wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Dec 20, 2016 – 05:06 PM EST

PDB ID	:	5MG3
EMDB ID:	:	EMD-3506
Title	:	EM fitted model of bacterial holo-translocon
Authors	:	Schaffitzel, C.; Botte, M.
Deposited on	:	2016-11-20
Resolution	:	14.00 Å(reported)

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 (i) symbol.

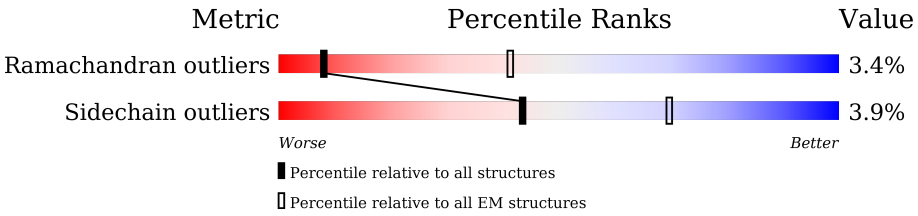
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 14.00 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)
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 <=5%

Mol	Chain	Length	Quality of chain
1	Y	458	70% 22%
2	E	140	33% 11% 54%
3	G	136	20% 76%
4	D	622	53% 11% 33%
5	F	323	68% 17% 5% 11%
6	C	559	63% 16% 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 26650 atoms, of which 13553 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 Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Y	443	7004	2259	3581	566	580	18	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-14	VAL	-	expression tag	UNP P0AGA2
Y	-13	TRP	-	expression tag	UNP P0AGA2
Y	-12	ASN	-	expression tag	UNP P0AGA2
Y	-11	CYS	-	expression tag	UNP P0AGA2
Y	-10	GLU	-	expression tag	UNP P0AGA2
Y	-9	ARG	-	expression tag	UNP P0AGA2
Y	-8	ILE	-	expression tag	UNP P0AGA2
Y	-7	THR	-	expression tag	UNP P0AGA2
Y	-6	ILE	-	expression tag	UNP P0AGA2
Y	-5	SER	-	expression tag	UNP P0AGA2
Y	-4	HIS	-	expression tag	UNP P0AGA2
Y	-3	ARG	-	expression tag	UNP P0AGA2
Y	-2	LYS	-	expression tag	UNP P0AGA2
Y	-1	GLN	-	expression tag	UNP P0AGA2
Y	0	THR	-	expression tag	UNP P0AGA2

- Molecule 2 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	65	1062	332	552	91	86	1	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	369	MET	-	initiating methionine	UNP P0AG96
E	370	HIS	-	expression tag	UNP P0AG96

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Chain	Residue	Modelled	Actual	Comment	Reference
E	371	HIS	-	expression tag	UNP P0AG96
E	372	HIS	-	expression tag	UNP P0AG96
E	373	HIS	-	expression tag	UNP P0AG96
E	374	HIS	-	expression tag	UNP P0AG96
E	375	HIS	-	expression tag	UNP P0AG96
E	376	ASP	-	expression tag	UNP P0AG96
E	377	ASP	-	expression tag	UNP P0AG96
E	378	ASP	-	expression tag	UNP P0AG96
E	379	ASP	-	expression tag	UNP P0AG96
E	380	LYS	-	expression tag	UNP P0AG96
E	381	ALA	-	expression tag	UNP P0AG96
E	382	MET	-	expression tag	UNP P0AG96
E	383	GLY	-	expression tag	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	G	32	480	151	244	39	44	2	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	439	VAL	-	expression tag	UNP P0AG99
G	440	GLY	-	expression tag	UNP P0AG99
G	441	THR	-	expression tag	UNP P0AG99
G	442	GLY	-	expression tag	UNP P0AG99
G	443	TRP	-	expression tag	UNP P0AG99
G	444	TYR	-	expression tag	UNP P0AG99
G	445	SER	-	expression tag	UNP P0AG99
G	446	GLY	-	expression tag	UNP P0AG99
G	447	SER	-	expression tag	UNP P0AG99
G	448	PRO	-	expression tag	UNP P0AG99
G	449	GLY	-	expression tag	UNP P0AG99
G	450	ILE	-	expression tag	UNP P0AG99
G	451	LEU	-	expression tag	UNP P0AG99
G	452	TYR	-	expression tag	UNP P0AG99
G	453	HIS	-	expression tag	UNP P0AG99
G	454	TRP	-	expression tag	UNP P0AG99
G	455	PRO	-	expression tag	UNP P0AG99
G	456	GLU	-	expression tag	UNP P0AG99
G	457	VAL	-	expression tag	UNP P0AG99

