VAL
3	A	197	SER
3	A	200	VAL
3	A	205	HIS
3	A	221	THR
3	A	230	ARG
3	A	239	ILE
3	A	249	LEU
3	A	253	LEU
3	A	297	MET
3	A	301	ARG
3	A	315	LEU
3	A	324	LYS
3	A	334	LYS
3	A	341	ILE
3	A	345	LEU
3	A	360	LEU
3	A	365	VAL
3	A	379	ILE
3	A	380	CYS
3	A	403	LEU
3	A	407	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	53	GLN
1	L	124	GLN
1	L	156	GLN
1	L	210	ASN
2	H	1	GLN
2	H	3	GLN
2	H	57	ASN
2	H	59	HIS
2	H	61	ASN
2	H	82	GLN
2	H	197	GLN
3	A	202	ASN
3	A	245	ASN
3	A	264	GLN
3	A	401	ASN
3	A	405	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](#)

1 ligand is 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	$\# Z > 2$
4	ERM	A	2001	-	50,50,50	1.13	4 (8%)	73,79,79	1.56	15 (20%)

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
4	ERM	A	2001	-	-	2/13/87/87	0/8/8/8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	ERM	O5-C25	3.59	1.43	1.38
4	A	2001	ERM	C14-C2	-3.13	1.36	1.43
4	A	2001	ERM	C9-C14	-2.78	1.37	1.41
4	A	2001	ERM	C14-C13	-2.02	1.38	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	ERM	O2-C25-C24	4.14	115.49	110.37
4	A	2001	ERM	C27-C19-N4	-4.04	107.49	112.60
4	A	2001	ERM	C3-C2-C1	-3.80	131.37	135.09
4	A	2001	ERM	C6-C16-N3	3.14	118.31	114.58
4	A	2001	ERM	O1-C16-C6	-3.10	118.10	121.44
4	A	2001	ERM	C24-N5-C20	-2.85	120.92	126.33
4	A	2001	ERM	C2-C1-N1	-2.50	107.56	110.31
4	A	2001	ERM	C23-C24-C25	-2.46	115.09	117.65
4	A	2001	ERM	C3-C2-C14	2.39	121.25	119.05
4	A	2001	ERM	C23-C24-N5	2.25	105.17	102.73
4	A	2001	ERM	C12-C13-N1	2.22	134.30	130.74
4	A	2001	ERM	C25-O2-C17	2.19	112.66	111.29
4	A	2001	ERM	C22-C23-C24	2.19	107.73	104.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	ERM	O5-C25-O2	-2.18	108.93	111.48
4	A	2001	ERM	C9-C8-C4	2.05	118.20	115.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

