



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:45 pm BST

PDB ID : 5TUD
Title : Structural Insights into the Extracellular Recognition of the Human Serotonin 2B Receptor by an Antibody
Authors : Ishchenko, A.; Wacker, D.; Kapoor, M.; Zhang, A.; Han, G.W.; Basu, S.; Boutet, S.; James, D.; Wang, D.; Weierstall, U.; Liu, W.; Katritch, V.; Stevens, R.C.; Cherezov, V.
Deposited on : 2016-11-05
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 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

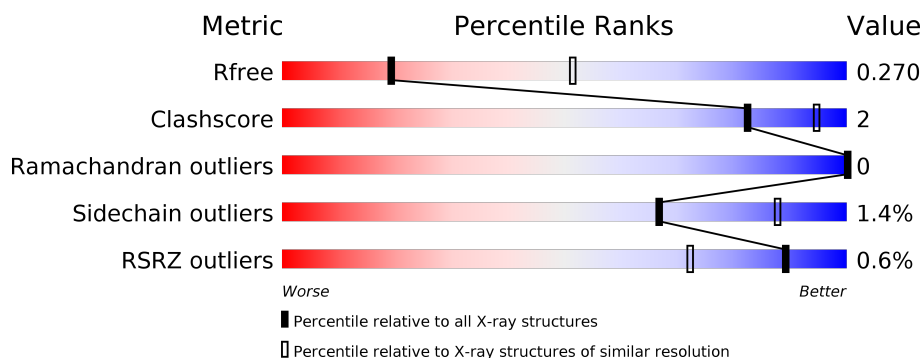
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on 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	457	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>6%</div> <div>18%</div> </div> </div>
1	D	457	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>7%</div> <div>19%</div> </div> </div>
2	B	213	<div> <div></div> <div>96%</div> <div>..</div> </div>
2	E	213	<div> <div></div> <div>96%</div> <div>..</div> </div>
3	C	236	<div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div>
3	F	236	<div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12395 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 2B,Soluble cytochrome b562 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	1	0
			2883	1901	460	505	17			
1	D	371	Total	C	N	O	S	0	0	0
			2875	1893	457	509	16			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP P41595
A	11	LYS	-	expression tag	UNP P41595
A	12	THR	-	expression tag	UNP P41595
A	13	ILE	-	expression tag	UNP P41595
A	14	ILE	-	expression tag	UNP P41595
A	15	ALA	-	expression tag	UNP P41595
A	16	LEU	-	expression tag	UNP P41595
A	17	SER	-	expression tag	UNP P41595
A	18	TYR	-	expression tag	UNP P41595
A	19	ILE	-	expression tag	UNP P41595
A	20	PHE	-	expression tag	UNP P41595
A	21	CYS	-	expression tag	UNP P41595
A	22	LEU	-	expression tag	UNP P41595
A	23	VAL	-	expression tag	UNP P41595
A	24	PHE	-	expression tag	UNP P41595
A	25	ALA	-	expression tag	UNP P41595
A	26	ASP	-	expression tag	UNP P41595
A	27	TYR	-	expression tag	UNP P41595
A	28	LYS	-	expression tag	UNP P41595
A	29	ASP	-	expression tag	UNP P41595
A	30	ASP	-	expression tag	UNP P41595
A	31	ASP	-	expression tag	UNP P41595
A	32	ASP	-	expression tag	UNP P41595
A	33	GLY	-	expression tag	UNP P41595

