wwPDB EM Validation Summary Report

Jan 23, 2024 – 08:13 PM JST

PDB ID	:	8H93
EMDB ID	:	EMD-34552
Title	:	Structure of dimeric mouse SCMC core complex
Authors	:	Chi, P.; Ou, G.; Han, Z.; Li, J.; Deng, D.
Deposited on	:	2022-10-24
Resolution	:	3.01 Å(reported)

This is a wwPDB EM Validation Summary 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/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:

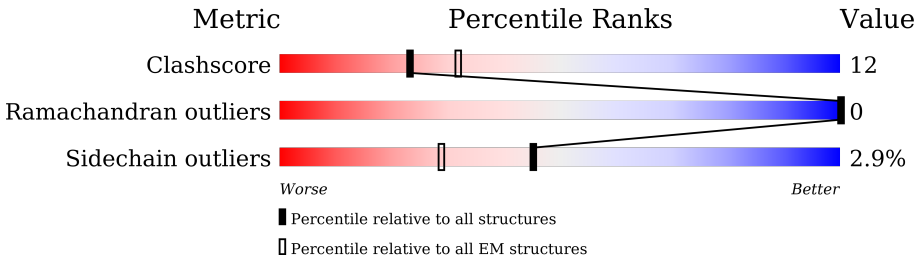
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.01 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1059	65% 24% • 10%
1	D	1059	68% 20% • 10%
2	B	581	38% 24% • 37%
2	E	581	47% 16% • 37%
3	C	164	23% 28% • • 46%
3	F	164	34% 18% • 46%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22191 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 NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7481	4760	1267	1388	66		
1	D	949	Total	C	N	O	S	0	0
			7476	4757	1266	1388	65		

- Molecule 2 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	367	Total	C	N	O	S	0	0
			2898	1837	508	533	20		
2	E	367	Total	C	N	O	S	0	0
			2898	1837	508	533	20		

- Molecule 3 is a protein called Oocyte-expressed protein homolog.

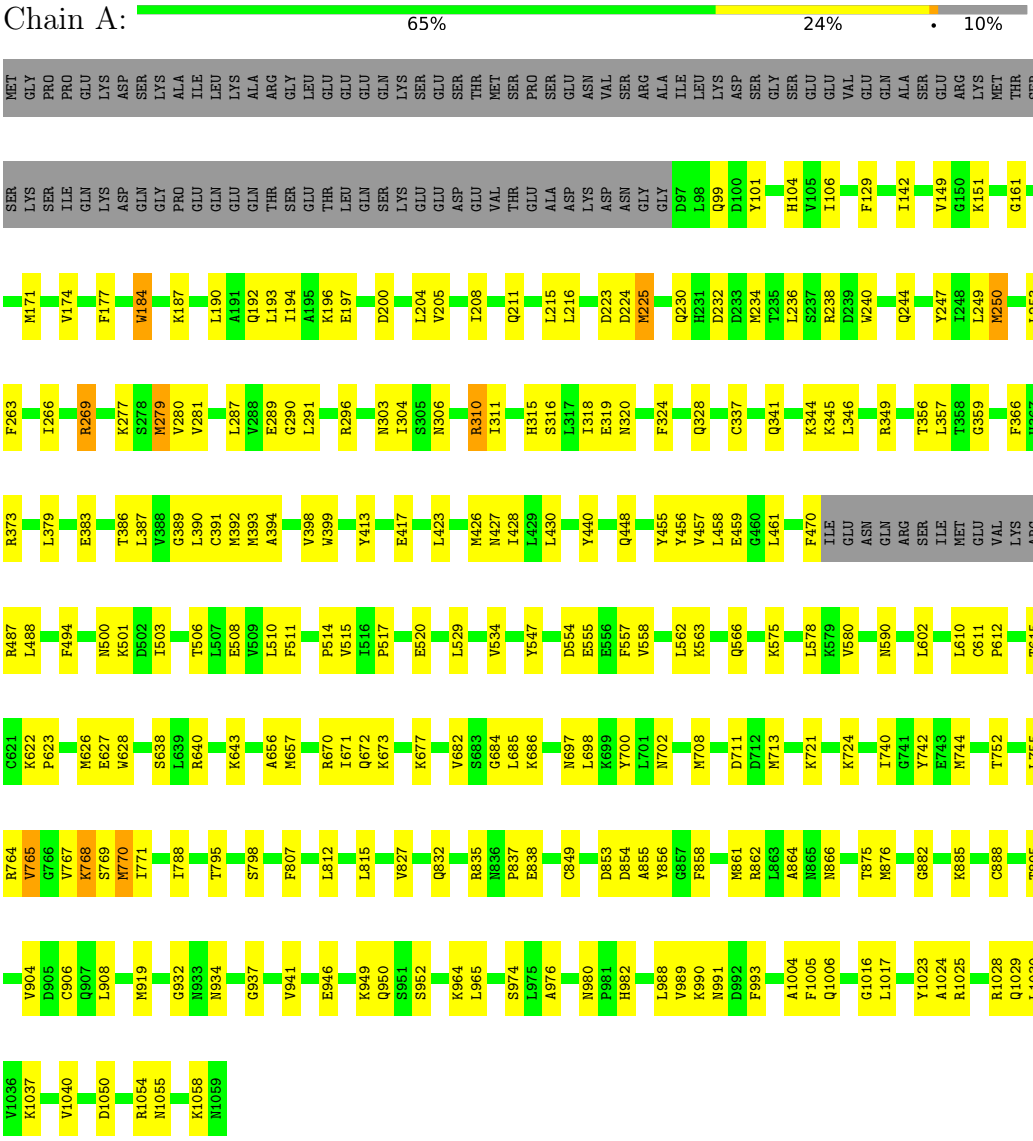
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	89	Total	C	N	O	S	0	0
			719	460	123	131	5		
3	F	89	Total	C	N	O	S	0	0
			719	460	123	131	5		