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Chain	Residue	Modelled	Actual	Comment	Reference
G	458	LEU	-	expression tag	UNP P0AG99
G	459	ARG	-	expression tag	UNP P0AG99
G	460	ILE	-	expression tag	UNP P0AG99
G	461	GLN	-	expression tag	UNP P0AG99
G	462	GLU	-	expression tag	UNP P0AG99
G	463	LEU	-	expression tag	UNP P0AG99
G	464	ILE	-	expression tag	UNP P0AG99

- Molecule 4 is a protein called Protein translocase subunit SecD.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	414	Total	C	H	N	O	S	0	0
			6419	1991	3291	545	582	10		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP P0AG90
D	-5	HIS	-	expression tag	UNP P0AG90
D	-4	HIS	-	expression tag	UNP P0AG90
D	-3	HIS	-	expression tag	UNP P0AG90
D	-2	HIS	-	expression tag	UNP P0AG90
D	-1	HIS	-	expression tag	UNP P0AG90
D	0	HIS	-	expression tag	UNP P0AG90
D	1	MET	-	expression tag	UNP P0AG90
D	142	VAL	ALA	conflict	UNP P0AG90

- Molecule 5 is a protein called Protein translocase subunit SecF.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	289	Total	C	H	N	O	S	0	0
			4502	1434	2291	366	398	13		

- Molecule 6 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	455	Total	C	H	N	O	S	0	0
			7183	2336	3594	582	650	21		

There are 17 discrepancies between the modelled and reference sequences:

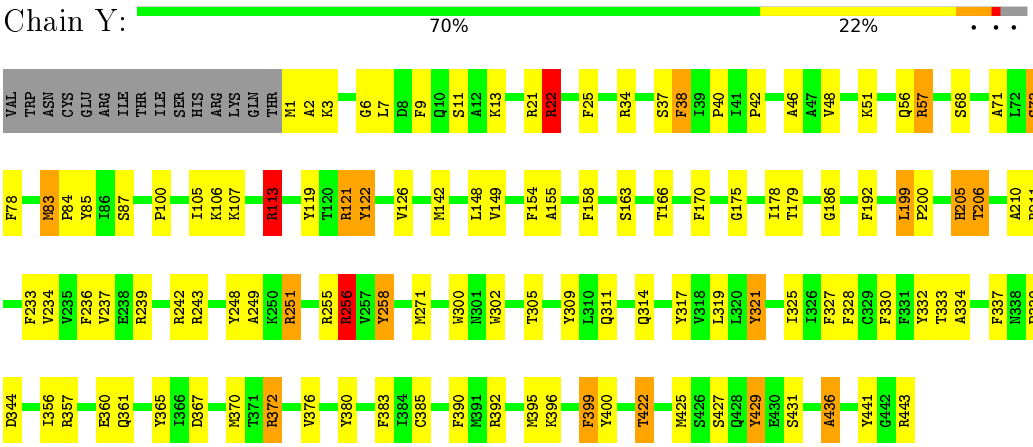
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	initiating methionine	UNP P25714
C	-3	ASP	-	expression tag	UNP P25714
C	-2	PRO	-	expression tag	UNP P25714
C	-1	SER	-	expression tag	UNP P25714
C	0	SER	-	expression tag	UNP P25714
C	1	ARG	-	expression tag	UNP P25714
C	228	ALA	GLU	conflict	UNP P25714
C	229	ALA	LYS	conflict	UNP P25714
C	231	ALA	GLU	conflict	UNP P25714
C	232	ALA	LYS	conflict	UNP P25714
C	234	ALA	LYS	conflict	UNP P25714
C	549	HIS	-	expression tag	UNP P25714
C	550	HIS	-	expression tag	UNP P25714
C	551	HIS	-	expression tag	UNP P25714
C	552	HIS	-	expression tag	UNP P25714
C	553	HIS	-	expression tag	UNP P25714
C	554	HIS	-	expression tag	UNP P25714