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Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	expression tag	UNP P41595
A	35	PRO	-	expression tag	UNP P41595
A	144	TRP	MET	engineered mutation	UNP P41595
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	406	GLY	-	expression tag	UNP P41595
A	407	ARG	-	expression tag	UNP P41595
A	408	PRO	-	expression tag	UNP P41595
A	409	LEU	-	expression tag	UNP P41595
A	410	GLU	-	expression tag	UNP P41595
A	411	VAL	-	expression tag	UNP P41595
A	412	LEU	-	expression tag	UNP P41595
A	413	PHE	-	expression tag	UNP P41595
A	414	GLN	-	expression tag	UNP P41595
A	415	GLY	-	expression tag	UNP P41595
A	416	PRO	-	expression tag	UNP P41595
A	417	HIS	-	expression tag	UNP P41595
A	418	HIS	-	expression tag	UNP P41595
A	419	HIS	-	expression tag	UNP P41595
A	420	HIS	-	expression tag	UNP P41595
A	421	HIS	-	expression tag	UNP P41595
A	422	HIS	-	expression tag	UNP P41595
A	423	HIS	-	expression tag	UNP P41595
A	424	HIS	-	expression tag	UNP P41595
A	425	HIS	-	expression tag	UNP P41595
D	10	MET	-	initiating methionine	UNP P41595
D	11	LYS	-	expression tag	UNP P41595
D	12	THR	-	expression tag	UNP P41595
D	13	ILE	-	expression tag	UNP P41595
D	14	ILE	-	expression tag	UNP P41595
D	15	ALA	-	expression tag	UNP P41595
D	16	LEU	-	expression tag	UNP P41595
D	17	SER	-	expression tag	UNP P41595
D	18	TYR	-	expression tag	UNP P41595
D	19	ILE	-	expression tag	UNP P41595
D	20	PHE	-	expression tag	UNP P41595
D	21	CYS	-	expression tag	UNP P41595
D	22	LEU	-	expression tag	UNP P41595
D	23	VAL	-	expression tag	UNP P41595
D	24	PHE	-	expression tag	UNP P41595
D	25	ALA	-	expression tag	UNP P41595

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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	ASP	-	expression tag	UNP P41595
D	27	TYR	-	expression tag	UNP P41595
D	28	LYS	-	expression tag	UNP P41595
D	29	ASP	-	expression tag	UNP P41595
D	30	ASP	-	expression tag	UNP P41595
D	31	ASP	-	expression tag	UNP P41595
D	32	ASP	-	expression tag	UNP P41595
D	33	GLY	-	expression tag	UNP P41595
D	34	ALA	-	expression tag	UNP P41595
D	35	PRO	-	expression tag	UNP P41595
D	144	TRP	MET	engineered mutation	UNP P41595
D	1007	TRP	MET	engineered mutation	UNP P0ABE7
D	1102	ILE	HIS	engineered mutation	UNP P0ABE7
D	1106	LEU	ARG	engineered mutation	UNP P0ABE7
D	406	GLY	-	expression tag	UNP P41595
D	407	ARG	-	expression tag	UNP P41595
D	408	PRO	-	expression tag	UNP P41595
D	409	LEU	-	expression tag	UNP P41595
D	410	GLU	-	expression tag	UNP P41595
D	411	VAL	-	expression tag	UNP P41595
D	412	LEU	-	expression tag	UNP P41595
D	413	PHE	-	expression tag	UNP P41595
D	414	GLN	-	expression tag	UNP P41595
D	415	GLY	-	expression tag	UNP P41595
D	416	PRO	-	expression tag	UNP P41595
D	417	HIS	-	expression tag	UNP P41595
D	418	HIS	-	expression tag	UNP P41595
D	419	HIS	-	expression tag	UNP P41595
D	420	HIS	-	expression tag	UNP P41595
D	421	HIS	-	expression tag	UNP P41595
D	422	HIS	-	expression tag	UNP P41595
D	423	HIS	-	expression tag	UNP P41595
D	424	HIS	-	expression tag	UNP P41595
D	425	HIS	-	expression tag	UNP P41595

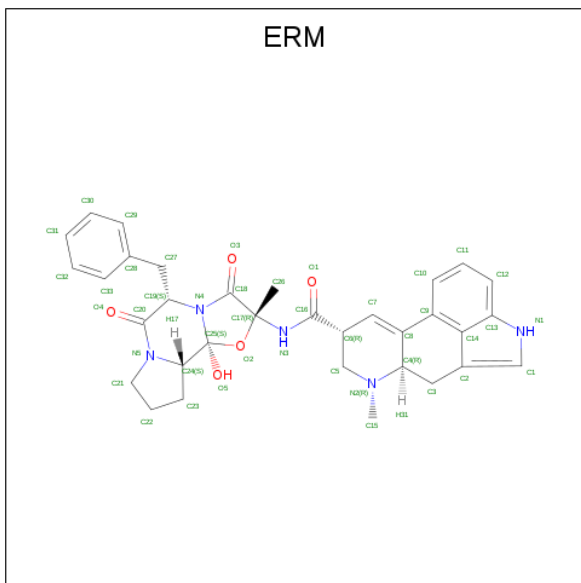
- Molecule 2 is a protein called Anti-5-HT2B Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1579	992	261	319	7			
2	E	211	Total	C	N	O	S	0	0	0
			1564	979	260	318	7			

