



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:02 PM BST

PDB ID : 3JBL
EMDB ID: : EMD-6458
Title : Cryo-EM Structure of the Activated NAIP2/NLRC4 Inflammasome Reveals Nucleated Polymerization
Authors : Zhang, L.; Chen, S.; Ruan, J.; Wu, J.; Tong, A.B.; Yin, Q.; Li, Y.; David, L.; Lu, A.; Wang, W.L.; Marks, C.; Ouyang, Q.; Zhang, X.; Mao, Y.; Wu, H.
Deposited on : 2015-09-05
Resolution : 4.50 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 : 1.7.1 (RC1), CSD as537be (2016)
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

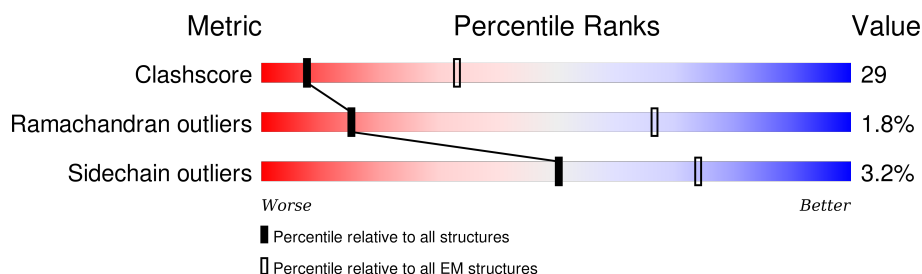
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	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	932	43% 51% . .
1	B	932	43% 51% . .
1	C	932	44% 50% . .
1	D	932	44% 50% . .
1	E	932	44% 50% . .
1	F	932	44% 50% . .
1	G	932	44% 50% . .
1	H	932	43% 50% . .
1	I	932	43% 51% . .

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Mol	Chain	Length	Quality of chain
1	J	932	<div><div></div><div>43%</div><div>51%</div><div></div><div>.</div><div>.</div></div>
