



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:37 PM BST

PDB ID : 2BG9
Title : REFINED STRUCTURE OF THE NICOTINIC ACETYLCHOLINE RE-
CEPTOR AT 4A RESOLUTION.
Authors : Unwin, N.
Deposited on : 2004-12-17
Resolution : 4.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

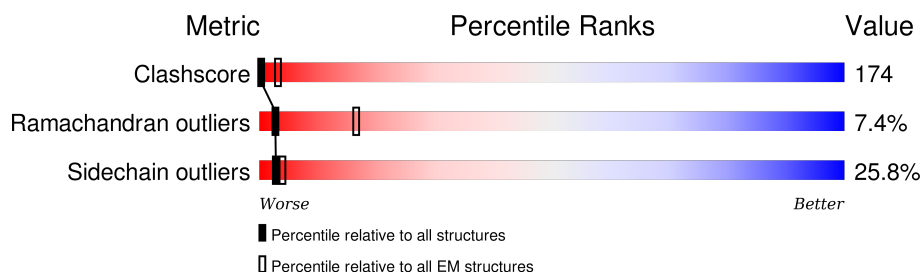
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	370	8% 63% 25% 5%
1	D	370	8% 64% 26% .
2	B	370	6% 66% 26% .
3	C	369	9% 62% 27% .
4	E	370	8% 63% 25% .

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 PROTEIN, ALPHA CHAIN.

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 PROTEIN, BETA CHAIN.

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 PROTEIN, DELTA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	369	Total	C	N	O	S	0	0
			2983	1944	488	537	14		

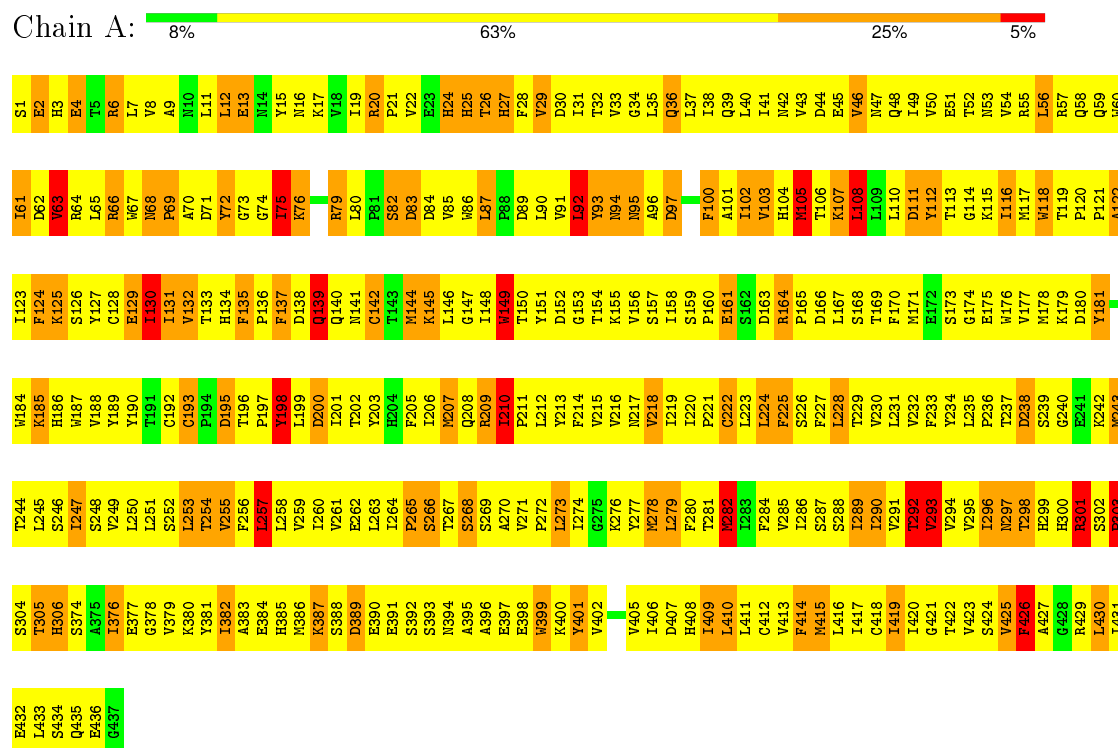
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR PROTEIN, GAMMA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	370	Total	C	N	O	S	0	0
			2987	1948	477	552	10		

