wwPDB EM Validation Summary Report

Mar 27, 2025 – 12:13 pm GMT

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

This is a wwPDB EM 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
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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:

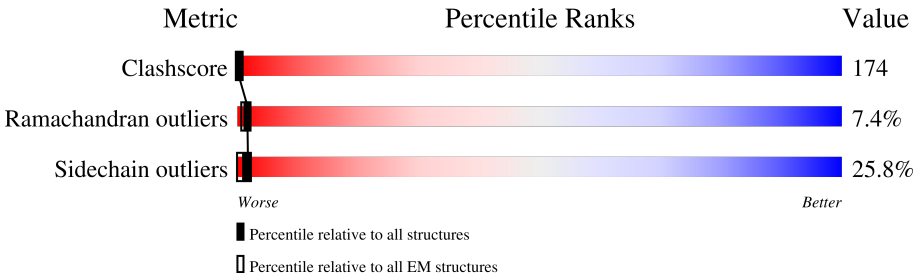
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

1 Overall quality at a glance (i)

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=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 (i)

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.

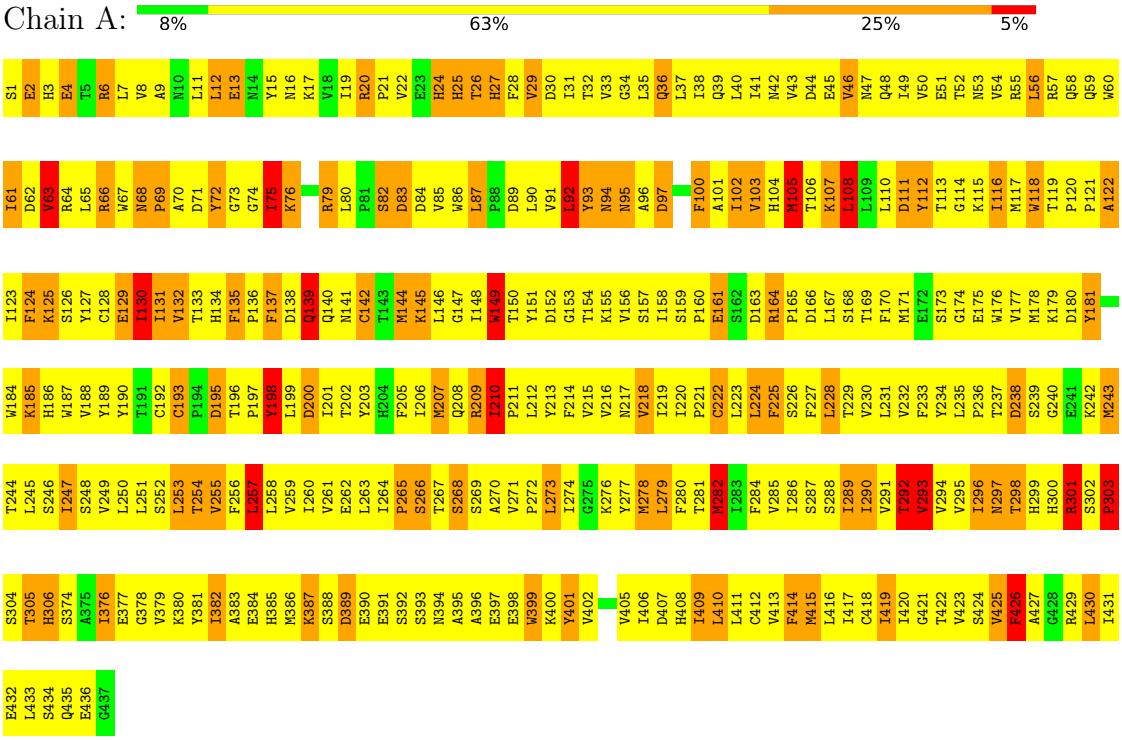
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	370	Total	C	N	O	S	0	0
			2987	1948	477	552	10		

3 Residue-property plots (i)

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. 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.