3 Residue-property plots (i)

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.

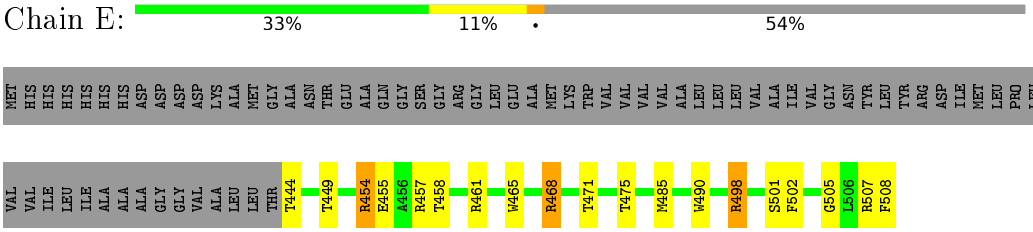
- Molecule 1: Protein translocase subunit SecY

Chain Y:



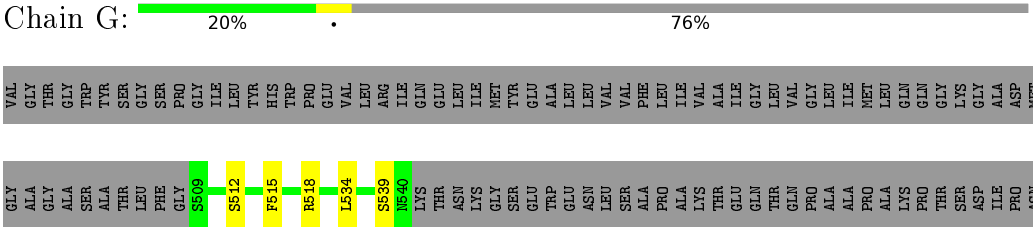
- Molecule 2: Protein translocase subunit SecE

Chain E:



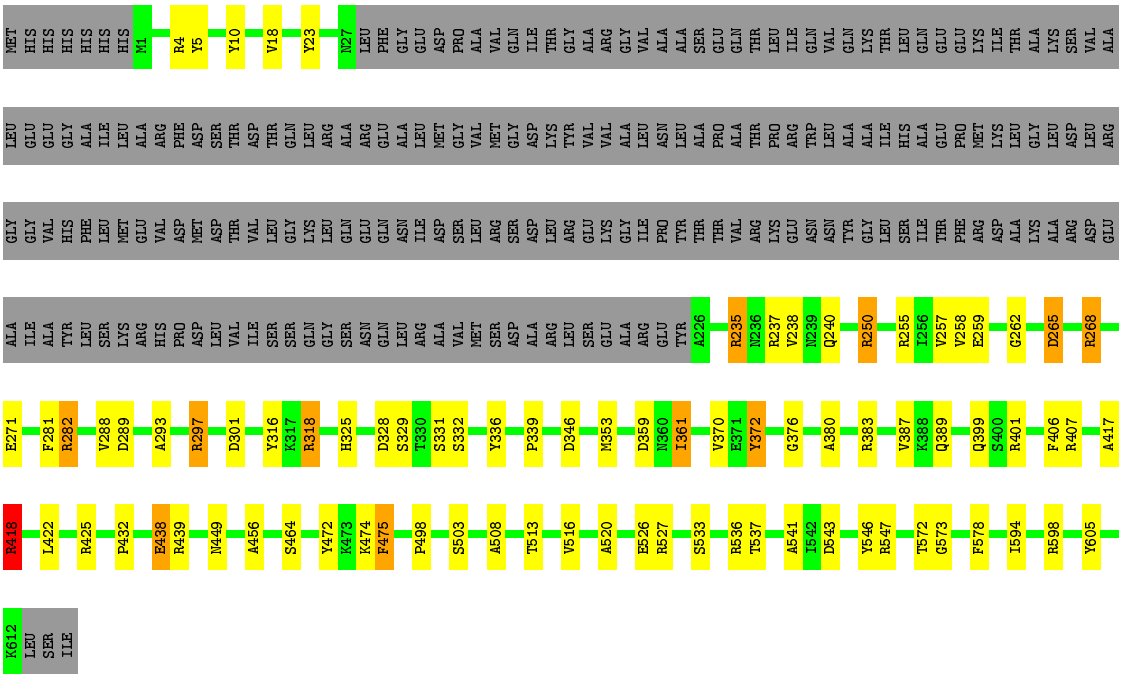
- Molecule 3: Protein-export membrane protein SecG