- Molecule 3 is a protein called Anti-5-HT2B Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	229	Total	C	N	O	S	0	0	0
			1692	1072	281	332	7			
3	F	233	Total	C	N	O	S	0	0	0
			1716	1082	283	344	7			

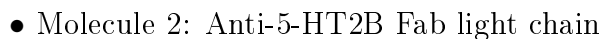
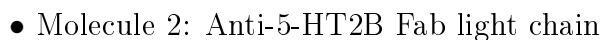
- Molecule 4 is Ergotamine (three-letter code: ERM) (formula: $C_{33}H_{35}N_5O_5$).



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

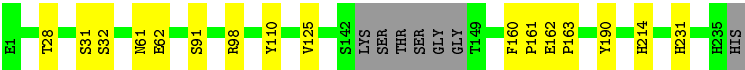
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- Molecule 1: 5-hydroxytryptamine receptor 2B, Soluble cytochrome b562 chimera

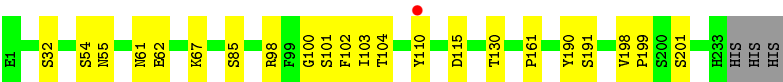
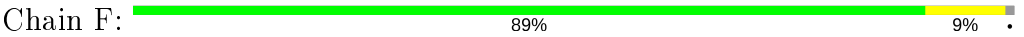




- Molecule 3: Anti-5-HT2B Fab heavy chain



- Molecule 3: Anti-5-HT2B Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.29 Å 118.86 Å 145.38 Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	35.64 – 3.00 35.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.64-3.00) 97.9 (35.64-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.90 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.227 , 0.247 0.248 , 0.270	Depositor DCC
R_{free} test set	2484 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	94.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12395	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.24	0/2945	0.38	0/4019
1	D	0.24	0/2936	0.38	0/4006
2	B	0.25	0/1615	0.43	0/2201
2	E	0.25	0/1600	0.44	0/2186
3	C	0.25	0/1740	0.43	0/2385
3	F	0.25	0/1763	0.43	0/2417
All	All	0.25	0/12599	0.41	0/17214

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	2883	0	2925	17	0
1	D	2875	0	2921	21	0
2	B	1579	0	1510	5	0
2	E	1564	0	1463	3	0
3	C	1692	0	1578	7	1
3	F	1716	0	1607	12	1
4	A	43	0	35	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	43	0	35	3	0
All	All	12395	0	12074	61	1

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 2.