1	K	932	<div><div></div><div>43%</div><div>51%</div><div></div><div>.</div><div>.</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 80124 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.

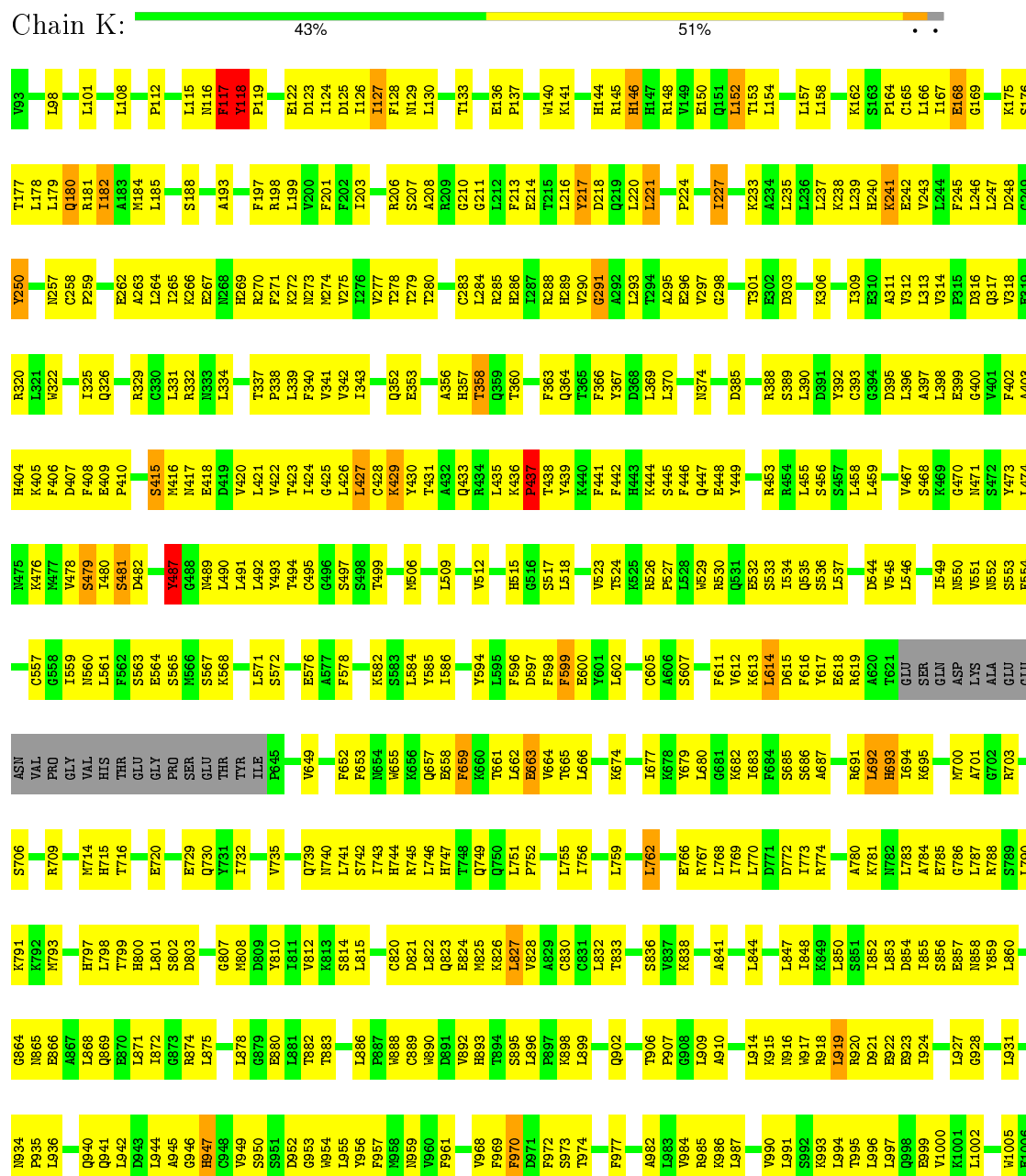
- Molecule 1 is a protein called NLR family CARD domain-containing protein 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	K	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	A	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	B	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	C	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	D	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	E	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	F	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	G	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	H	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	I	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		
1	J	909	Total	C	N	O	P	S	0	0
			7284	4647	1233	1363	1	40		