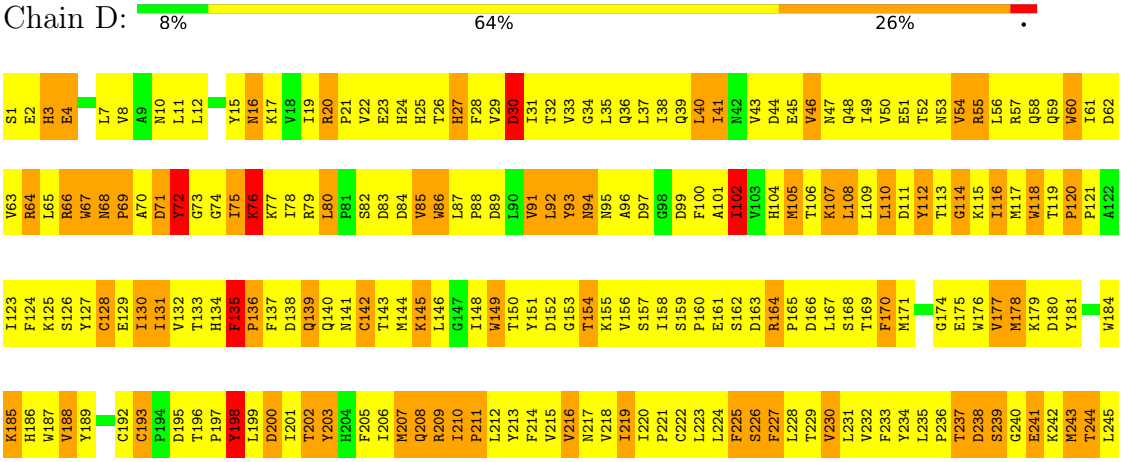
• Molecule 1: ACETYLCHOLINE RECEPTOR PROTEIN, ALPHA CHAIN

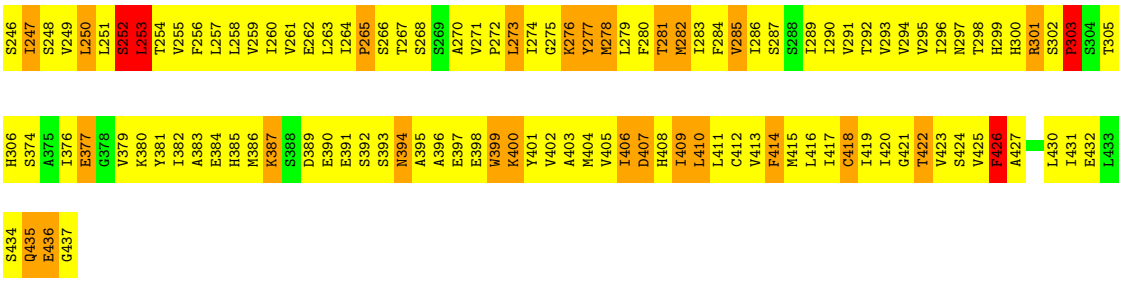
Chain A:



• Molecule 1: ACETYLCHOLINE RECEPTOR PROTEIN, ALPHA CHAIN

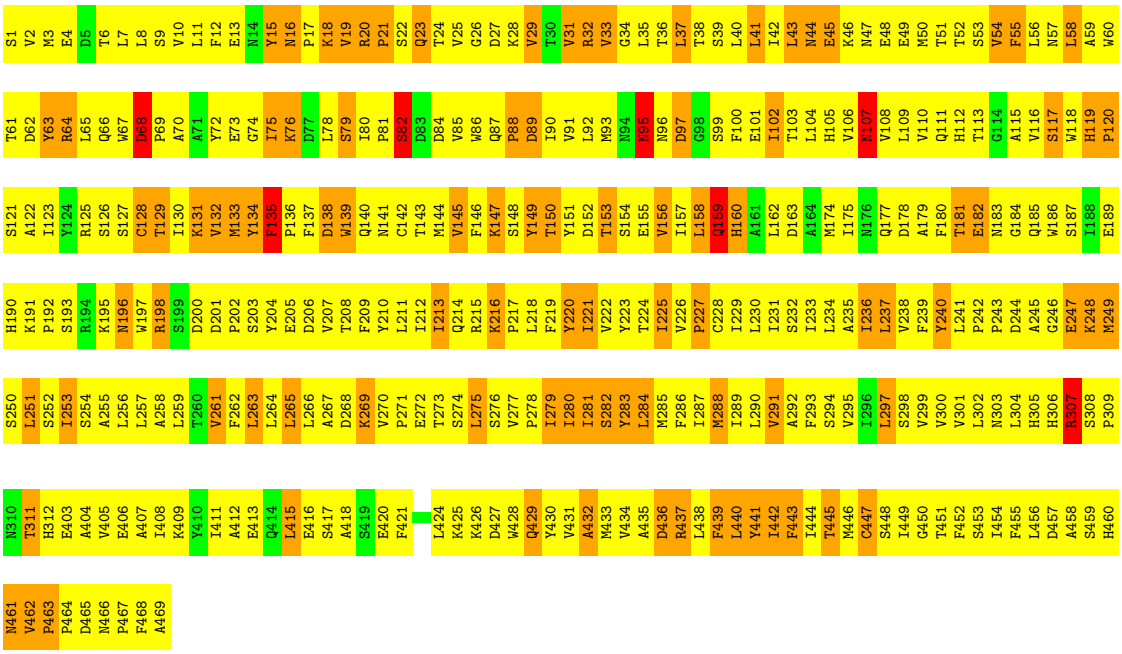
Chain D:





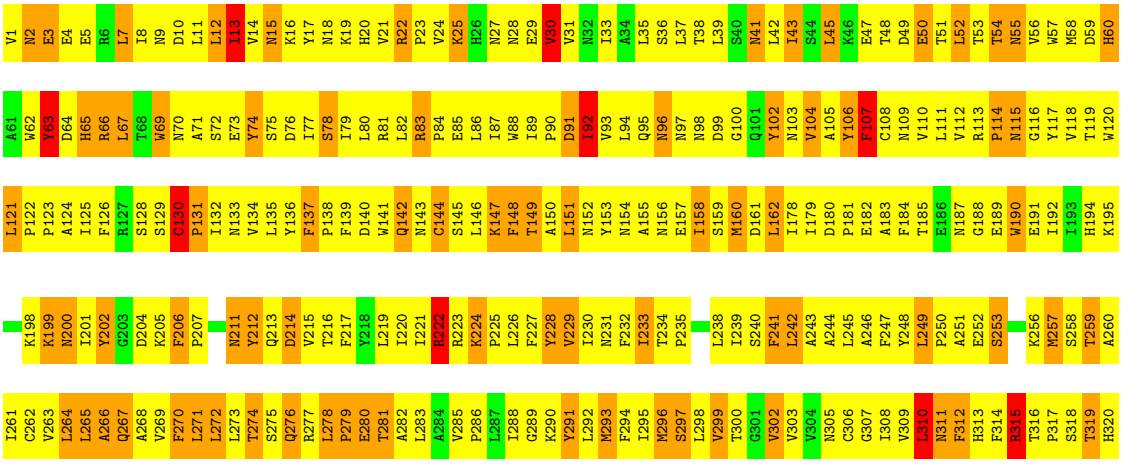
• Molecule 2: ACETYLCHOLINE RECEPTOR PROTEIN, BETA CHAIN