All (61) 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:D:359:GLN:HG3	4:D:1201:ERM:H12	1.55	0.88
1:D:376:ASN:O	1:D:380:TYR:HD2	1.59	0.84
1:D:359:GLN:CG	4:D:1201:ERM:H12	2.09	0.81
1:D:193:LYS:NZ	1:D:213:ARG:O	2.15	0.80
1:D:329:VAL:HG21	1:D:380:TYR:OH	1.84	0.77
1:D:329:VAL:CG2	1:D:380:TYR:OH	2.38	0.71
2:E:90:ARG:NH2	3:F:100:GLY:O	2.25	0.69
1:A:359:GLN:HB2	4:A:2001:ERM:H12	1.77	0.66
1:D:198:ASP:O	2:E:90:ARG:NH1	2.33	0.61
3:C:61:ASN:OD1	3:C:62:GLU:N	2.35	0.60
1:A:359:GLN:CB	4:A:2001:ERM:H12	2.34	0.58
3:C:28:THR:OG1	3:C:31:SER:OG	2.22	0.58
3:F:100:GLY:N	3:F:115:ASP:OD1	2.37	0.57
1:D:1076:LEU:O	1:D:1080:ASN:ND2	2.39	0.56
1:D:376:ASN:O	1:D:380:TYR:CD2	2.51	0.55
1:A:1076:LEU:O	1:A:1080:ASN:ND2	2.40	0.55
1:A:314:GLN:O	1:A:318:ASN:ND2	2.41	0.54
1:D:153:ARG:NH2	1:D:326:LEU:HD23	2.22	0.54
3:F:54:SER:OG	3:F:55:ASN:N	2.41	0.53
3:F:61:ASN:OD1	3:F:62:GLU:N	2.42	0.53
3:F:103:ILE:O	3:F:110:TYR:N	2.41	0.53
1:A:1005:ASP:OD1	1:A:1006:ASN:N	2.42	0.52
1:D:197:THR:O	3:F:102:PHE:N	2.31	0.49
2:B:60:ARG:O	2:B:75:SER:N	2.46	0.49
1:D:376:ASN:N	1:D:377:PRO:HD2	2.28	0.49
1:A:194:GLY:O	1:A:213:ARG:NE	2.39	0.49
2:B:18:LYS:HE2	2:B:18:LYS:HA	1.94	0.48
1:A:359:GLN:HB2	4:A:2001:ERM:C21	2.42	0.48
1:A:193:LYS:NZ	1:A:213:ARG:O	2.45	0.48
1:A:246:LYS:O	1:A:1002:ASP:N	2.40	0.47
1:D:188:ILE:N	1:D:189:PRO:HD2	2.29	0.47
1:A:188:ILE:N	1:A:189:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:O	1:A:175:LYS:HB2	2.15	0.47
2:B:18:LYS:HZ3	2:B:74:ILE:HB	1.79	0.47
1:D:188:ILE:N	1:D:189:PRO:CD	2.78	0.47
1:A:188:ILE:N	1:A:189:PRO:CD	2.78	0.46
1:D:171:THR:O	1:D:175:LYS:HG3	2.14	0.46
3:F:190:TYR:O	3:F:191:SER:OG	2.34	0.45
3:F:67:LYS:NZ	3:F:85:SER:O	2.49	0.44
3:F:104:THR:HG23	3:F:104:THR:O	2.18	0.44
3:C:161:PRO:HG2	3:C:214:HIS:CE1	2.53	0.43
1:A:1026:VAL:O	1:A:1030:LEU:HB2	2.19	0.43
1:D:198:ASP:OD2	2:E:93:TYR:OH	2.35	0.43
3:F:32:SER:OG	3:F:98:ARG:NH1	2.48	0.42
1:A:208:VAL:HG23	4:A:2001:ERM:H19	2.01	0.42
1:D:338:CYS:N	1:D:339:PRO:HD2	2.35	0.42
2:B:197:HIS:ND1	2:B:198:GLN:N	2.68	0.42
3:C:160:PHE:O	3:C:190:TYR:CD1	2.73	0.42
3:C:32:SER:OG	3:C:98:ARG:NH2	2.53	0.41
2:B:74:ILE:HG22	2:B:75:SER:H	1.85	0.41
1:D:171:THR:O	1:D:174:ILE:HG13	2.21	0.41
3:F:130:THR:HG22	3:F:161:PRO:HD3	2.03	0.41
1:D:217:PHE:O	1:D:221:GLY:N	2.51	0.41
3:C:162:GLU:N	3:C:163:PRO:CD	2.84	0.41
3:C:91:SER:HB3	3:C:125:VAL:HG12	2.03	0.41
1:A:338:CYS:N	1:A:339:PRO:HD2	2.35	0.41
1:A:66:ILE:HB	1:A:67:PRO:HD3	2.03	0.41
1:D:153:ARG:NH2	1:D:326:LEU:CD2	2.83	0.40
1:A:355:GLN:O	1:A:359:GLN:HG2	2.20	0.40
1:D:218:MET:HG3	4:D:1201:ERM:C31	2.51	0.40
3:F:198:VAL:HB	3:F:199:PRO:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:GLU:OE2	3:F:201:SER:OG[2_657]	1.99	0.21

