



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 23, 2017 – 07:41 PM EDT

PDB ID : 4BOT
EMDB ID: : EMD-2383
Title : The structure and super-organization of acetylcholine receptor- rapsyn complexes class E
Authors : Zuber, B.; Unwin, N.
Deposited on : unknown
Resolution : 42.00 Å(reported)
Based on PDB ID : 2BG9

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

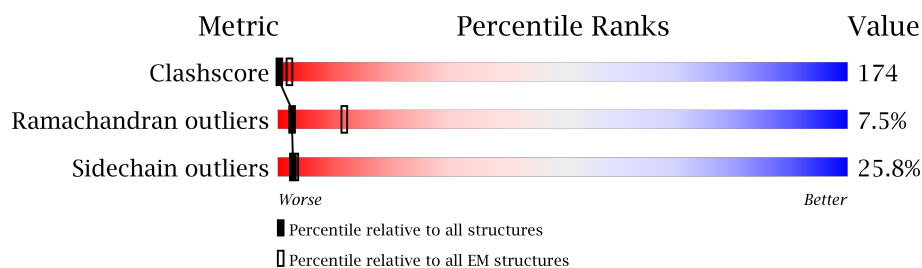
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 42.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	461	6% 51% 20% . 20%
1	D	461	7% 51% 21% . 20%
2	B	493	5% 49% 19% . 25%
3	C	522	7% 43% 19% . 29%
4	E	505	6% 46% 18% . 27%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14924 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
1	D	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		

- Molecule 2 is a protein called ACETYLCHOLINE RECEPTOR BETA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		

- Molecule 3 is a protein called ACETYLCHOLINE RECEPTOR DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		

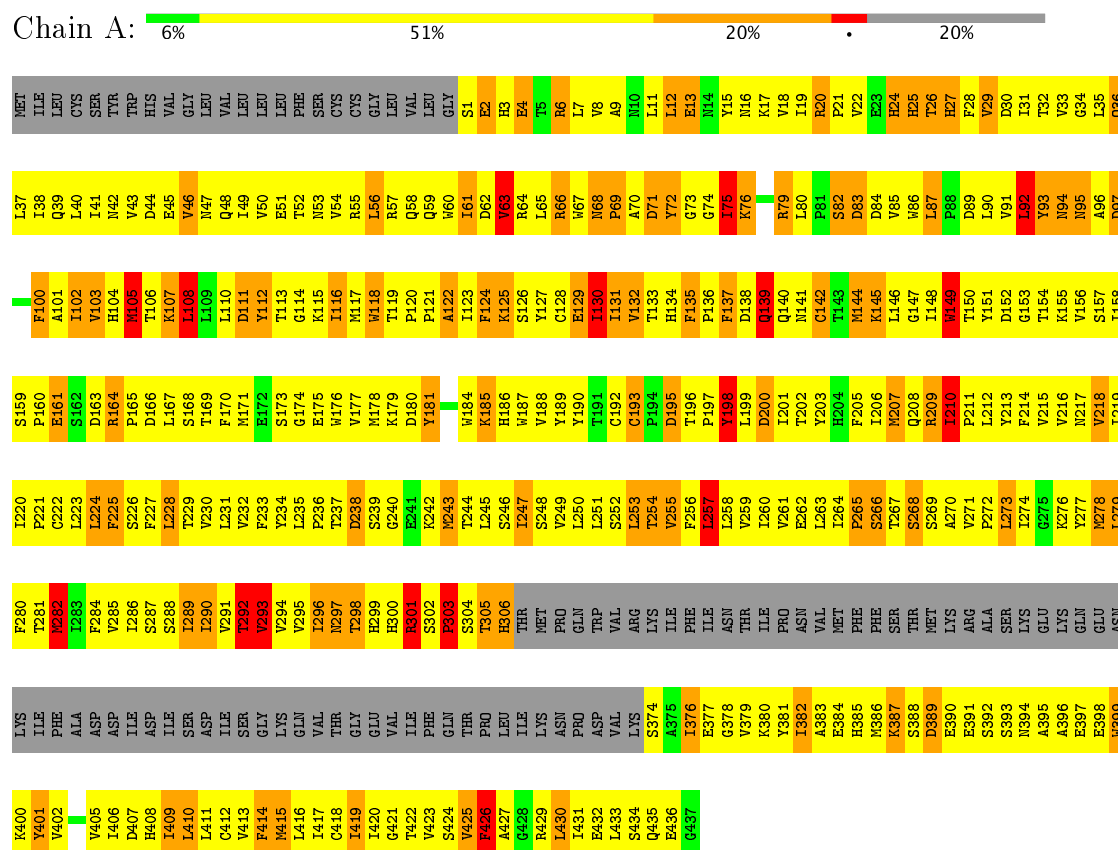
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