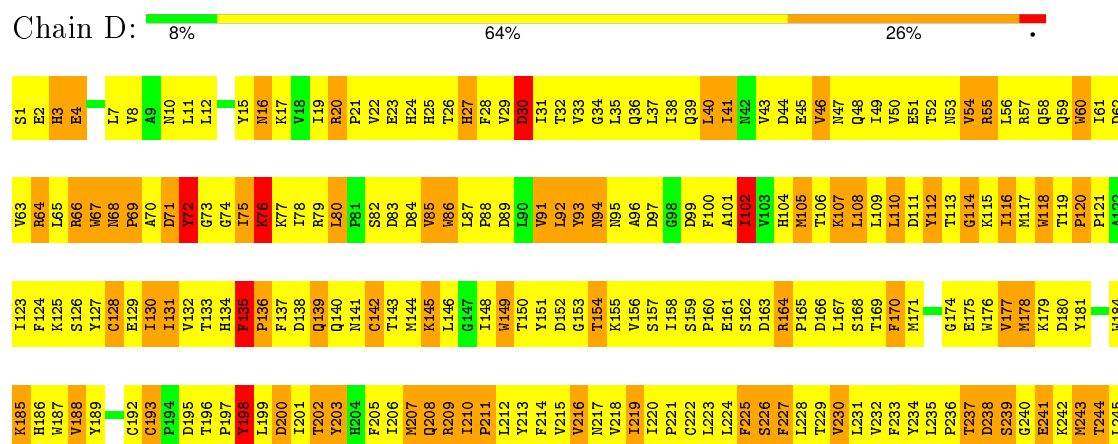
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 PROTEIN, ALPHA CHAIN



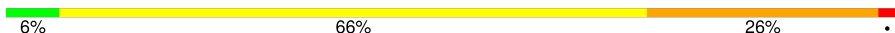
• Molecule 1: ACETYLCHOLINE RECEPTOR PROTEIN, ALPHA CHAIN



S246	H306
1247	S374
S248	A376
V249	I376
L250	E377
L251	G378
S252	V379
L253	K380
T254	Y381
V255	I382
F256	A383
L257	E384
L258	H385
V259	M386
L260	K387
V261	S388
E262	D389
L263	E390
L264	E391
F265	S392
S266	S393
T267	N394
S268	A395
S269	A396
A270	E397
V271	E398
P272	M399
L273	K400
L274	Y401
G275	V402
K276	A403
Y277	M404
M278	V405
L279	I406
F280	D407
T281	H408
M282	I409
L283	L410
F284	L411
V285	C412
L286	V413
S287	F414
L288	M415
L289	M416
L290	I417
V291	C418
T292	I419
V293	I420
V294	G421
V295	T422
L296	V423
M297	S424
T298	V425
H299	F426
H300	A427
R301	L430
S302	I431
P303	E432
S304	L433
T305	

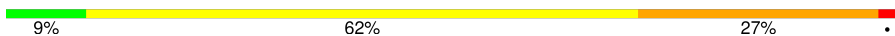
S434
Q435
E436
G437

• Molecule 2: ACETYLCHOLINE RECEPTOR PROTEIN, BETA CHAIN

Chain B:  6% 66% 26%

S1	T61	S121	H190	S250	R310	N461
V2	D62	A122	K191	L261	T311	V462
M3	Y63	I123	P192	S262	H312	P463
E4	R64	Y124	S193	I263	E403	P464
D5	L65	R125	A194	S254	A404	N465
T6	D66	S126	K195	A255	V405	D466
L7	H67	S127	N196	L256	E406	P467
L8	D68	C128	H197	L257	A407	F468
S9	P69	T129	I198	A258	K409	A469
V10	A70	K130	S199	L259	V410	
L11	Y72	V132	D201	T260	L411	
F12	E73	M133	P202	F262	A412	
E13	G74	Y134	S203	L263	E413	
N14	I75	F135	Y204	L264	Q414	
Y15	K76	D137	D206	L266	E416	
M16	D77	F138	V207	A267	S417	
P17	L78	M139	T208	D268	A418	
K18	S79	Q140	F209	K269	S419	
R20	L80	C142	V210	V270	E420	
S22	S82	T143	T212	E272	F421	
Q23	D83	M144	D214	T273	L424	
T24	H84	V145	R215	S274	K425	
V25	E85	F146	R216	L275	K426	
G26	H86	K147	P217	S276	D427	
D27	Q87	S148	L218	V277	N428	
K28	D89	T149	F219	P278	Q429	
V29	I90	T150	V220	L279	Y430	
T30	V91	D152	T221	L280	V431	
R32	L92	T153	V222	I281	A432	
V33	H93	S154	Y223	S282	N433	
G34	N95	E155	T224	Y283	V434	
L35	I96	D156	I225	L284	A435	
T36	D97	V157	V226	M285	D436	
L37	I98	L158	P227	F286	R437	
T38	S99	Q159	C228	L287	L438	
S39	F100	H160	L229	M288	F439	
L41	E101	A161	L230	L289	L440	
I42	T102	L162	T231	L290	Y441	
L43	T103	D163	S232	V291	L442	
M44	L104	A164	L233	A292	F443	
E45	H105	M174	L234	F293	T444	
K46	V106	N176	A235	S294	T445	
M47	I108	Q177	T236	I296	N446	
E48	E109	D178	L237	L297	C447	
E49	V110	A179	V238	S298	S448	
M50	T51	F180	F239	V299	T449	
T52	H112	I181	Y240	V300	G450	
S53	T113	E182	L241	V301	T451	
V54	G114	N183	P242	L302	F452	
F55	A115	L184	N303	L303	S453	
L56	V116	Q185	D244	L304	L454	
M57	S117	Q186	A245	H305	F455	
L58	H118	M187	G246	H306	L456	
A59	P120	I188	E247	R307	D457	
M60		E189	T248	P309	A458	
			V249		S459	
					H460	