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.

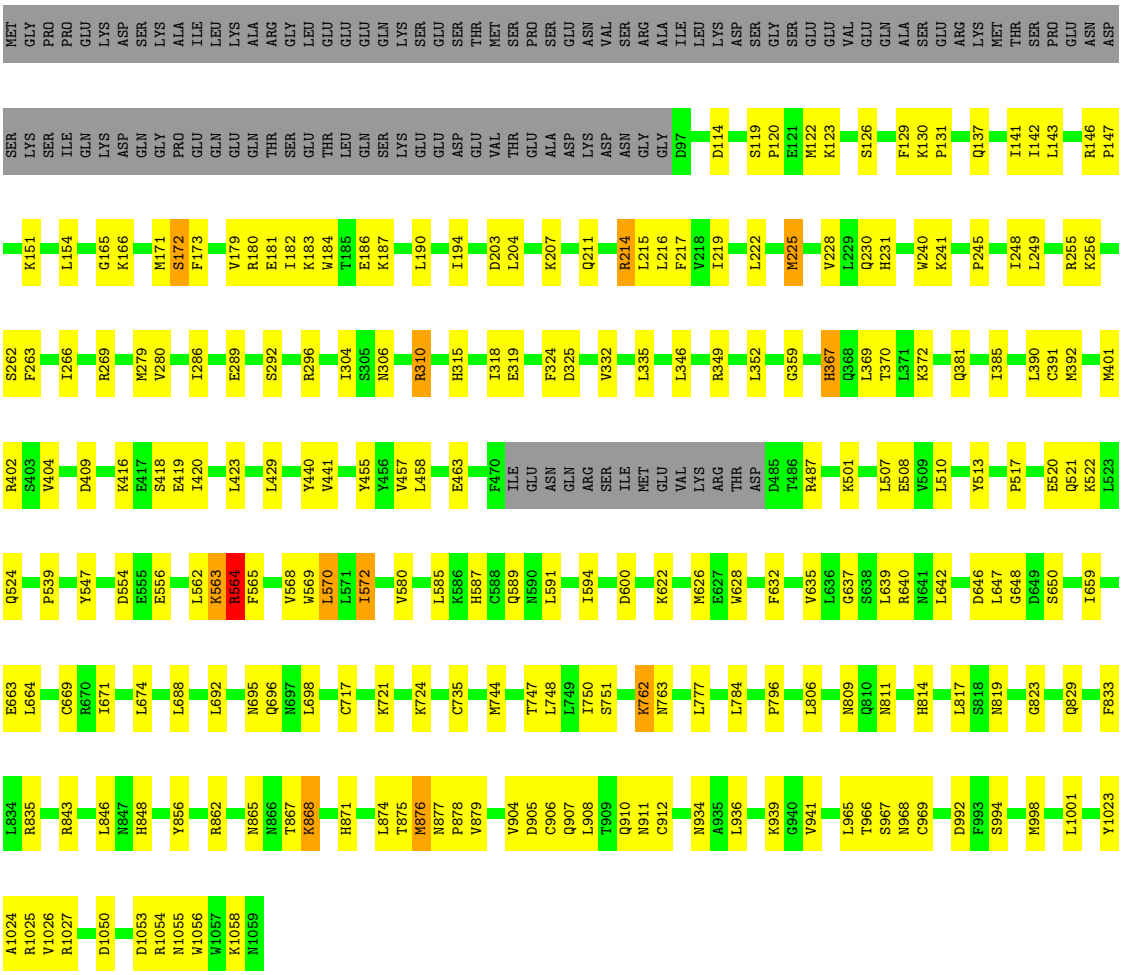
• Molecule 1: NACHT, LRR and PYD domains-containing protein 5

