



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2024 – 12:09 AM JST

PDB ID : 8JCB
EMDB ID : EMD-36156
Title : Vgamma5 Vdelta1 T cell receptor complex
Authors : Xin, W.; Huang, B.; Chi, X.; Xu, M.; Zhang, Y.; Li, X.; Su, Q.; Zhou, Q.
Deposited on : 2023-05-10
Resolution : 9.50 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) : 2.36.2

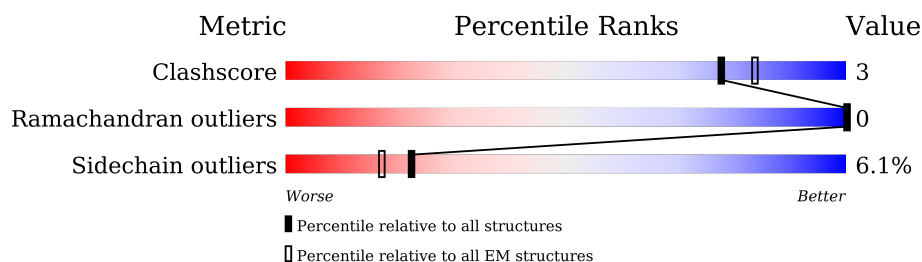
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	195	15% 84%
1	B	195	12% 86%
1	a	195	16% 84%
1	b	195	14% 86%
2	D	171	46% 15% 39%
2	d	171	61% 39%
3	E	207	53% 5% 42%
3	F	207	47% 10% 43%
3	e	207	58% 42%

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Mol	Chain	Length	Quality of chain
3	f	207	 57%43%
4	G	182	 56%7%37%
4	g	182	 63%37%
5	M	307	 59%15%•24%
5	m	307	 66%9%24%
6	N	331	 57%17%•24%
6	n	331	 67%8%•24%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15950 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 T-cell surface glycoprotein CD3 zeta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	31	Total	C	N	O	S	0	0
			251	175	36	39	1		
1	B	28	Total	C	N	O	S	0	0
			226	157	33	35	1		
1	a	31	Total	C	N	O	S	0	0
			251	175	36	39	1		
1	b	28	Total	C	N	O	S	0	0
			226	157	33	35	1		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ALA	-	expression tag	UNP P20963
A	166	ALA	-	expression tag	UNP P20963
A	167	ALA	-	expression tag	UNP P20963
A	168	TRP	-	expression tag	UNP P20963
A	169	SER	-	expression tag	UNP P20963
A	170	HIS	-	expression tag	UNP P20963
A	171	PRO	-	expression tag	UNP P20963
A	172	GLN	-	expression tag	UNP P20963
A	173	PHE	-	expression tag	UNP P20963
A	174	GLU	-	expression tag	UNP P20963
A	175	LYS	-	expression tag	UNP P20963
A	176	GLY	-	expression tag	UNP P20963
A	177	GLY	-	expression tag	UNP P20963
A	178	GLY	-	expression tag	UNP P20963
A	179	SER	-	expression tag	UNP P20963
A	180	GLY	-	expression tag	UNP P20963
A	181	GLY	-	expression tag	UNP P20963
A	182	GLY	-	expression tag	UNP P20963
A	183	SER	-	expression tag	UNP P20963
A	184	GLY	-	expression tag	UNP P20963
A	185	GLY	-	expression tag	UNP P20963
A	186	SER	-	expression tag	UNP P20963

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Chain	Residue	Modelled	Actual	Comment	Reference
A	187	ALA	-	expression tag	UNP P20963
A	188	TRP	-	expression tag	UNP P20963
A	189	SER	-	expression tag	UNP P20963
A	190	HIS	-	expression tag	UNP P20963
A	191	PRO	-	expression tag	UNP P20963
A	192	GLN	-	expression tag	UNP P20963
A	193	PHE	-	expression tag	UNP P20963
A	194	GLU	-	expression tag	UNP P20963
A	195	LYS	-	expression tag	UNP P20963
B	165	ALA	-	expression tag	UNP P20963
B	166	ALA	-	expression tag	UNP P20963
B	167	ALA	-	expression tag	UNP P20963
B	168	TRP	-	expression tag	UNP P20963
B	169	SER	-	expression tag	UNP P20963
B	170	HIS	-	expression tag	UNP P20963
B	171	PRO	-	expression tag	UNP P20963
B	172	GLN	-	expression tag	UNP P20963
B	173	PHE	-	expression tag	UNP P20963
B	174	GLU	-	expression tag	UNP P20963
B	175	LYS	-	expression tag	UNP P20963
B	176	GLY	-	expression tag	UNP P20963
B	177	GLY	-	expression tag	UNP P20963
B	178	GLY	-	expression tag	UNP P20963
B	179	SER	-	expression tag	UNP P20963
B	180	GLY	-	expression tag	UNP P20963
B	181	GLY	-	expression tag	UNP P20963
B	182	GLY	-	expression tag	UNP P20963
B	183	SER	-	expression tag	UNP P20963
B	184	GLY	-	expression tag	UNP P20963
B	185	GLY	-	expression tag	UNP P20963
B	186	SER	-	expression tag	UNP P20963
B	187	ALA	-	expression tag	UNP P20963
B	188	TRP	-	expression tag	UNP P20963
B	189	SER	-	expression tag	UNP P20963
B	190	HIS	-	expression tag	UNP P20963
B	191	PRO	-	expression tag	UNP P20963
B	192	GLN	-	expression tag	UNP P20963
B	193	PHE	-	expression tag	UNP P20963
B	194	GLU	-	expression tag	UNP P20963
B	195	LYS	-	expression tag	UNP P20963
a	165	ALA	-	expression tag	UNP P20963
a	166	ALA	-	expression tag	UNP P20963