• Molecule 3: ACETYLCHOLINE RECEPTOR PROTEIN, DELTA CHAIN

Chain C:  9% 62% 27%

V1	A61	L121	K198	T261
N2	H62	P122	K199	C262
E3	Y63	P123	N200	V263
E4	D64	A124	I201	L264
E5	H65	I125	Y202	L265
R6	R66	F126	G203	A266
L7	L67	A127	D204	Q267
L8	T68	S128	K205	A268
N9	H69	S129	F206	V269
D10	N70	C130	P207	F270
L11	A71	P131	N211	L271
L12	S72	I132	Y212	L272
T13	E73	K133	Q213	T274
Y14	Y74	V134	D214	S275
M15	S75	L135	L215	Q276
K16	D76	F137	T216	R277
Y17	I77	P138	F217	L278
N18	S78	F139	E218	P279
K19	I79	D140	L219	E280
H20	L80	M141	A220	T281
V21	R81	Q142	T221	A282
R22	L82	N143	R223	L283
F23	R83	C144	R224	T284
V24	P84	S145	P225	V285
K25	E85	L146	K226	P286
H26	L86	K147	P227	L287
I27	I87	F148	F228	L288
N28	H88	T149	K290	G289
E29	I89	A150	V291	K290
V30	P90	L151	L292	Y291
V31	D91	N152	K293	L292
R32	I92	Y153	F294	M293
I33	L94	A154	I295	F294
A34	Q95	M155	T296	L295
L35	N96	T234	S297	M296
S36	I97	P335	L298	S297
L37	N98			L298
T38	N98			V299
L39	D99			S300
G100	G100			G301
N41	Q101			S302
L42	L102			V303
L43	N103			V304
S44	V104			N305
L45	A105			C306
R46	Y106			G307
F47	F107			I308
C108	C108			V309
T48	N109			L310
D49	F184			N311
E50	T185			F312
T51	L111			H313
L52	V112			F314
T53	R113			S253
T54	P114			K315
N55	N115			T316
V56	G116			P317
N57	Y117			S318
M58	V118			T319
P59	T119			H320
H60	W120			

S421 G422 T423 D424 S425 T426 T427 Y428 T429 V430 K431 Q432 T433 K434 E435 K436 N437 A438 Y439 D440 E441 E442 V443 G444 N445 K446 N447 V449 G450 G451 Q452 T453 D454 R455 L456 S457 K458 F459 T460 T461 T462 P463 V464 M465 V466 V467 G468 T469 T470 F471 T472 F473 V474 M475 G476 N477 F478 N479 R480

P481
P482
K484

• Molecule 4: ACETYLCHOLINE RECEPTOR PROTEIN, GAMMA CHAIN

Chain E: 8% 63% 25% *

N1 E2 E3 G4 R5 L6 L7 E8 S9 K9 L10 L11 L12 G12 D13 G73 Y14 Y15 D15 L16 L17 R17 R18 K19 P20 A21 K22 T23 T24 L24 D25 H26 V27 D88 T28 D29 V30 T31 T32 R33 K34 L34 T35 T36 D36 T37 N38 F39 L39 T40 S41 A102 L42 L43 G44 A104 A105 M106 E107 L108 A109 V109 T50 T51 N52 N53 G54 T55 E56 E57 L58 P59 M60