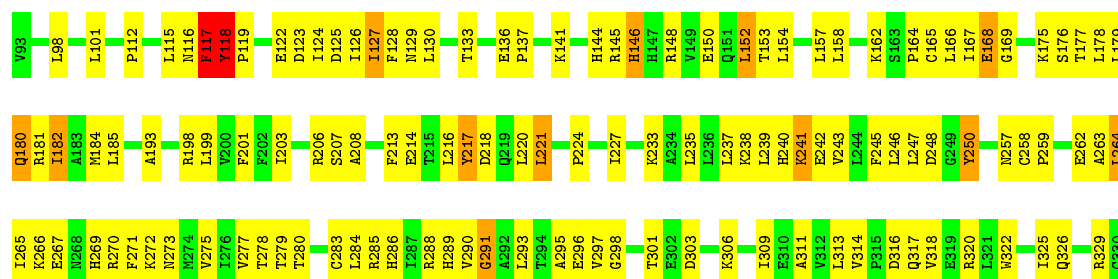
3 Residue-property plots

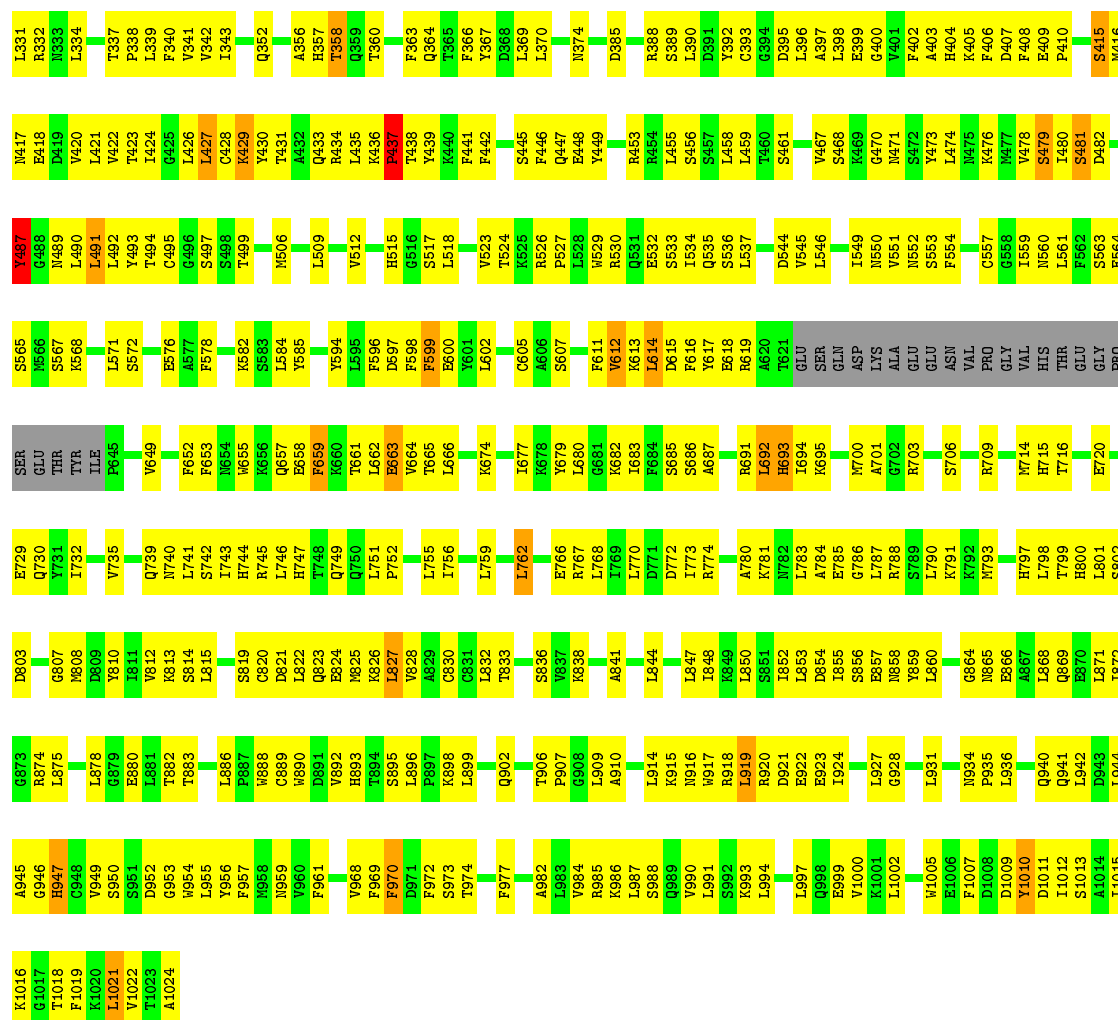
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: NLR family CARD domain-containing protein 4