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Chain	Residue	Modelled	Actual	Comment	Reference
a	167	ALA	-	expression tag	UNP P20963
a	168	TRP	-	expression tag	UNP P20963
a	169	SER	-	expression tag	UNP P20963
a	170	HIS	-	expression tag	UNP P20963
a	171	PRO	-	expression tag	UNP P20963
a	172	GLN	-	expression tag	UNP P20963
a	173	PHE	-	expression tag	UNP P20963
a	174	GLU	-	expression tag	UNP P20963
a	175	LYS	-	expression tag	UNP P20963
a	176	GLY	-	expression tag	UNP P20963
a	177	GLY	-	expression tag	UNP P20963
a	178	GLY	-	expression tag	UNP P20963
a	179	SER	-	expression tag	UNP P20963
a	180	GLY	-	expression tag	UNP P20963
a	181	GLY	-	expression tag	UNP P20963
a	182	GLY	-	expression tag	UNP P20963
a	183	SER	-	expression tag	UNP P20963
a	184	GLY	-	expression tag	UNP P20963
a	185	GLY	-	expression tag	UNP P20963
a	186	SER	-	expression tag	UNP P20963
a	187	ALA	-	expression tag	UNP P20963
a	188	TRP	-	expression tag	UNP P20963
a	189	SER	-	expression tag	UNP P20963
a	190	HIS	-	expression tag	UNP P20963
a	191	PRO	-	expression tag	UNP P20963
a	192	GLN	-	expression tag	UNP P20963
a	193	PHE	-	expression tag	UNP P20963
a	194	GLU	-	expression tag	UNP P20963
a	195	LYS	-	expression tag	UNP P20963
b	165	ALA	-	expression tag	UNP P20963
b	166	ALA	-	expression tag	UNP P20963
b	167	ALA	-	expression tag	UNP P20963
b	168	TRP	-	expression tag	UNP P20963
b	169	SER	-	expression tag	UNP P20963
b	170	HIS	-	expression tag	UNP P20963
b	171	PRO	-	expression tag	UNP P20963
b	172	GLN	-	expression tag	UNP P20963
b	173	PHE	-	expression tag	UNP P20963
b	174	GLU	-	expression tag	UNP P20963
b	175	LYS	-	expression tag	UNP P20963
b	176	GLY	-	expression tag	UNP P20963
b	177	GLY	-	expression tag	UNP P20963

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Chain	Residue	Modelled	Actual	Comment	Reference
b	178	GLY	-	expression tag	UNP P20963
b	179	SER	-	expression tag	UNP P20963
b	180	GLY	-	expression tag	UNP P20963
b	181	GLY	-	expression tag	UNP P20963
b	182	GLY	-	expression tag	UNP P20963
b	183	SER	-	expression tag	UNP P20963
b	184	GLY	-	expression tag	UNP P20963
b	185	GLY	-	expression tag	UNP P20963
b	186	SER	-	expression tag	UNP P20963
b	187	ALA	-	expression tag	UNP P20963
b	188	TRP	-	expression tag	UNP P20963
b	189	SER	-	expression tag	UNP P20963
b	190	HIS	-	expression tag	UNP P20963
b	191	PRO	-	expression tag	UNP P20963
b	192	GLN	-	expression tag	UNP P20963
b	193	PHE	-	expression tag	UNP P20963
b	194	GLU	-	expression tag	UNP P20963
b	195	LYS	-	expression tag	UNP P20963

- Molecule 2 is a protein called T-cell surface glycoprotein CD3 delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	105	Total	C	N	O	S	0	0
			817	521	135	155	6		
2	d	105	Total	C	N	O	S	0	0
			817	521	135	155	6		

- Molecule 3 is a protein called T-cell surface glycoprotein CD3 epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	121	Total	C	N	O	S	0	0
			959	609	151	191	8		
3	F	118	Total	C	N	O	S	0	0
			933	594	148	183	8		
3	e	121	Total	C	N	O	S	0	0
			959	609	151	191	8		
3	f	118	Total	C	N	O	S	0	0
			933	594	148	183	8		

- Molecule 4 is a protein called T-cell surface glycoprotein CD3 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	115	Total	C	N	O	S	0	0
			907	582	150	168	7		
4	g	115	Total	C	N	O	S	0	0
			907	582	150	168	7		