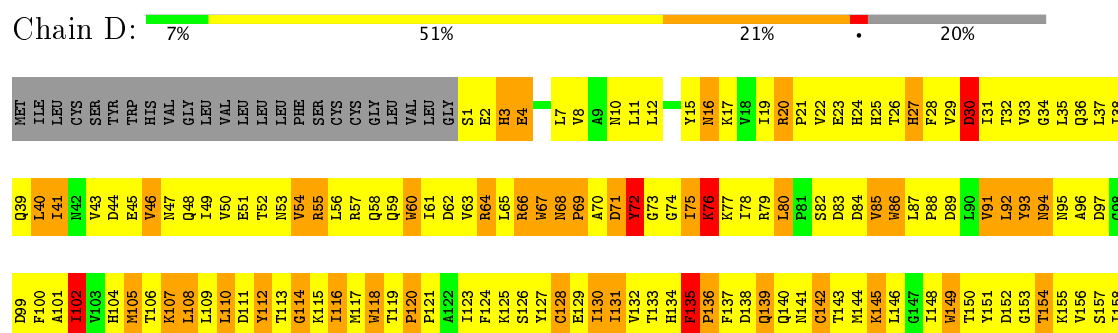
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA



• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA





M465	ASN	GLU	V285	R223	M160	G100	S40
M466	ASN	ILE	P286	K224	D161	Q101	M41
M467	GLU	GLU	L287	P225	L162	I102	L42
G468	ASN	GLN	I288	L226	NET	N103	I43
M469	ILE	PRO	G289	G227	THR	A104	S44
I470	ALA	ASP	K290	Y228	ASP	A105	L45
F471	ALA	TRP	Y291	Y229	THR	Y106	F46
I472	SER	GLN	L292	I230	ILE	F107	E47
F473	ASP	ASN	M293	P231	ASP	C108	T48
F474	GLN	ASP	F294	F232	GLY	M109	D49
M475	LEU	LEU	L295	I233	LYS	V110	E50
G476	HIS	LYS	M296	T234	ASP	L111	T51
M477	ASP	LEU	S297	P235	TYR	V112	L52
F478	GLU	ARG	L298	L238	ILE	R113	T53
M479	ILE	ARG	F299	I239	GLU	P114	T54
R480	LYS	SER	T300	S240	TRP	N115	M55
P481	S421	SER	G301	F241	ILE	G116	V56
P482	G422	SER	V302	L242	ILE	Y117	M57
A483	I423	VAL	V303	A243	I178	V118	M58
K484	D424	GLY	V304	A244	I179	T119	D59
P485	S425	TYR	N305	A244	D180	M120	H60
PHE	T426	ILE	G306	A246	P181	L121	A61
GLU	M427	SER	G307	A246	E182	P122	M62
GLY	Y428	LYS	I308	F247	A183	P123	M63
ASP	I429	ALA	V309	Y248	F184	A124	D64
PRO	V430	GLN	L310	L249	T185	I125	M65
PHE	K431	GLU	N311	P250	I186	F126	R66
ASP	D432	TYR	F312	A251	N187	G127	L67
T433	I433	PHE	H313	E252	G188	A128	T68
TYR	L434	ASN	F314	S253	E189	S129	M69
SER	K434	ASN	F315	S253	E190	C130	M70
SER	E435	ILE	R316	K256	E191	P131	A71
ASP	K436	LYS	T316	M257	I192	I132	S72
HIS	M437	SER	P317	S258	I193	N133	E73
PRO	A438	ARG	S318	T259	H194	V134	Y74
ARG	Y439	SER	T319	G260	K195	L135	S75
CYS	P440	GLU	H320	A261		L136	D76
ALA	E441	LEU	VAL	L261		Y136	F77
	E442	MET	LEU	C262	K198	F137	S78
	V443	PHE	SER	V263	K199	P138	I79
	G444	GLU	THR	L264	M200	F139	L80
	M445	LYS	ARG	L265	T201	D140	L81
	M446	GLN	VAL	A266	Y202	W141	R81
	M447	SER	LYS	G267	G203	Q142	L82
	L448	GLU	GLN	A268	D204	N143	R83
	V449	ARG	ILE	V269	K205	C144	P84
	G450	HIS	PHE	F270	F206	S145	B85
	O451	GLY	LEU	L271	P207	L146	L86
	F452	LEU	GLU	L272		K147	I87
	I453	VAL	LYS	L273	M211	F148	M88
	D454	PRO	LEU	T274	Y212	T149	P89
	R455	ARG	PRO	S275	Q213	A150	P90
	L456	VAL	ARG	Q276	D214	L151	D91
	S457	THR	ILE	R277	V215	N152	I92
	M458	PRO	LEU	L278	T216	Y153	V93
	F459	ARG	HIS	P279	F217	N154	L94
	I460	ILE	MET	E280	Y218	A155	Q95
	T461	GLY	SER	T281	L219	N156	N96
	M462	PHE	ARG	A282	T220	E157	M97
	F463	GLY	VAL	L283	T221	I158	N98
	V464	ASN	ASP	E284	S222	S159	D99

- Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain E:  6% 46% 18% 2% 27%

ASP	LEU	LYS	GLU	K284	N224	G164	Y104	E44	NET
ALA	ASN	PRO	PRO	L286	I226	VAL	A105	K45	VAL
PHE	ARG	GLN	GLN	I287	A227	VAL	Y107	E47	THR
ALA	ARG	PRO	ARG	F288	P228	GLU	L108	A48	LEU
PRO	ARG	V289	TRP	I289	C229	TRP	Y109	L49	LEU
GLU	ARG	M290	ILE	F290	V230	ILE	Y110	T50	LEU
LYS	SER	F291	HIS	F291	L231	HIS	M111	T51	ILE
LYS	SER	S292	D172	F292	I232	D172	D112	N52	ILE
S414	PHE	S293	D173	S293	S233	D173	G113	V53	CYS
C415	GLY	L294	P174	S234	S234	P174	S114	H54	LEU
V416	ILE	V295	E175	L295	L235	E175	M115	I55	ALA
E417	MET	I296	D176	V236	V237	D176	Y116	E56	LEU
A418	ILE	F297	F177	V237	F177	F178	M117	I57	VAL
A419	LYS	T298	T178	L238	T178	E179	M118	Q58	GLU
M420	ALA	N299	E179	V239	E179	P119	P119	N59	ARG
F421	ALA	C300	M180	Y240	M180	P120	P120	N60	SER
I422	GLU	F301	G181	F241	G181	A121	A121	D61	M1
A423	GLU	I302	E182	L242	E182	I122	I122	Y62	E2
K424	TYR	F303	M183	P243	M183	Y123	Y123	R63	E3
S425	ILE	L304	T184	K244	T184	S124	L124	L64	G4
S425	LEU	N305	I185	Q245	I185	R125	R125	S65	R5
T426	LYS	V306	R186	A246	R186	L126	L126	H66	L6
K427	LYS	S307	H187	G247	H187	G127	G127	M67	F7
E428	PRO	L308	R188	G248	R188	P128	P128	T68	E8
Q429	ARG	R309	P189	Q249	P189	I129	I129	S69	K9
D431	SER	T310	A190	K250	A190	A130	A130	E70	L10
S432	GLU	F311	K191	C251	K191	Y131	Y131	Y71	L11
S432	LEU	N312	N192	T252	N192	T132	T132	E72	G12
G433	MET	T313	N193	L253	N193	R133	R133	G73	D13
S434	PHE	H314	Y194	S254	Y194	P134	P134	I74	Y14
E435	GLU	SER	N195	T255	N195	F135	F135	D75	D15
A436	GLU	LEU	H196	S256	H196	F136	F136	L76	K16
E437	GLN	SER	V257	V257	V257	D137	D137	V77	R17
M438	LYS	GLU	L258	L258	L258	M138	M138	R78	I18
M439	ASP	LYS	T599	L259	T599	Q139	Q139	I79	K19
V440	ARG	ILE	K200	A260	K200	M140	M140	P80	P20
L441	HIS	LYS	D201	Q261	D201	C141	C141	S81	A21
I442	GLY	HIS	T262	T262	T262	S142	S142	E82	K22
G443	LEU	LEU	L263	L263	L263	L143	L143	L83	T23
K444	LYS	PHE	F264	F264	F264	D204	D204	L84	L24
V445	ARG	LEU	L265	L265	L265	F205	F145	H85	E25
L446	VAL	GLU	F266	F266	F266	Q206	Q206	L86	E26
D447	ASN	PHI	L267	L267	L267	E207	S147	P87	V27
A448	LYS	LEU	L268	L268	L268	I209	Q148	D88	T28
A449	MET	PRO	A269	A269	A269	I209	T149	V89	D29
C450	THR	LYS	Q270	Q270	Q270	F210	Y150	V90	V30
F451	SER	TYR	K271	K271	K271	F211	M151	L91	T31
M452	ASP	LEU	V272	V272	V272	L212	A152	E92	L32
I453	ILE	GLY	F273	F273	F273	L213	H153	N93	K33
A454	ASP	MET	E274	E274	E274	I214	E154	N94	L34
L455	ILE	HIS	T275	T275	T275	Q215	V155	V95	T35
L456	GLY	LEU	S276	S276	S276	R216	M156	D96	L36
L457	THR	GLU	L277	L277	L277	K217	L157	G97	T37
	THR	PRO	P218	P218	P218	L218	Q158	Q98	N38
L460	VAL	SER	V279	V279	V279	L219	M159	F99	L39
G461	ASP	GLU	P280	P280	P280	G220	S160	E100	I40
T462	LEU	GLU	L281	L281	L281	Y221	A161	V101	S41
L463	TYR	THR	P282	P282	P282	I222	E162	L402	M42
L463	LYS	THR	C282	C282	C282	L222	F162	X102	L42