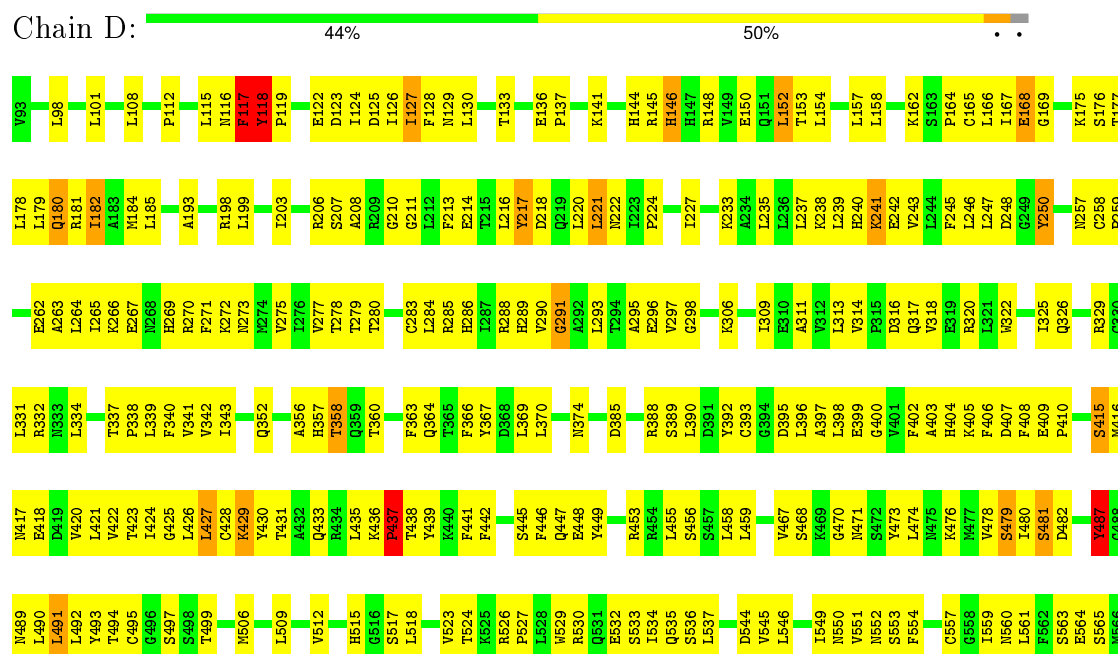


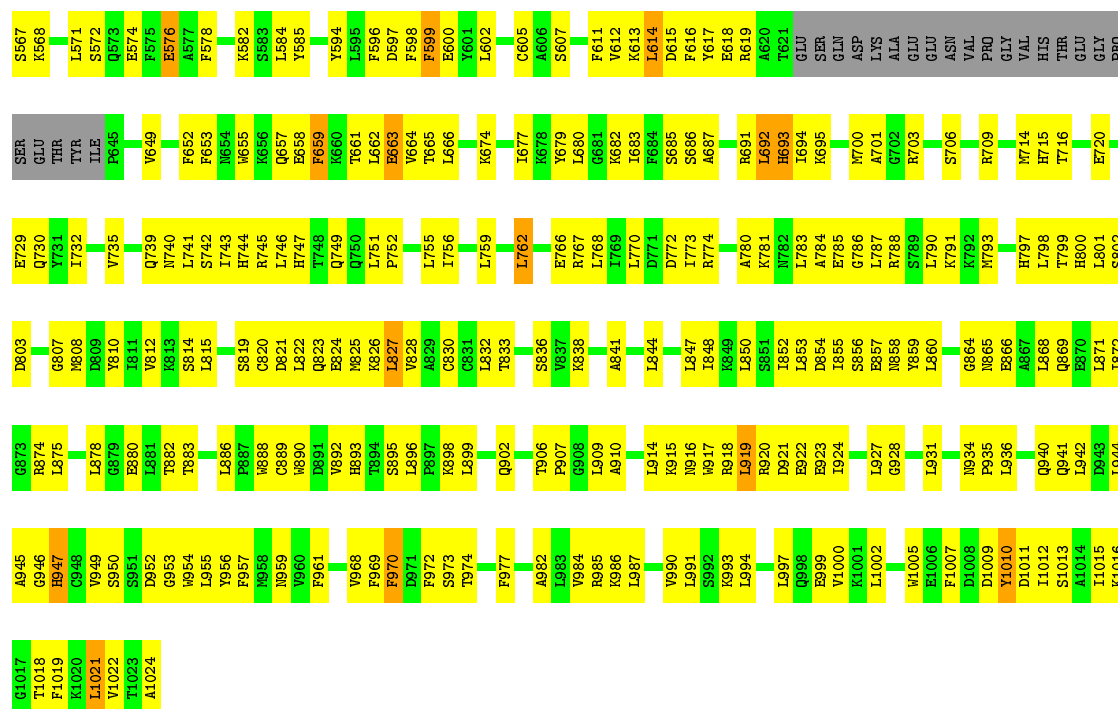




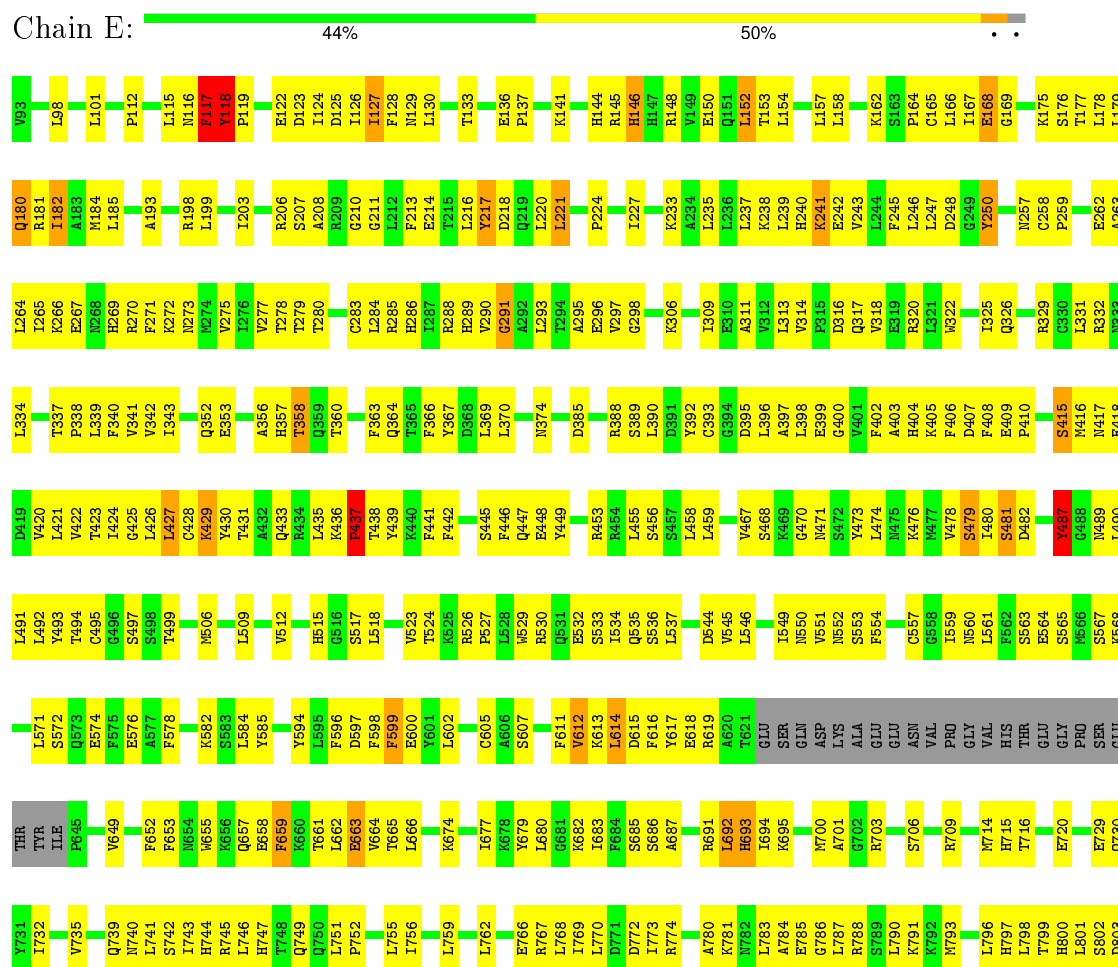