- Molecule 5 is a protein called T cell receptor delta variable 1,T cell receptor delta constant.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	233	Total	C	N	O	S	0	0
			1844	1187	308	339	10		
5	m	233	Total	C	N	O	S	0	0
			1844	1187	308	339	10		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-16	MET	-	initiating methionine	UNP A0A1B0GX56
M	-15	ASP	-	expression tag	UNP A0A1B0GX56
M	-14	MET	-	expression tag	UNP A0A1B0GX56
M	-13	ARG	-	expression tag	UNP A0A1B0GX56
M	-12	VAL	-	expression tag	UNP A0A1B0GX56
M	-11	PRO	-	expression tag	UNP A0A1B0GX56
M	-10	ALA	-	expression tag	UNP A0A1B0GX56
M	-9	GLN	-	expression tag	UNP A0A1B0GX56
M	-8	LEU	-	expression tag	UNP A0A1B0GX56
M	-7	LEU	-	expression tag	UNP A0A1B0GX56
M	-6	GLY	-	expression tag	UNP A0A1B0GX56
M	-5	LEU	-	expression tag	UNP A0A1B0GX56
M	-4	LEU	-	expression tag	UNP A0A1B0GX56
M	-3	LEU	-	expression tag	UNP A0A1B0GX56
M	-2	LEU	-	expression tag	UNP A0A1B0GX56
M	-1	TRP	-	expression tag	UNP A0A1B0GX56
M	0	LEU	-	expression tag	UNP A0A1B0GX56
M	1	SER	-	expression tag	UNP A0A1B0GX56
M	2	GLY	-	expression tag	UNP A0A1B0GX56
M	3	ALA	-	expression tag	UNP A0A1B0GX56
M	4	ARG	-	expression tag	UNP A0A1B0GX56
M	5	CYS	-	expression tag	UNP A0A1B0GX56
M	6	MET	-	expression tag	UNP A0A1B0GX56
M	7	ASP	-	expression tag	UNP A0A1B0GX56
M	8	TYR	-	expression tag	UNP A0A1B0GX56
M	9	LYS	-	expression tag	UNP A0A1B0GX56
M	10	ASP	-	expression tag	UNP A0A1B0GX56

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Chain	Residue	Modelled	Actual	Comment	Reference
M	11	ASP	-	expression tag	UNP A0A1B0GX56
M	12	ASP	-	expression tag	UNP A0A1B0GX56
M	13	ASP	-	expression tag	UNP A0A1B0GX56
M	14	LYS	-	expression tag	UNP A0A1B0GX56
M	15	GLY	-	expression tag	UNP A0A1B0GX56
M	16	GLY	-	expression tag	UNP A0A1B0GX56
M	17	SER	-	expression tag	UNP A0A1B0GX56
M	18	GLU	-	expression tag	UNP A0A1B0GX56
M	19	THR	-	expression tag	UNP A0A1B0GX56
M	20	GLY	-	expression tag	UNP A0A1B0GX56
M	115	ASP	-	linker	UNP A0A1B0GX56
M	116	PRO	-	linker	UNP A0A1B0GX56
M	117	GLY	-	linker	UNP A0A1B0GX56
M	118	GLY	-	linker	UNP A0A1B0GX56
M	119	LEU	-	linker	UNP A0A1B0GX56
M	120	ASN	-	linker	UNP A0A1B0GX56
M	121	THR	-	linker	UNP A0A1B0GX56
M	122	ASP	-	linker	UNP A0A1B0GX56
M	123	LYS	-	linker	UNP A0A1B0GX56
M	124	LEU	-	linker	UNP A0A1B0GX56
M	125	ILE	-	linker	UNP A0A1B0GX56
M	126	PHE	-	linker	UNP A0A1B0GX56
M	127	GLY	-	linker	UNP A0A1B0GX56
M	128	LYS	-	linker	UNP A0A1B0GX56
M	129	GLY	-	linker	UNP A0A1B0GX56
M	130	THR	-	linker	UNP A0A1B0GX56
M	131	ARG	-	linker	UNP A0A1B0GX56
M	132	VAL	-	linker	UNP A0A1B0GX56
M	133	THR	-	linker	UNP A0A1B0GX56
M	134	VAL	-	linker	UNP A0A1B0GX56
M	135	GLU	-	linker	UNP A0A1B0GX56
M	136	PRO	-	linker	UNP A0A1B0GX56
M	137	ARG	-	linker	UNP A0A1B0GX56
m	-16	MET	-	initiating methionine	UNP A0A1B0GX56
m	-15	ASP	-	expression tag	UNP A0A1B0GX56
m	-14	MET	-	expression tag	UNP A0A1B0GX56
m	-13	ARG	-	expression tag	UNP A0A1B0GX56
m	-12	VAL	-	expression tag	UNP A0A1B0GX56
m	-11	PRO	-	expression tag	UNP A0A1B0GX56
m	-10	ALA	-	expression tag	UNP A0A1B0GX56
m	-9	GLN	-	expression tag	UNP A0A1B0GX56
m	-8	LEU	-	expression tag	UNP A0A1B0GX56

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Chain	Residue	Modelled	Actual	Comment	Reference
m	-7	LEU	-	expression tag	UNP A0A1B0GX56
m	-6	GLY	-	expression tag	UNP A0A1B0GX56
m	-5	LEU	-	expression tag	UNP A0A1B0GX56
m	-4	LEU	-	expression tag	UNP A0A1B0GX56
m	-3	LEU	-	expression tag	UNP A0A1B0GX56
m	-2	LEU	-	expression tag	UNP A0A1B0GX56
m	-1	TRP	-	expression tag	UNP A0A1B0GX56
m	0	LEU	-	expression tag	UNP A0A1B0GX56
m	1	SER	-	expression tag	UNP A0A1B0GX56
m	2	GLY	-	expression tag	UNP A0A1B0GX56
m	3	ALA	-	expression tag	UNP A0A1B0GX56
m	4	ARG	-	expression tag	UNP A0A1B0GX56
m	5	CYS	-	expression tag	UNP A0A1B0GX56
m	6	MET	-	expression tag	UNP A0A1B0GX56
m	7	ASP	-	expression tag	UNP A0A1B0GX56
m	8	TYR	-	expression tag	UNP A0A1B0GX56
m	9	LYS	-	expression tag	UNP A0A1B0GX56
m	10	ASP	-	expression tag	UNP A0A1B0GX56
m	11	ASP	-	expression tag	UNP A0A1B0GX56
m	12	ASP	-	expression tag	UNP A0A1B0GX56
m	13	ASP	-	expression tag	UNP A0A1B0GX56
m	14	LYS	-	expression tag	UNP A0A1B0GX56
m	15	GLY	-	expression tag	UNP A0A1B0GX56
m	16	GLY	-	expression tag	UNP A0A1B0GX56
m	17	SER	-	expression tag	UNP A0A1B0GX56
m	18	GLU	-	expression tag	UNP A0A1B0GX56
m	19	THR	-	expression tag	UNP A0A1B0GX56
m	20	GLY	-	expression tag	UNP A0A1B0GX56
m	115	ASP	-	linker	UNP A0A1B0GX56
m	116	PRO	-	linker	UNP A0A1B0GX56
m	117	GLY	-	linker	UNP A0A1B0GX56
m	118	GLY	-	linker	UNP A0A1B0GX56
m	119	LEU	-	linker	UNP A0A1B0GX56
m	120	ASN	-	linker	UNP A0A1B0GX56
m	121	THR	-	linker	UNP A0A1B0GX56
m	122	ASP	-	linker	UNP A0A1B0GX56
m	123	LYS	-	linker	UNP A0A1B0GX56
m	124	LEU	-	linker	UNP A0A1B0GX56
m	125	ILE	-	linker	UNP A0A1B0GX56
m	126	PHE	-	linker	UNP A0A1B0GX56
m	127	GLY	-	linker	UNP A0A1B0GX56
m	128	LYS	-	linker	UNP A0A1B0GX56