Chain A:



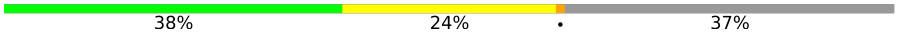
• Molecule 1: NACHT, LRR and PYD domains-containing protein 5

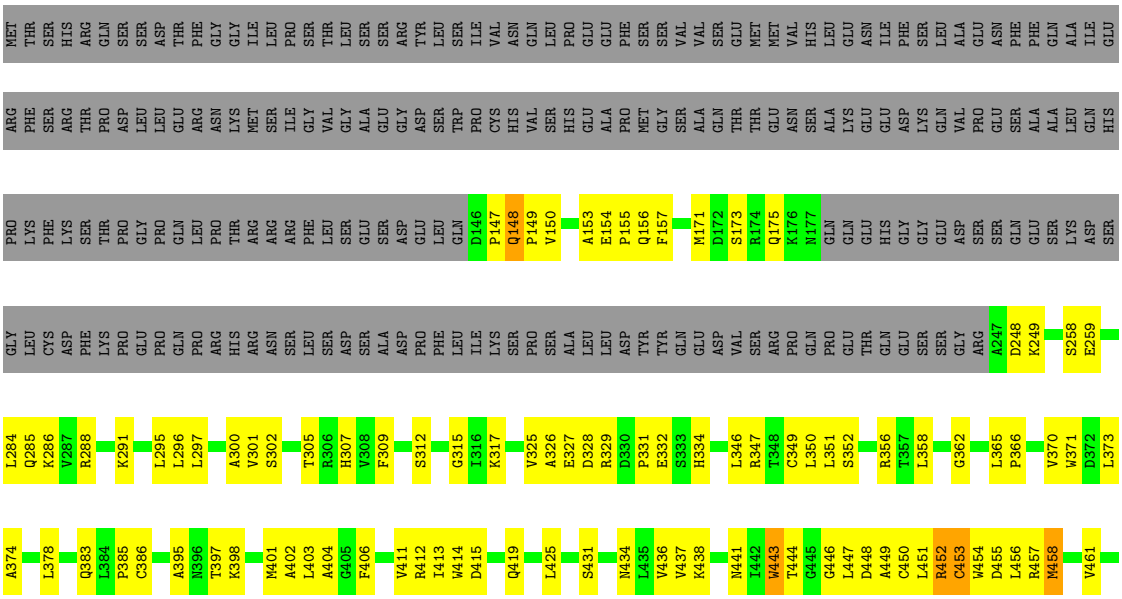
Chain D:

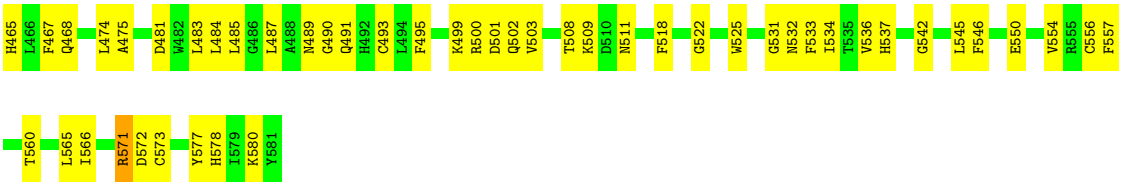


• Molecule 2: Transducin-like enhancer protein 6

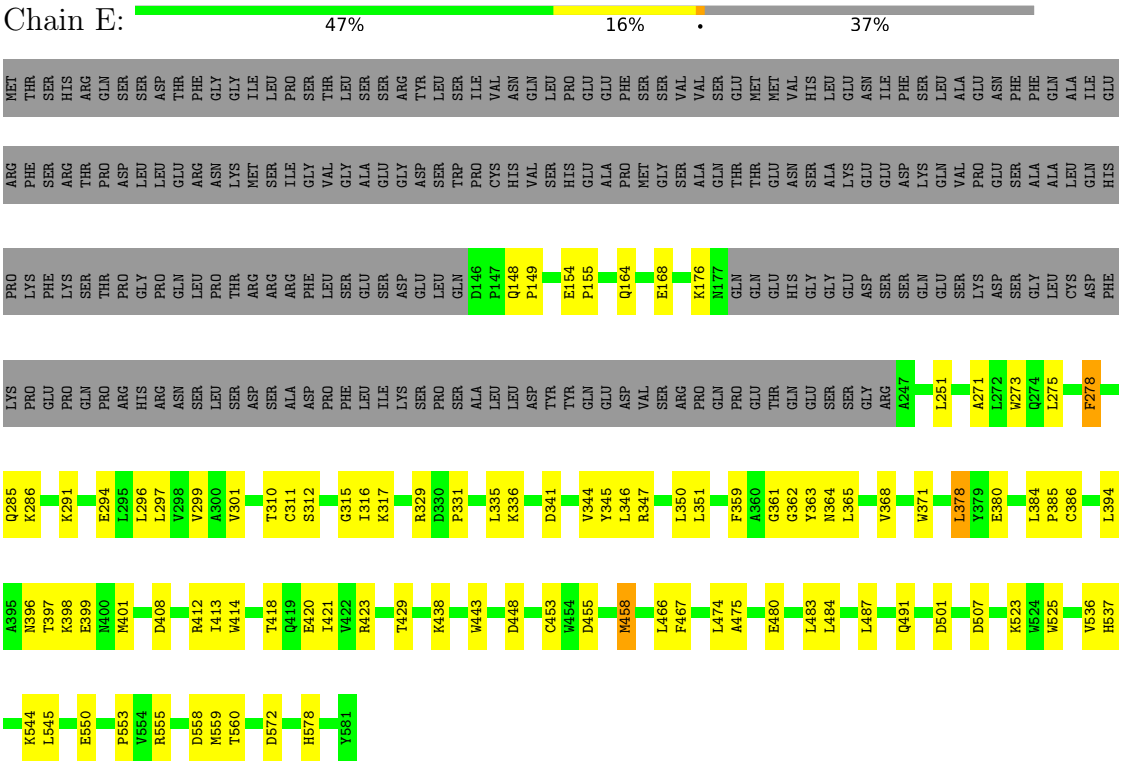
Chain B:



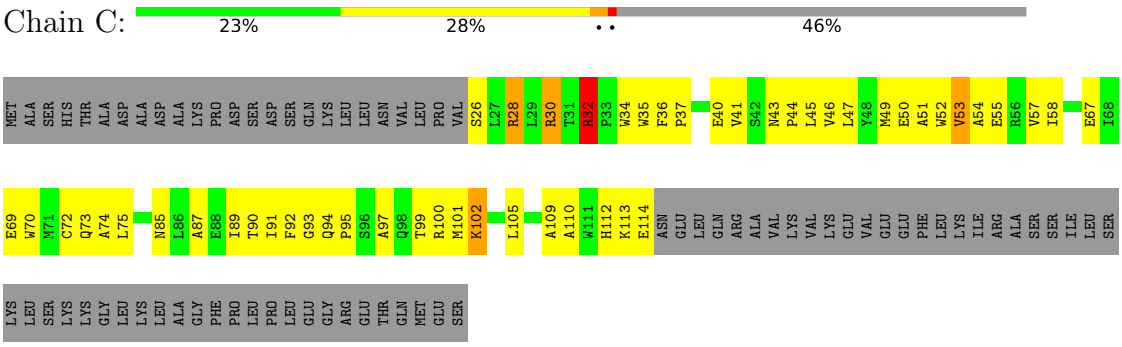




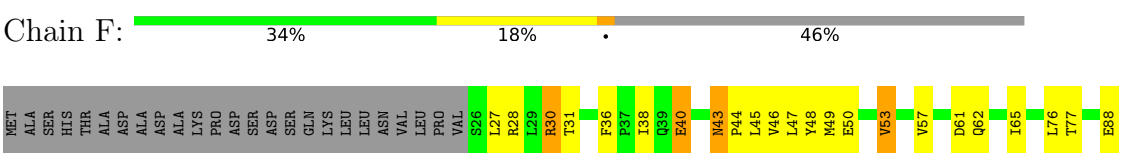
• Molecule 2: Transducin-like enhancer protein 6