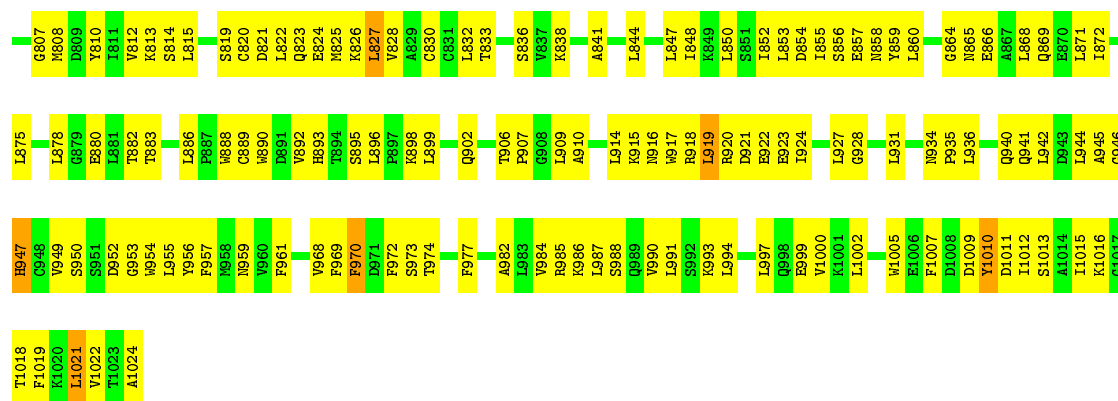
- Molecule 1: NLR family CARD domain-containing protein 4