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Chain	Residue	Modelled	Actual	Comment	Reference
m	129	GLY	-	linker	UNP A0A1B0GX56
m	130	THR	-	linker	UNP A0A1B0GX56
m	131	ARG	-	linker	UNP A0A1B0GX56
m	132	VAL	-	linker	UNP A0A1B0GX56
m	133	THR	-	linker	UNP A0A1B0GX56
m	134	VAL	-	linker	UNP A0A1B0GX56
m	135	GLU	-	linker	UNP A0A1B0GX56
m	136	PRO	-	linker	UNP A0A1B0GX56
m	137	ARG	-	linker	UNP A0A1B0GX56

- Molecule 6 is a protein called T cell receptor gamma variable 5,T cell receptor gamma constant 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	250	Total	C	N	O	S	0	0
			2038	1318	337	374	9		
6	n	250	Total	C	N	O	S	0	0
			2038	1318	337	374	9		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-33	MET	-	initiating methionine	UNP A0A0B4J1U4
N	-32	ASP	-	expression tag	UNP A0A0B4J1U4
N	-31	MET	-	expression tag	UNP A0A0B4J1U4
N	-30	ARG	-	expression tag	UNP A0A0B4J1U4
N	-29	VAL	-	expression tag	UNP A0A0B4J1U4
N	-28	PRO	-	expression tag	UNP A0A0B4J1U4
N	-27	ALA	-	expression tag	UNP A0A0B4J1U4
N	-26	GLN	-	expression tag	UNP A0A0B4J1U4
N	-25	LEU	-	expression tag	UNP A0A0B4J1U4
N	-24	LEU	-	expression tag	UNP A0A0B4J1U4
N	-23	GLY	-	expression tag	UNP A0A0B4J1U4
N	-22	LEU	-	expression tag	UNP A0A0B4J1U4
N	-21	LEU	-	expression tag	UNP A0A0B4J1U4
N	-20	LEU	-	expression tag	UNP A0A0B4J1U4
N	-19	LEU	-	expression tag	UNP A0A0B4J1U4
N	-18	TRP	-	expression tag	UNP A0A0B4J1U4
N	-17	LEU	-	expression tag	UNP A0A0B4J1U4
N	-16	SER	-	expression tag	UNP A0A0B4J1U4
N	-15	GLY	-	expression tag	UNP A0A0B4J1U4
N	-14	ALA	-	expression tag	UNP A0A0B4J1U4

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-13	ARG	-	expression tag	UNP A0A0B4J1U4
N	-12	CYS	-	expression tag	UNP A0A0B4J1U4
N	-11	MET	-	expression tag	UNP A0A0B4J1U4
N	-10	ASP	-	expression tag	UNP A0A0B4J1U4
N	-9	TYR	-	expression tag	UNP A0A0B4J1U4
N	-8	LYS	-	expression tag	UNP A0A0B4J1U4
N	-7	ASP	-	expression tag	UNP A0A0B4J1U4
N	-6	ASP	-	expression tag	UNP A0A0B4J1U4
N	-5	ASP	-	expression tag	UNP A0A0B4J1U4
N	-4	ASP	-	expression tag	UNP A0A0B4J1U4
N	-3	LYS	-	expression tag	UNP A0A0B4J1U4
N	-2	GLY	-	expression tag	UNP A0A0B4J1U4
N	-1	GLY	-	expression tag	UNP A0A0B4J1U4
N	0	SER	-	expression tag	UNP A0A0B4J1U4
N	1	GLU	-	expression tag	UNP A0A0B4J1U4
N	2	THR	-	expression tag	UNP A0A0B4J1U4
N	3	GLY	-	expression tag	UNP A0A0B4J1U4
N	104	GLY	-	linker	UNP A0A0B4J1U4
N	105	ASN	-	linker	UNP A0A0B4J1U4
N	106	PRO	-	linker	UNP A0A0B4J1U4
N	107	LYS	-	linker	UNP A0A0B4J1U4
N	108	THR	-	linker	UNP A0A0B4J1U4
N	109	HIS	-	linker	UNP A0A0B4J1U4
N	110	TYR	-	linker	UNP A0A0B4J1U4
N	111	TYR	-	linker	UNP A0A0B4J1U4
N	112	LYS	-	linker	UNP A0A0B4J1U4
N	113	LYS	-	linker	UNP A0A0B4J1U4
N	114	LEU	-	linker	UNP A0A0B4J1U4
N	115	PHE	-	linker	UNP A0A0B4J1U4
N	116	GLY	-	linker	UNP A0A0B4J1U4
N	117	SER	-	linker	UNP A0A0B4J1U4
N	118	GLY	-	linker	UNP A0A0B4J1U4
N	119	THR	-	linker	UNP A0A0B4J1U4
N	120	THR	-	linker	UNP A0A0B4J1U4
N	121	LEU	-	linker	UNP A0A0B4J1U4
N	122	VAL	-	linker	UNP A0A0B4J1U4
N	123	VAL	-	linker	UNP A0A0B4J1U4
N	124	THR	-	linker	UNP A0A0B4J1U4
n	-33	MET	-	initiating methionine	UNP A0A0B4J1U4
n	-32	ASP	-	expression tag	UNP A0A0B4J1U4
n	-31	MET	-	expression tag	UNP A0A0B4J1U4
n	-30	ARG	-	expression tag	UNP A0A0B4J1U4