Chain G:



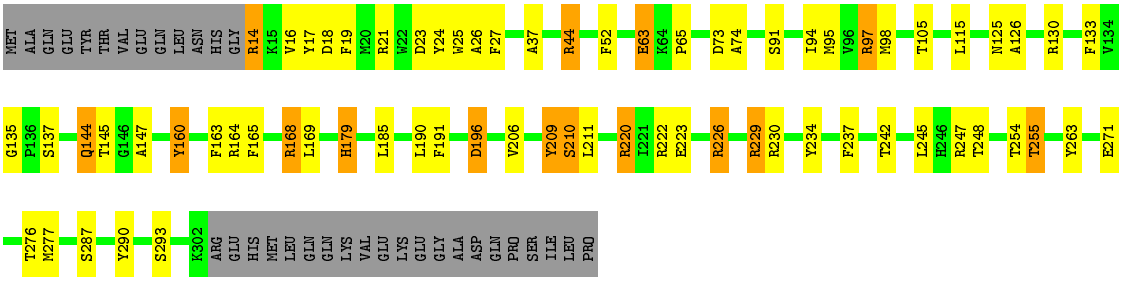
- Molecule 4: Protein translocase subunit SecD

Chain D:



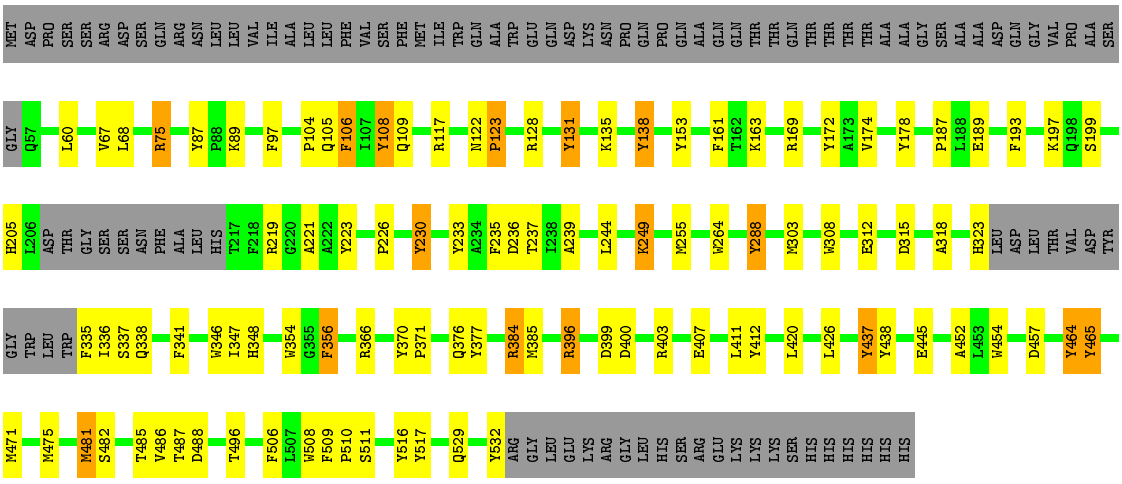
• Molecule 5: Protein translocase subunit SecF