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	370/457 (81%)	361 (98%)	9 (2%)	0	100	100
1	D	367/457 (80%)	354 (96%)	13 (4%)	0	100	100
2	B	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
2	E	209/213 (98%)	201 (96%)	8 (4%)	0	100	100
3	C	225/236 (95%)	210 (93%)	15 (7%)	0	100	100
3	F	231/236 (98%)	211 (91%)	20 (9%)	0	100	100
All	All	1611/1812 (89%)	1536 (95%)	75 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	302/395 (76%)	300 (99%)	2 (1%)	84	94
1	D	304/395 (77%)	297 (98%)	7 (2%)	50	80
2	B	175/185 (95%)	173 (99%)	2 (1%)	73	90
2	E	170/185 (92%)	165 (97%)	5 (3%)	42	76
3	C	185/205 (90%)	183 (99%)	2 (1%)	73	90
3	F	190/205 (93%)	189 (100%)	1 (0%)	88	96
All	All	1326/1570 (84%)	1307 (99%)	19 (1%)	67	88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	60	LEU
2	B	46	TRP
2	B	197	HIS
3	C	110	TYR
3	C	231	HIS
1	D	212	GLU
1	D	234	ILE
1	D	1014	LEU
1	D	1102	ILE
1	D	356	THR
1	D	362	LEU
1	D	375	VAL
2	E	46	TRP
2	E	76	ARG
2	E	89	GLN
2	E	136	ASN
2	E	145	VAL
3	F	101	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	ASN
2	B	151	ASN

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 carbohydrates 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	$\# Z > 2$
4	ERM	D	1201	-	46,50,50	0.62	0	66,79,79	0.89	2 (3%)
4	ERM	A	2001	-	46,50,50	0.74	1 (2%)	66,79,79	1.61	8 (12%)

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	D	1201	-	-	3/13/87/87	0/7/8/8
4	ERM	A	2001	-	-	0/13/87/87	0/7/8/8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	ERM	C9-C8	2.66	1.50	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	ERM	C19-N4-C18	-5.73	119.78	125.93
4	A	2001	ERM	O2-C25-N4	-5.15	99.43	104.00
4	A	2001	ERM	C25-N4-C18	4.48	117.12	112.64
4	A	2001	ERM	O2-C25-C24	4.13	115.47	110.37
4	A	2001	ERM	C26-C17-N3	4.02	113.88	108.39
4	A	2001	ERM	C25-O2-C17	3.58	113.52	111.29
4	D	1201	ERM	C27-C19-N4	2.75	116.00	112.54
4	A	2001	ERM	C10-C9-C14	-2.65	116.37	120.10
4	D	1201	ERM	C10-C9-C14	-2.50	116.59	120.10
4	A	2001	ERM	C27-C19-C20	2.31	114.72	109.84

There are no chirality outliers.

All (3) torsion outliers are listed below:

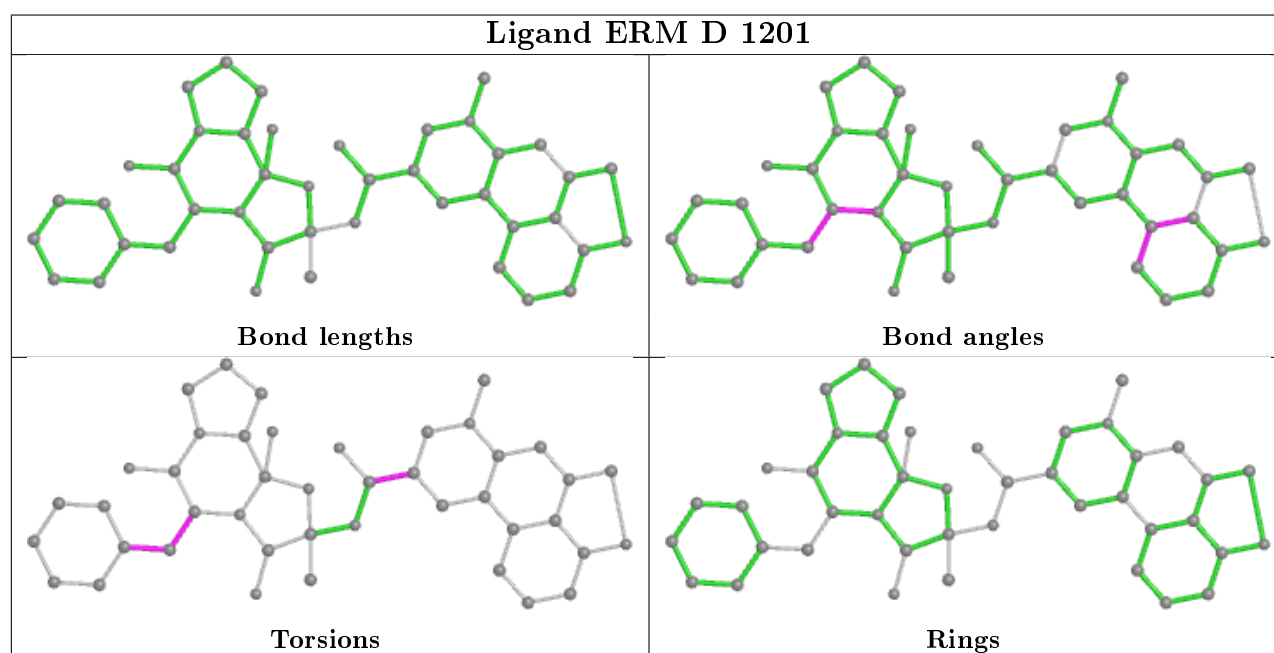
Mol	Chain	Res	Type	Atoms
4	D	1201	ERM	N4-C19-C27-C28
4	D	1201	ERM	O1-C16-C6-C7
4	D	1201	ERM	C19-C27-C28-C33