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Chain	Residue	Modelled	Actual	Comment	Reference
n	-29	VAL	-	expression tag	UNP A0A0B4J1U4
n	-28	PRO	-	expression tag	UNP A0A0B4J1U4
n	-27	ALA	-	expression tag	UNP A0A0B4J1U4
n	-26	GLN	-	expression tag	UNP A0A0B4J1U4
n	-25	LEU	-	expression tag	UNP A0A0B4J1U4
n	-24	LEU	-	expression tag	UNP A0A0B4J1U4
n	-23	GLY	-	expression tag	UNP A0A0B4J1U4
n	-22	LEU	-	expression tag	UNP A0A0B4J1U4
n	-21	LEU	-	expression tag	UNP A0A0B4J1U4
n	-20	LEU	-	expression tag	UNP A0A0B4J1U4
n	-19	LEU	-	expression tag	UNP A0A0B4J1U4
n	-18	TRP	-	expression tag	UNP A0A0B4J1U4
n	-17	LEU	-	expression tag	UNP A0A0B4J1U4
n	-16	SER	-	expression tag	UNP A0A0B4J1U4
n	-15	GLY	-	expression tag	UNP A0A0B4J1U4
n	-14	ALA	-	expression tag	UNP A0A0B4J1U4
n	-13	ARG	-	expression tag	UNP A0A0B4J1U4
n	-12	CYS	-	expression tag	UNP A0A0B4J1U4
n	-11	MET	-	expression tag	UNP A0A0B4J1U4
n	-10	ASP	-	expression tag	UNP A0A0B4J1U4
n	-9	TYR	-	expression tag	UNP A0A0B4J1U4
n	-8	LYS	-	expression tag	UNP A0A0B4J1U4
n	-7	ASP	-	expression tag	UNP A0A0B4J1U4
n	-6	ASP	-	expression tag	UNP A0A0B4J1U4
n	-5	ASP	-	expression tag	UNP A0A0B4J1U4
n	-4	ASP	-	expression tag	UNP A0A0B4J1U4
n	-3	LYS	-	expression tag	UNP A0A0B4J1U4
n	-2	GLY	-	expression tag	UNP A0A0B4J1U4
n	-1	GLY	-	expression tag	UNP A0A0B4J1U4
n	0	SER	-	expression tag	UNP A0A0B4J1U4
n	1	GLU	-	expression tag	UNP A0A0B4J1U4
n	2	THR	-	expression tag	UNP A0A0B4J1U4
n	3	GLY	-	expression tag	UNP A0A0B4J1U4
n	104	GLY	-	linker	UNP A0A0B4J1U4
n	105	ASN	-	linker	UNP A0A0B4J1U4
n	106	PRO	-	linker	UNP A0A0B4J1U4
n	107	LYS	-	linker	UNP A0A0B4J1U4
n	108	THR	-	linker	UNP A0A0B4J1U4
n	109	HIS	-	linker	UNP A0A0B4J1U4
n	110	TYR	-	linker	UNP A0A0B4J1U4
n	111	TYR	-	linker	UNP A0A0B4J1U4
n	112	LYS	-	linker	UNP A0A0B4J1U4

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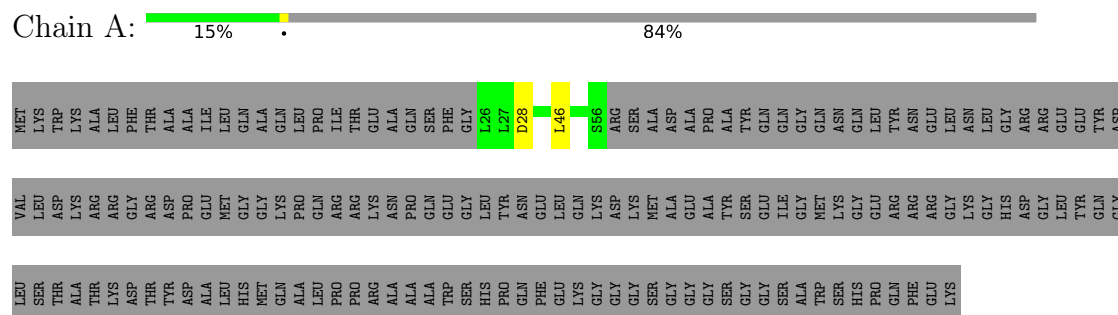
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Chain	Residue	Modelled	Actual	Comment	Reference
n	113	LYS	-	linker	UNP A0A0B4J1U4
n	114	LEU	-	linker	UNP A0A0B4J1U4
n	115	PHE	-	linker	UNP A0A0B4J1U4
n	116	GLY	-	linker	UNP A0A0B4J1U4
n	117	SER	-	linker	UNP A0A0B4J1U4
n	118	GLY	-	linker	UNP A0A0B4J1U4
n	119	THR	-	linker	UNP A0A0B4J1U4
n	120	THR	-	linker	UNP A0A0B4J1U4
n	121	LEU	-	linker	UNP A0A0B4J1U4
n	122	VAL	-	linker	UNP A0A0B4J1U4
n	123	VAL	-	linker	UNP A0A0B4J1U4
n	124	THR	-	linker	UNP A0A0B4J1U4