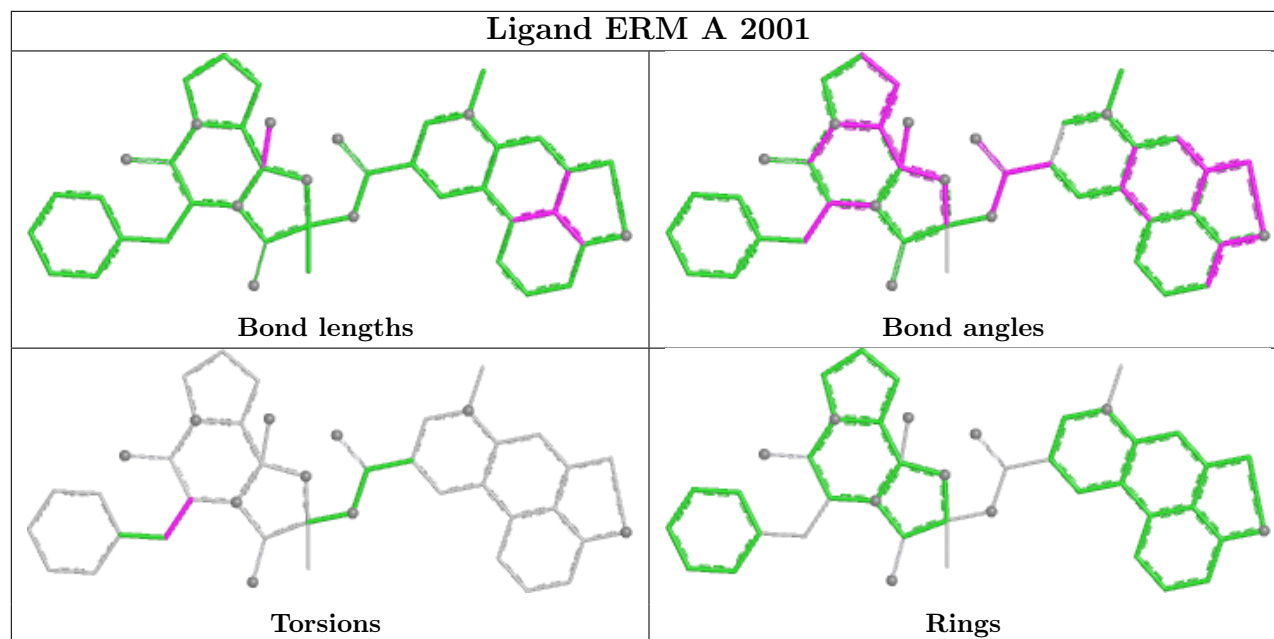
Mol	Chain	Res	Type	Atoms
4	A	2001	ERM	N4-C19-C27-C28
4	A	2001	ERM	C20-C19-C27-C28

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	ERM	2	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	L	213/214 (99%)	0.24	5 (2%) 61 38	51, 100, 164, 199	0
2	H	215/323 (66%)	0.29	7 (3%) 49 28	53, 96, 190, 230	0
3	A	362/399 (90%)	1.40	90 (24%) 2 1	45, 282, 328, 354	0
All	All	790/936 (84%)	0.79	102 (12%) 7 5	45, 123, 318, 354	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	207	LEU	6.8
3	A	61	LEU	5.6
3	A	374	SER	5.5
3	A	222	LEU	5.0
3	A	368	LEU	4.9
3	A	79	LYS	4.8
3	A	52	LEU	4.5
3	A	221	THR	4.3
3	A	145	LEU	4.2
3	A	227	LEU	4.2
3	A	223	LEU	4.0
3	A	235	ALA	4.0
3	A	121	VAL	3.9
3	A	375	LEU	3.8
3	A	323	VAL	3.7
3	A	225	ILE	3.7
3	A	321	GLY	3.7
3	A	218	TYR	3.6
3	A	239	ILE	3.4
3	A	215	GLY	3.3
3	A	206	ILE	3.3
3	A	175	VAL	3.3
3	A	141	CYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	172	LEU	3.2
3	A	261	ASN	3.1
3	A	216	ALA	3.1
3	A	319	ASN	3.1
2	H	184	SER	3.1
3	A	142	VAL	3.1
3	A	246	TRP	3.1
3	A	101	LEU	3.1
3	A	224	LEU	3.0
3	A	176	PHE	3.0
3	A	208	TYR	3.0
2	H	142	VAL	3.0
3	A	209	THR	3.0
3	A	231	ILE	3.0
3	A	400	LEU	3.0
3	A	364	ILE	3.0
3	A	138	TRP	2.9
3	A	258	LYS	2.9
3	A	54	MET	2.9
2	H	217	GLU	2.9
3	A	233	VAL	2.9
2	H	194	TRP	2.9
3	A	143	ILE	2.9
3	A	144	ALA	2.8
3	A	65	LEU	2.8
3	A	370	PHE	2.8
3	A	372	ILE	2.8
3	A	151	ILE	2.8
3	A	243	GLU	2.7
3	A	42	ASP	2.7
3	A	87	LEU	2.7
1	L	117	ILE	2.6
3	A	59	ILE	2.6
3	A	58	LEU	2.6
3	A	211	TYR	2.6
3	A	363	PHE	2.6
3	A	318	ALA	2.5
1	L	115	VAL	2.5
3	A	367	TRP	2.4
1	L	40	SER	2.4
3	A	156	GLU	2.4
2	H	166	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	197	SER	2.4
3	A	213	THR	2.3
3	A	300	PHE	2.3
3	A	43	SER	2.3
3	A	232	TYR	2.3
3	A	278	ASP	2.3
3	A	118	GLY	2.3
3	A	394	PHE	2.3
3	A	327	GLN	2.3
3	A	360	LEU	2.3
3	A	219	PHE	2.3
3	A	55	LEU	2.2
2	H	141	SER	2.2
3	A	245	ASN	2.2
3	A	260	ASP	2.2
3	A	420	PHE	2.2
3	A	70	VAL	2.2
3	A	210	VAL	2.2
3	A	212	SER	2.2
3	A	317	LEU	2.2
3	A	393	PHE	2.2
3	A	116	THR	2.2
3	A	88	ILE	2.2
3	A	169	MET	2.2
3	A	376	VAL	2.1
3	A	237	SER	2.1
3	A	320	GLU	2.1
1	L	152	GLY	2.1
3	A	196	VAL	2.1
3	A	340	TYR	2.1
3	A	217	PHE	2.1
3	A	50	VAL	2.1
3	A	148	TYR	2.1
3	A	168	VAL	2.1
3	A	344	TYR	2.0
1	L	206	VAL	2.0
2	H	144	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