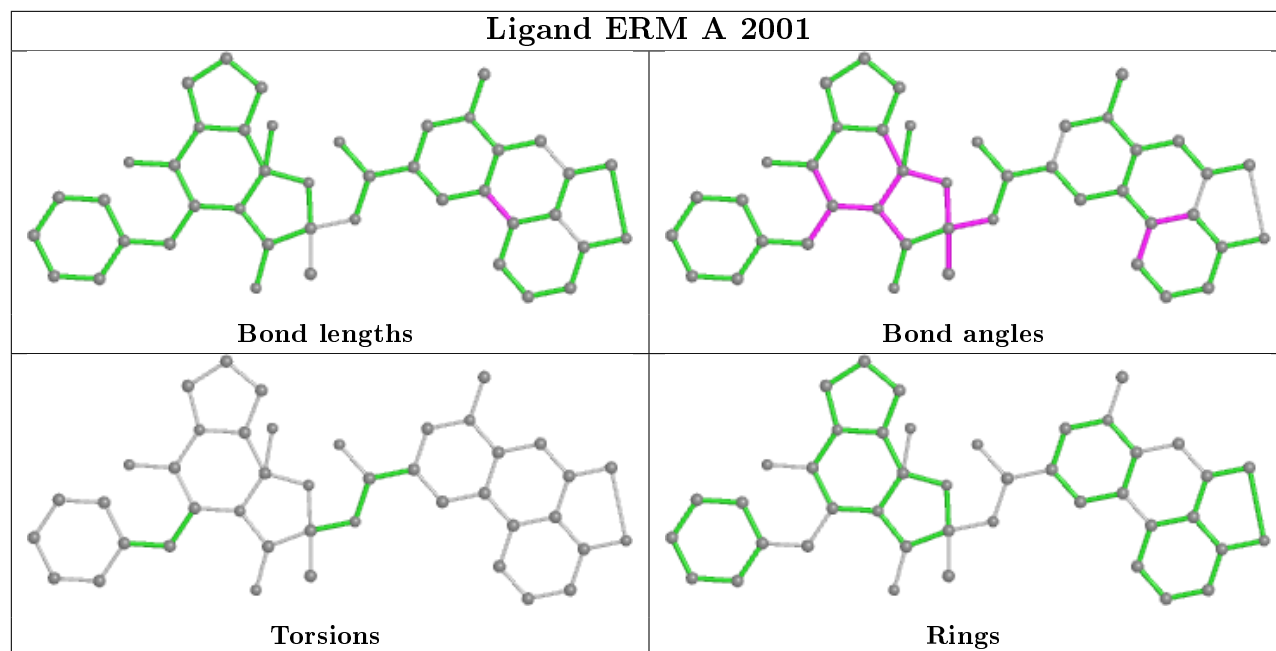
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1201	ERM	3	0
4	A	2001	ERM	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	373/457 (81%)	-0.26	4 (1%) 80 56	75, 103, 144, 186	0
1	D	371/457 (81%)	-0.26	4 (1%) 80 56	58, 107, 142, 193	0
2	B	211/213 (99%)	-0.30	0 100 100	69, 105, 128, 143	0
2	E	211/213 (99%)	-0.37	0 100 100	75, 99, 132, 151	0
3	C	229/236 (97%)	-0.40	0 100 100	76, 107, 131, 159	0
3	F	233/236 (98%)	-0.41	1 (0%) 92 79	67, 104, 132, 157	0
All	All	1628/1812 (89%)	-0.32	9 (0%) 89 72	58, 105, 136, 193	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	165	GLN	6.6
1	A	166	TYR	3.9
1	D	380	TYR	3.8
1	A	380	TYR	3.6
1	D	165	GLN	3.1
1	D	166	TYR	2.5
1	A	167	ASN	2.3
3	F	110	TYR	2.2
1	D	1105	TYR	2.1