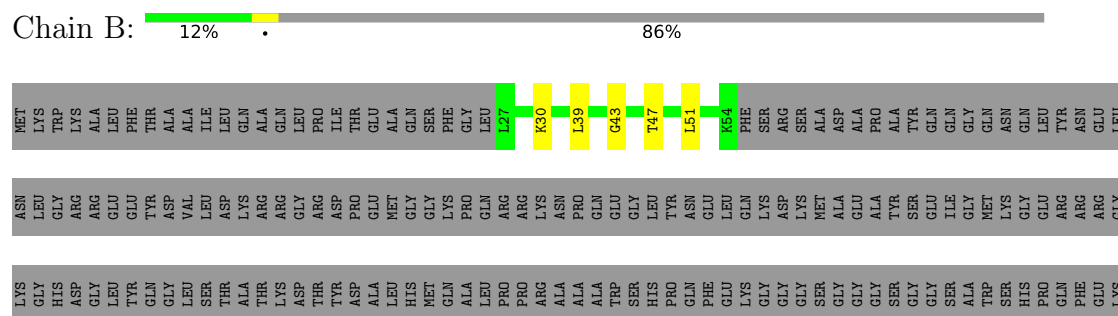
3 Residue-property plots

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.

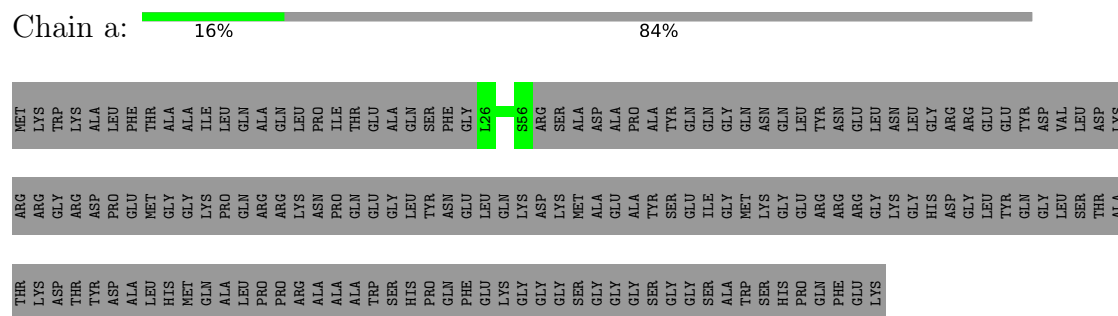
- Molecule 1: T-cell surface glycoprotein CD3 zeta chain