D61 Y62 R63 L64 S65 M66 N67 T68 S69 E70 Y71 Y72 E73 E74 D75 V77 V78 P80 S81 E82 L83 L84 L85 L86 P87 D88 V89 V90 T91 E92 R93 N94 V95 D96 G97 Q98 F99 E100 A101 A102 Y103 G104 A105 M106 E107 L108 A109 V109 T110 N111 D112 G113 S114 M115 Y116 M117 L118 P119 P120

A121 T122 Y123 R124 S125 T126 C127 F128 T129 A130 Y131 Y132 T132 E133 Y134 F135 F136 D137 Y138 Q139 N140 S141 S142 L143 Y144 F145 R146 S147 Q148 T149 Y150 N151 A152 H153 E154 V155 M156 L157 Q158 L159 S160 A161 E162 E163 G164 T172 D173 P174 E175 D176 F177 T178 E179 N180 G181 E182 M183 T184 L185 R186 H187

R188 P189 K190 K191 K192 N193 Y194 M195 M196 L198 T199 K200 D201 D202 D203 F204 F205 Q206 E207 I208 T209 F210 F211 L212 L213 L214 Q215 R216 K217 P218 L219 F220 Y221 I222 I223 N224 I225 I226 A227 P228 C229 V230 L231 L232 S233 S234 L235 V236 V237 L238 V239 Y240 F241 L242 P243 A244 Q245 A246 G247

G248 Q249 R250 C251 T252 L253 S254 I255 S256 V257 L258 L259 A260 Q261 T262 L263 F264 L265 F266 L267 I268 A269 Q270 Q271 V272 V273 E274 T275 S276 L277 V278 V279 F280 L281 L282 G283 K284 V285 L286 L287 F288 V289 N290 F291 V292 S293 L294 V295 L296 V297 T298 N299 C300 V301 I302 V303 L304 N305 V306 S307

L308 R309 T310 P311 N312 T313 H314 A315 V316 E317 A318 C319 N320 F321 I322 A323 K324 S325 T326 K327 E328 Q329 N330 D331 S332 G333 S334 E335 N336 E337 N338 F339 V340 L341 I342 G343 K344 V345 I346 D347 A348 A349 C350 F351 W352 I353 A354 L355 L356 L357 L360 G361 T362 L363 A364 L365 F366

G469 H470 L471 N472 Q473 V474 P475 E476

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEM300SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	40000	Depositor
Image detector	SO-163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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	9/4173 (0.2%)
4	E	0.73	6/3057 (0.2%)	1.01	9/4172 (0.2%)
All	All	0.74	15/15302 (0.1%)	1.01	38/20879 (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	-8.41	1.14	1.34
1	A	118	TRP	CB-CG	7.90	1.64	1.50
1	D	208	GLN	C-N	7.57	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	10.39	124.64	110.10
4	E	198	LEU	CA-CB-CG	7.19	131.83	115.30
3	C	315	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	A	209	ARG	NE-CZ-NH2	7.04	123.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	263	ILE	CG1-CB-CG2	-6.66	96.74	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	1069	0
1	D	2991	0	3006	1060	0
2	B	2972	0	2952	1081	0
3	C	2983	0	2987	1148	0
4	E	2987	0	2994	1090	0
All	All	14924	0	14944	5190	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 5190 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	1.50
1:A:167:LEU:HD12	1:A:178:MET:CB	1.43	1.47
1:A:167:LEU:CD1	1:A:178:MET:HB2	1.46	1.44
3:C:316:THR:CG2	3:C:447:ASN:HB3	1.53	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	366/370 (99%)	288 (79%)	50 (14%)	28 (8%)	1	20
1	D	366/370 (99%)	294 (80%)	41 (11%)	31 (8%)	1	17
2	B	364/370 (98%)	274 (75%)	58 (16%)	32 (9%)	1	17
3	C	363/369 (98%)	288 (79%)	57 (16%)	18 (5%)	3	32
4	E	364/370 (98%)	280 (77%)	58 (16%)	26 (7%)	1	23
All	All	1823/1849 (99%)	1424 (78%)	264 (14%)	135 (7%)	3	21

5 of 135 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	343/343 (100%)	248 (72%)	95 (28%)	0	4
1	D	343/343 (100%)	258 (75%)	85 (25%)	1	7
2	B	340/340 (100%)	262 (77%)	78 (23%)	1	9
3	C	335/335 (100%)	243 (72%)	92 (28%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	337/337 (100%)	249 (74%)	88 (26%)	0	6
All	All	1698/1698 (100%)	1260 (74%)	438 (26%)	3	6

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 64 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	152	ASN
1	D	36	GLN
4	E	197	GLN
3	C	200	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.