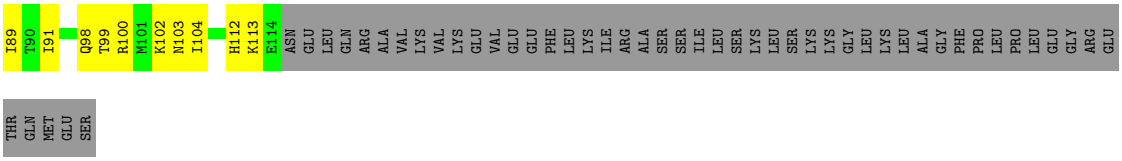


• Molecule 3: Oocyte-expressed protein homolog



• Molecule 3: Oocyte-expressed protein homolog




I89
T90
I91
Q98
T99
R100
M101
K102
N103
I104
H112
K113
E114
ASN GLU LEU GLN ARG ALA VAL LYS VAL LYS GLU VAL GLU GLU PHE LEU LYS ILE ARG ALA SER SER ILE LEU SER LYS LEU SER LYS LYS GLY LEU LYS LEU ALA GLY PHE PRO LEU PRO LEU GLU GLY ARG GLU
THR GLN MET GLU SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197574	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/7613	0.48	0/10294
1	D	0.25	0/7608	0.48	0/10289
2	B	0.28	0/2964	0.53	0/4023
2	E	0.26	0/2964	0.53	0/4023
3	C	0.40	0/736	0.58	0/1003
3	F	0.37	0/736	0.58	0/1003
All	All	0.27	0/22621	0.50	0/30635

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	1
2	B	0	1
3	C	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	452	ARG	Sidechain
3	C	30	ARG	Sidechain
3	C	32	ARG	Sidechain
1	D	564	ARG	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	7481	0	7571	184	0
1	D	7476	0	7557	143	0
2	B	2898	0	2875	116	0
2	E	2898	0	2875	68	0
3	C	719	0	713	40	0
3	F	719	0	713	24	0
All	All	22191	0	22304	547	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 12.

The worst 5 of 547 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)
2:E:386:CYS:HB3	2:E:412:ARG:HH22	1.35	0.91
3:C:47:LEU:HD23	3:C:91:ILE:HD11	1.53	0.89
2:B:434:ASN:HD21	2:B:474:LEU:HB2	1.39	0.86
2:E:344:VAL:HG22	2:E:364:ASN:HB3	1.62	0.80
3:C:47:LEU:HG	3:C:89:ILE:HB	1.64	0.80

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	945/1059 (89%)	912 (96%)	33 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	945/1059 (89%)	913 (97%)	32 (3%)	0	100	100
2	B	363/581 (62%)	347 (96%)	16 (4%)	0	100	100
2	E	363/581 (62%)	340 (94%)	23 (6%)	0	100	100
3	C	87/164 (53%)	86 (99%)	1 (1%)	0	100	100
3	F	87/164 (53%)	86 (99%)	1 (1%)	0	100	100
All	All	2790/3608 (77%)	2684 (96%)	106 (4%)	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 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	849/960 (88%)	831 (98%)	18 (2%)	53	81
1	D	847/960 (88%)	823 (97%)	24 (3%)	43	76
2	B	323/516 (63%)	313 (97%)	10 (3%)	40	74
2	E	323/516 (63%)	317 (98%)	6 (2%)	57	83
3	C	78/143 (54%)	71 (91%)	7 (9%)	9	33
3	F	78/143 (54%)	71 (91%)	7 (9%)	9	33
All	All	2498/3238 (77%)	2426 (97%)	72 (3%)	45	75

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	868	LYS
3	F	53	VAL
2	E	148	GLN
3	F	30	ARG
2	B	458	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	574	GLN
3	F	43	ASN
3	F	112	HIS
1	D	1011	ASN
2	B	441	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 monosaccharides 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

There are no chain breaks in this entry.