- Molecule 1: T-cell surface glycoprotein CD3 zeta chain

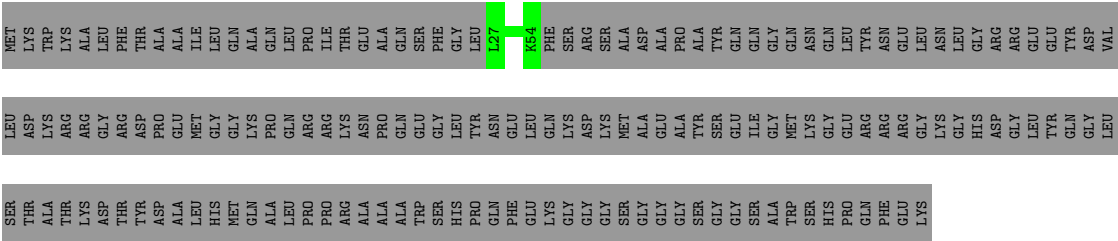


- Molecule 1: T-cell surface glycoprotein CD3 zeta chain

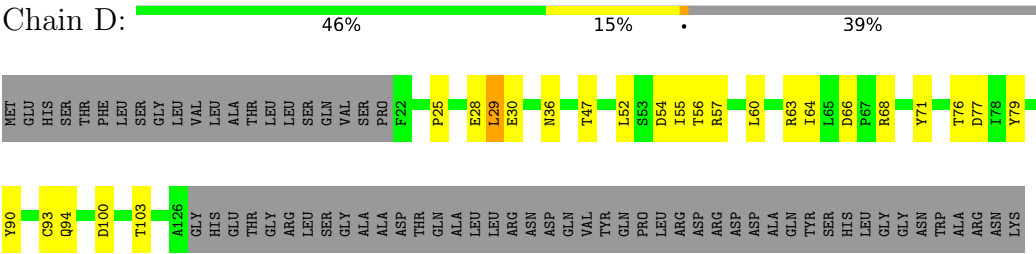


- Molecule 1: T-cell surface glycoprotein CD3 zeta chain

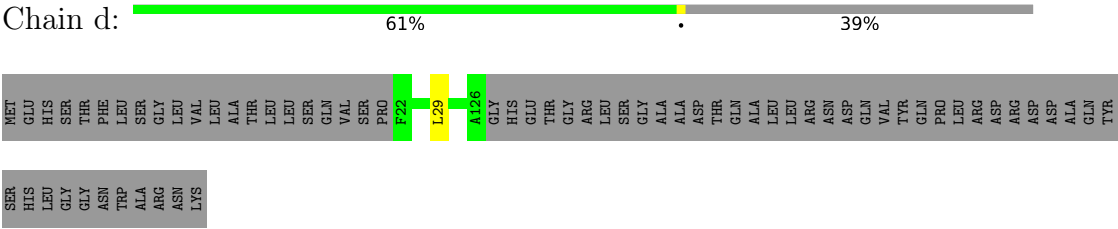




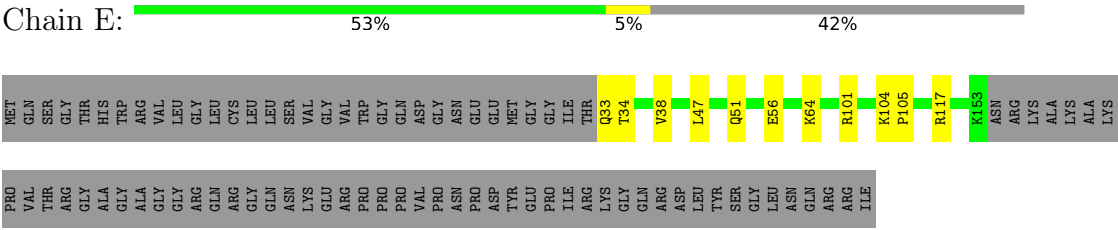
• Molecule 2: T-cell surface glycoprotein CD3 delta chain



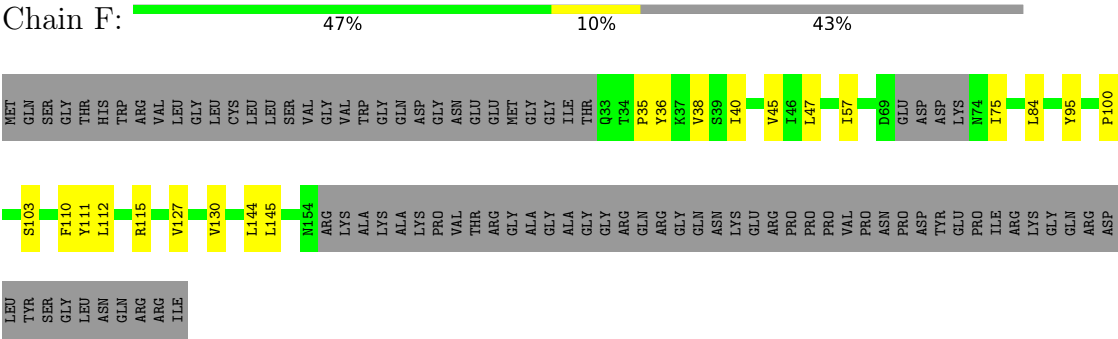
• Molecule 2: T-cell surface glycoprotein CD3 delta chain

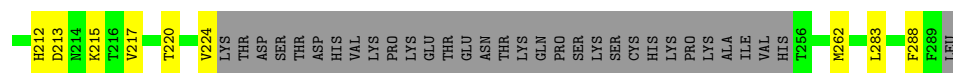


• Molecule 3: T-cell surface glycoprotein CD3 epsilon chain



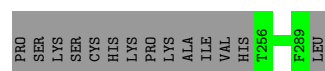
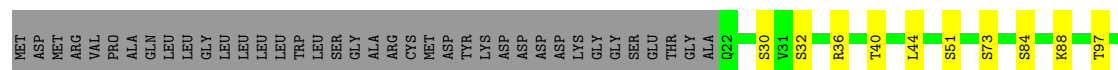
• Molecule 3: T-cell surface glycoprotein CD3 epsilon chain





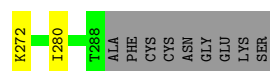
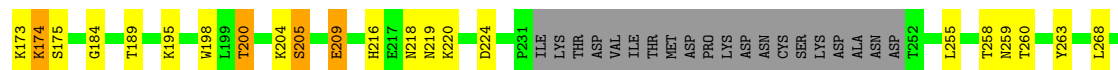
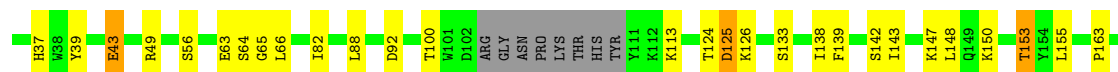
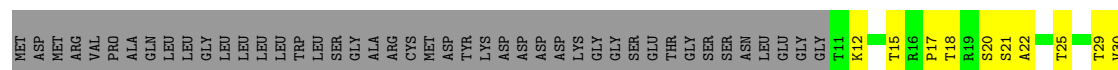
- Molecule 5: T cell receptor delta variable 1,T cell receptor delta constant

Chain m: 66% 9% 24%



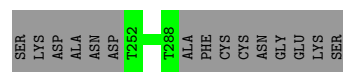
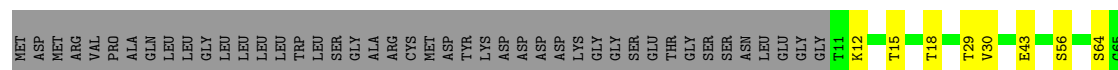
- Molecule 6: T cell receptor gamma variable 5,T cell receptor gamma constant 1