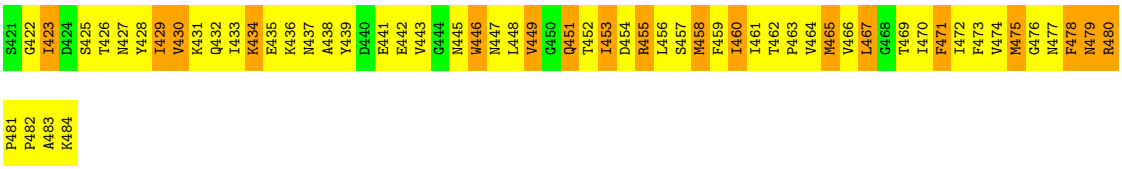
Chain B: 6% 66% 26%



• Molecule 3: ACETYLCHOLINE RECEPTOR PROTEIN, DELTA CHAIN

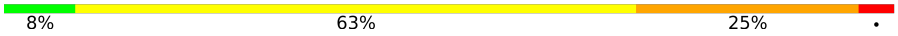
Chain C: 9% 62% 27%

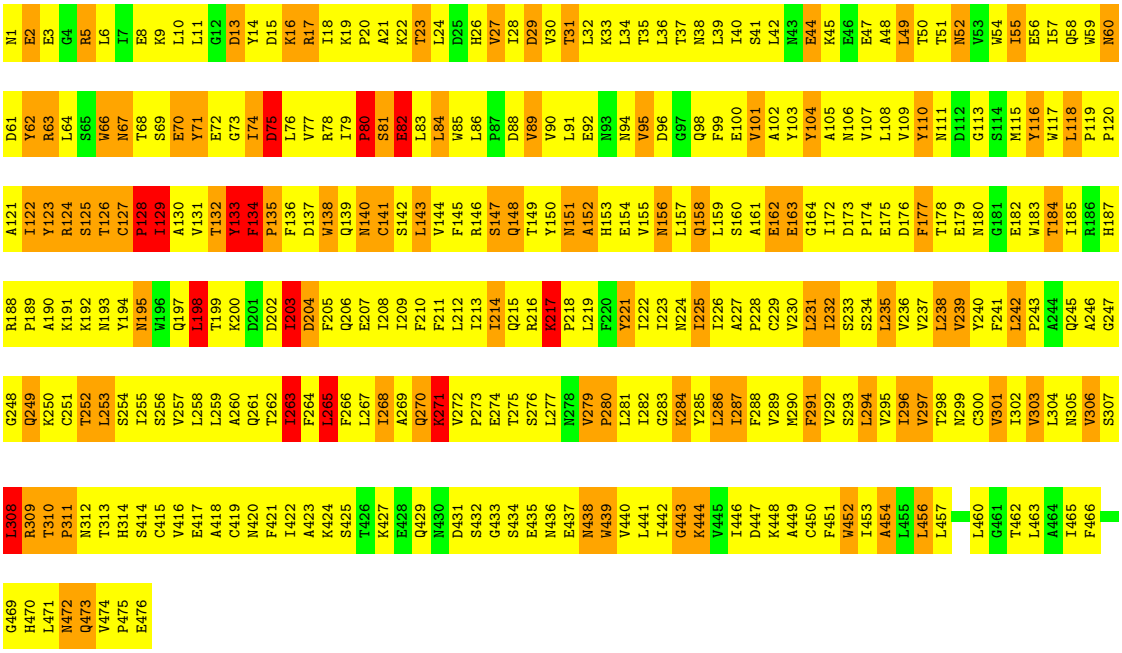




• Molecule 4: ACETYLCHOLINE RECEPTOR PROTEIN, GAMMA CHAIN

Chain E:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14924	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	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 (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 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 13
1	D	366/370 (99%)	294 (80%)	41 (11%)	31 (8%)	0 11
2	B	364/370 (98%)	274 (75%)	58 (16%)	32 (9%)	0 11
3	C	363/369 (98%)	288 (79%)	57 (16%)	18 (5%)	1 19
4	E	364/370 (98%)	280 (77%)	58 (16%)	26 (7%)	1 14
All	All	1823/1849 (99%)	1424 (78%)	264 (14%)	135 (7%)	2 13

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 (i)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	337/337 (100%)	249 (74%)	88 (26%)	0 3
All	All	1698/1698 (100%)	1260 (74%)	438 (26%)	2 3

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

Mol	Chain	Res	Type
3	C	274	THR
1	D	94	ASN
4	E	184	THR
3	C	296	MET
3	C	471	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	158	GLN
4	E	197	GLN
3	C	70	ASN
3	C	65	HIS
4	E	206	GLN

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)

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	3
3	C	2
4	E	2
1	A	1
1	D	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	312:HIS	C	403:GLU	N	45.08
1	C	320:HIS	C	421:SER	N	45.05
1	E	314:HIS	C	414:SER	N	44.81
1	A	306:HIS	C	374:SER	N	44.46
1	D	306:HIS	C	374:SER	N	43.93