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](#)

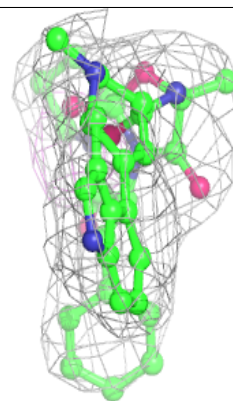
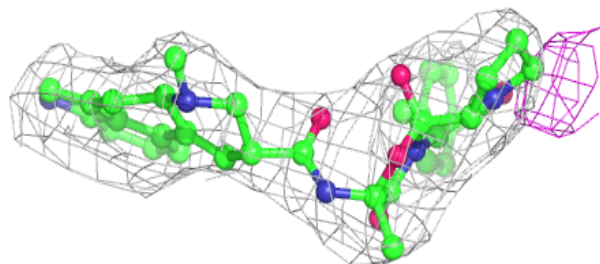
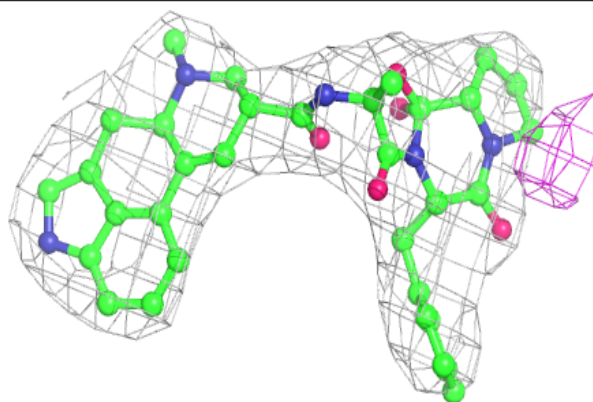
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ERM	A	2001	43/43	0.96	0.22	78,88,101,103	0
4	ERM	D	1201	43/43	0.97	0.24	85,97,106,107	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.

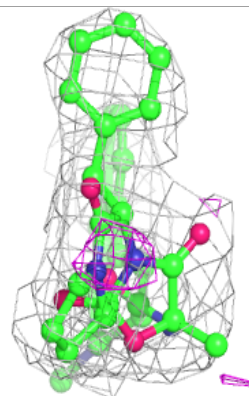
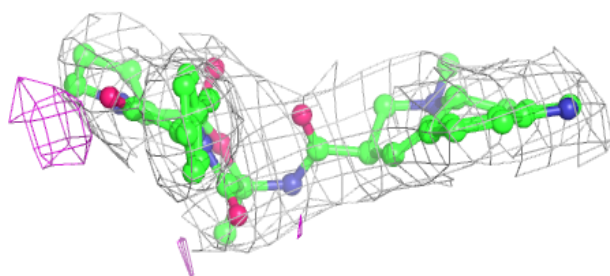
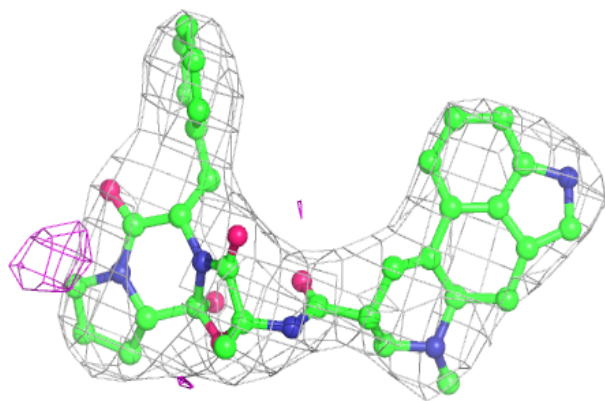
Electron density around ERM A 2001:

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



Electron density around ERM D 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 [i](#)

There are no such residues in this entry.