Chain N: 57% 17% 24%



- Molecule 6: T cell receptor gamma variable 5,T cell receptor gamma constant 1

Chain n: 67% 8% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/256	0.65	0/346
1	B	0.36	0/230	0.70	0/311
1	a	0.38	0/256	0.65	0/346
1	b	0.36	0/230	0.70	0/311
2	D	0.36	0/829	0.66	1/1127 (0.1%)
2	d	0.35	0/829	0.66	1/1127 (0.1%)
3	E	0.37	0/980	0.63	0/1331
3	F	0.34	0/953	0.60	0/1294
3	e	0.37	0/980	0.63	0/1331
3	f	0.34	0/953	0.60	0/1294
4	G	0.36	0/925	0.58	0/1244
4	g	0.36	0/925	0.58	0/1244
5	M	0.41	0/1880	0.62	2/2537 (0.1%)
5	m	0.41	0/1880	0.62	2/2537 (0.1%)
6	N	0.42	0/2087	0.61	2/2834 (0.1%)
6	n	0.43	0/2087	0.63	3/2834 (0.1%)
All	All	0.39	0/16280	0.62	11/22048 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	m	104	GLU	CA-CB-CG	7.27	129.40	113.40
5	M	104	GLU	CA-CB-CG	7.25	129.35	113.40
5	M	134	VAL	C-N-CA	6.09	136.94	121.70
5	m	134	VAL	C-N-CA	6.08	136.91	121.70
6	n	219	ASN	CB-CA-C	-5.98	98.45	110.40

There are no chirality outliers.

There are no planarity outliers.

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	251	0	275	2	0
1	B	226	0	250	4	0
1	a	251	0	275	0	0
1	b	226	0	250	0	0
2	D	817	0	828	19	0
2	d	817	0	828	0	0
3	E	959	0	919	8	0
3	F	933	0	897	12	0
3	e	959	0	919	0	0
3	f	933	0	897	0	0
4	G	907	0	897	8	0
4	g	907	0	897	0	0
5	M	1844	0	1884	19	0
5	m	1844	0	1884	0	0
6	N	2038	0	2052	28	0
6	n	2038	0	2052	0	0
All	All	15950	0	16004	92	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 3.

The worst 5 of 92 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)
5:M:151:ASN:ND2	6:N:138:ILE:O	2.37	0.64
2:D:66:ASP:HB3	2:D:68:ARG:HH21	1.63	0.64
5:M:82:ARG:NH2	5:M:105:ASP:OD2	2.33	0.62
2:D:85:THR:HG21	3:E:33:GLN:HE22	1.65	0.62
6:N:139:PHE:HB2	6:N:155:LEU:HB3	1.81	0.62

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	29/195 (15%)	29 (100%)	0	0	100	100
1	B	26/195 (13%)	23 (88%)	3 (12%)	0	100	100
1	a	29/195 (15%)	29 (100%)	0	0	100	100
1	b	26/195 (13%)	23 (88%)	3 (12%)	0	100	100
2	D	103/171 (60%)	92 (89%)	11 (11%)	0	100	100
2	d	103/171 (60%)	92 (89%)	11 (11%)	0	100	100
3	E	119/207 (58%)	109 (92%)	10 (8%)	0	100	100
3	F	114/207 (55%)	101 (89%)	13 (11%)	0	100	100
3	e	119/207 (58%)	109 (92%)	10 (8%)	0	100	100
3	f	114/207 (55%)	101 (89%)	13 (11%)	0	100	100
4	G	113/182 (62%)	100 (88%)	13 (12%)	0	100	100
4	g	113/182 (62%)	100 (88%)	13 (12%)	0	100	100
5	M	227/307 (74%)	208 (92%)	19 (8%)	0	100	100
5	m	227/307 (74%)	208 (92%)	19 (8%)	0	100	100
6	N	244/331 (74%)	213 (87%)	31 (13%)	0	100	100
6	n	244/331 (74%)	212 (87%)	32 (13%)	0	100	100
All	All	1950/3590 (54%)	1749 (90%)	201 (10%)	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	28/154 (18%)	28 (100%)	0	100	100
1	B	25/154 (16%)	25 (100%)	0	100	100
1	a	28/154 (18%)	28 (100%)	0	100	100
1	b	25/154 (16%)	25 (100%)	0	100	100
2	D	93/147 (63%)	93 (100%)	0	100	100
2	d	93/147 (63%)	93 (100%)	0	100	100
3	E	109/177 (62%)	109 (100%)	0	100	100
3	F	106/177 (60%)	106 (100%)	0	100	100
3	e	109/177 (62%)	109 (100%)	0	100	100
3	f	106/177 (60%)	106 (100%)	0	100	100
4	G	97/155 (63%)	97 (100%)	0	100	100
4	g	97/155 (63%)	97 (100%)	0	100	100
5	M	209/272 (77%)	181 (87%)	28 (13%)	4	17
5	m	209/272 (77%)	181 (87%)	28 (13%)	4	17
6	N	231/299 (77%)	204 (88%)	27 (12%)	5	21
6	n	231/299 (77%)	204 (88%)	27 (12%)	5	21
All	All	1796/3070 (58%)	1686 (94%)	110 (6%)	22	44

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	m	36	ARG
5	m	145	SER
6	n	209	GLU
6	n	148	LEU
5	m	44	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	f	121	ASN
5	m	77	ASN
5	m	22	GLN
5	m	102	GLN
5	M	102	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 monosaccharides 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](#)

There are no chain breaks in this entry.