I465		G469	N472	Q473	PRO
F466		H470	N473	V474	PHE
		L471	P475	P475	PRO
			E476	E476	GLY
			F477	F477	ASP
					PRO
					ARG
					LYS
					TYR
					VAL
					PRO

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	3564	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	80213	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
1	D	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
2	B	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
3	C	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
4	E	0.74	6/3057 (0.2%)	1.01	9/4174 (0.2%)
All	All	0.74	15/15302 (0.1%)	1.01	38/20883 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
3	C	0	2
All	All	0	4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-8.40	1.14	1.34
1	A	118	TRP	CB-CG	7.91	1.64	1.50
1	D	208	GLN	C-N	7.58	1.51	1.34
4	E	8	GLU	CB-CG	6.52	1.64	1.52
3	C	265	LEU	C-N	6.18	1.48	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	266	ALA	N-CA-CB	10.40	124.66	110.10
4	E	198	LEU	CA-CB-CG	7.18	131.82	115.30
3	C	315	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	209	ARG	NE-CZ-NH2	6.96	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	263	ILE	CG1-CB-CG2	-6.67	96.73	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	63	TYR	Sidechain
3	C	74	TYR	Sidechain
1	D	277	TYR	Sidechain
1	D	72	TYR	Sidechain

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	2991	0	3005	1072	0
1	D	2991	0	3006	1056	0
2	B	2972	0	2952	1088	0
3	C	2983	0	2987	1159	0
4	E	2987	0	2994	1090	0
All	All	14924	0	14944	5204	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 174.

The worst 5 of 5204 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)
4:E:183:TRP:CB	4:E:216:ARG:HG2	1.33	1.53
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.44	1.51
1:A:167:LEU:HD12	1:A:178:MET:CB	1.43	1.48
1:A:167:LEU:CD1	1:A:178:MET:HB2	1.46	1.45
1:D:261:VAL:O	1:D:265:PRO:HD2	1.22	1.38

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 PDB entries followed by that with respect to all EM entries.

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	366/461 (79%)	288 (79%)	49 (13%)	29 (8%)	1	17
1	D	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	15
2	B	364/493 (74%)	274 (75%)	58 (16%)	32 (9%)	1	15
3	C	364/522 (70%)	288 (79%)	58 (16%)	18 (5%)	2	27
4	E	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	19
All	All	1825/2442 (75%)	1425 (78%)	264 (14%)	136 (8%)	2	18

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	27	HIS
1	A	76	LYS
1	A	83	ASP
1	A	102	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 PDB entries followed by that with respect to all EM entries.

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	343/427 (80%)	248 (72%)	95 (28%)	0	3
1	D	343/427 (80%)	258 (75%)	85 (25%)	1	5
2	B	340/449 (76%)	262 (77%)	78 (23%)	1	6
3	C	335/475 (70%)	243 (72%)	92 (28%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	337/463 (73%)	249 (74%)	88 (26%)	0	4
All	All	1698/2241 (76%)	1260 (74%)	438 (26%)	2	4

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	106	TYR
3	C	315	ARG
4	E	217	LYS
3	C	130	CYS
3	C	241	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	200	ASN
1	D	42	ASN
4	E	197	GLN
3	C	231	ASN
3	C	447	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	129:THR	C	130:ILE	N	1.14