Chain F:



• Molecule 6: Membrane protein insertase YidC

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	53648	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	Y	2.09	27/3501 (0.8%)	2.13	116/4744 (2.4%)
2	E	1.78	6/518 (1.2%)	2.24	19/702 (2.7%)
3	G	1.72	3/238 (1.3%)	1.91	5/320 (1.6%)
4	D	1.62	20/3163 (0.6%)	2.06	82/4288 (1.9%)
5	F	1.59	4/2250 (0.2%)	2.18	77/3049 (2.5%)
6	C	1.62	16/3683 (0.4%)	1.99	97/5013 (1.9%)
All	All	1.76	76/13353 (0.6%)	2.09	396/18116 (2.2%)

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	Y	0	11
2	E	0	3
4	D	0	9
5	F	0	13
6	C	0	21
All	All	0	57

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	317	TYR	CG-CD2	35.73	1.85	1.39
1	Y	317	TYR	CG-CD1	34.43	1.83	1.39
1	Y	317	TYR	CE2-CZ	33.58	1.82	1.38
1	Y	317	TYR	CE1-CZ	33.16	1.81	1.38
1	Y	317	TYR	CD1-CE1	23.16	1.74	1.39

The worst 5 of 396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	226	ARG	NE-CZ-NH1	28.99	134.80	120.30
4	D	297	ARG	NE-CZ-NH1	22.63	131.61	120.30
1	Y	392	ARG	NE-CZ-NH1	18.04	129.32	120.30
4	D	268	ARG	NE-CZ-NH1	17.26	128.93	120.30
5	F	168	ARG	NE-CZ-NH1	17.14	128.87	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	113	ARG	Sidechain
1	Y	122	TYR	Sidechain
1	Y	22	ARG	Sidechain
1	Y	38	PHE	Sidechain
1	Y	7	LEU	Peptide

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	Y	3423	3581	3583	0	0
2	E	510	552	551	0	0
3	G	236	244	243	0	0
4	D	3128	3291	3292	0	0
5	F	2211	2291	2290	0	0
6	C	3589	3594	3591	0	0
All	All	13097	13553	13550	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	Y	441/458 (96%)	367 (83%)	50 (11%)	24 (5%)	2 29
2	E	63/140 (45%)	57 (90%)	5 (8%)	1 (2%)	12 56
3	G	30/136 (22%)	29 (97%)	1 (3%)	0	100 100
4	D	410/622 (66%)	373 (91%)	25 (6%)	12 (3%)	6 43
5	F	287/323 (89%)	257 (90%)	24 (8%)	6 (2%)	9 50
6	C	449/559 (80%)	395 (88%)	40 (9%)	14 (3%)	5 42
All	All	1680/2238 (75%)	1478 (88%)	145 (9%)	57 (3%)	8 40

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	48	VAL
1	Y	71	ALA
1	Y	113	ARG
1	Y	199	LEU
1	Y	305	THR

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	Y	359/374 (96%)	338 (94%)	21 (6%)	25 61
2	E	54/110 (49%)	52 (96%)	2 (4%)	41 73
3	G	27/106 (26%)	27 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	337/509 (66%)	328 (97%)	9 (3%)	52 79
5	F	237/267 (89%)	227 (96%)	10 (4%)	36 70
6	C	387/475 (82%)	375 (97%)	12 (3%)	47 77
All	All	1401/1841 (76%)	1347 (96%)	54 (4%)	43 72

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	297	ARG
4	D	474	LYS
6	C	376	GLN
4	D	339	PRO
4	D	418	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.