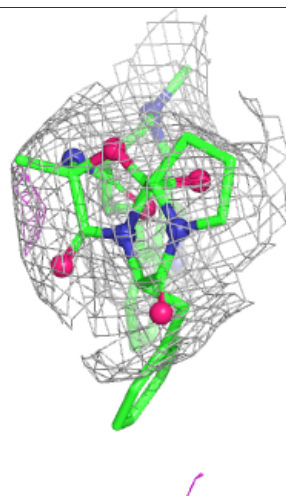
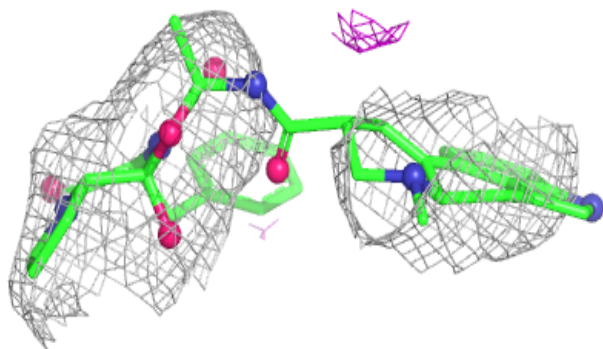
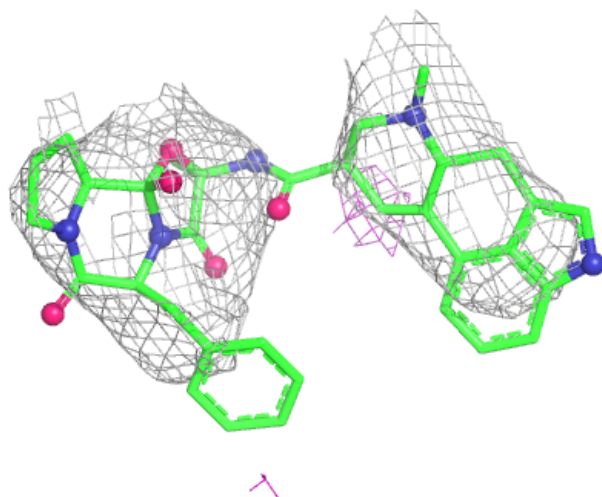
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ERM	A	2001	43/43	0.84	0.20	273,288,298,299	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 ERM A 2001:

$2mF_o-DF_c$ (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.