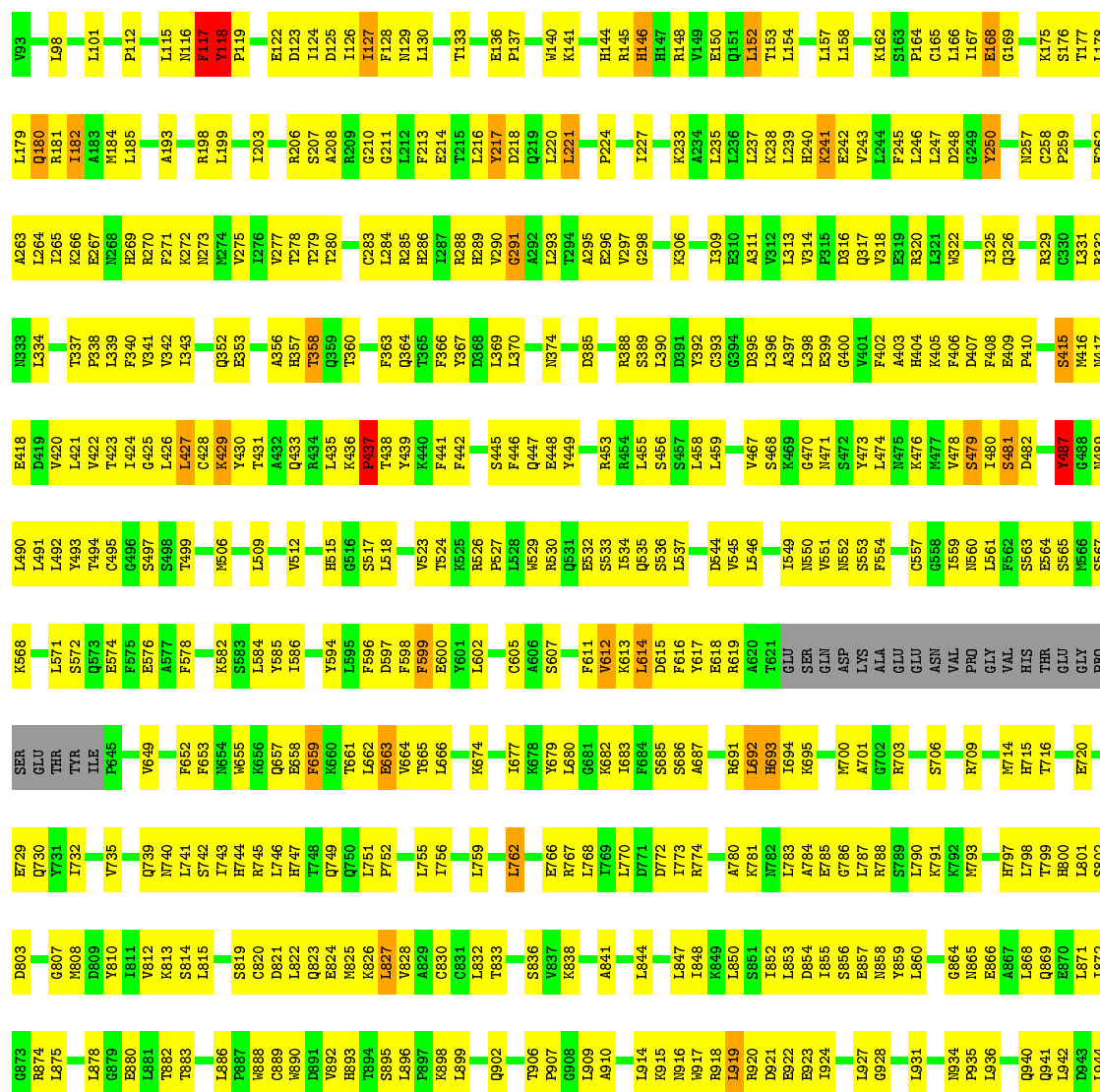
• Molecule 1: NLR family CARD domain-containing protein 4



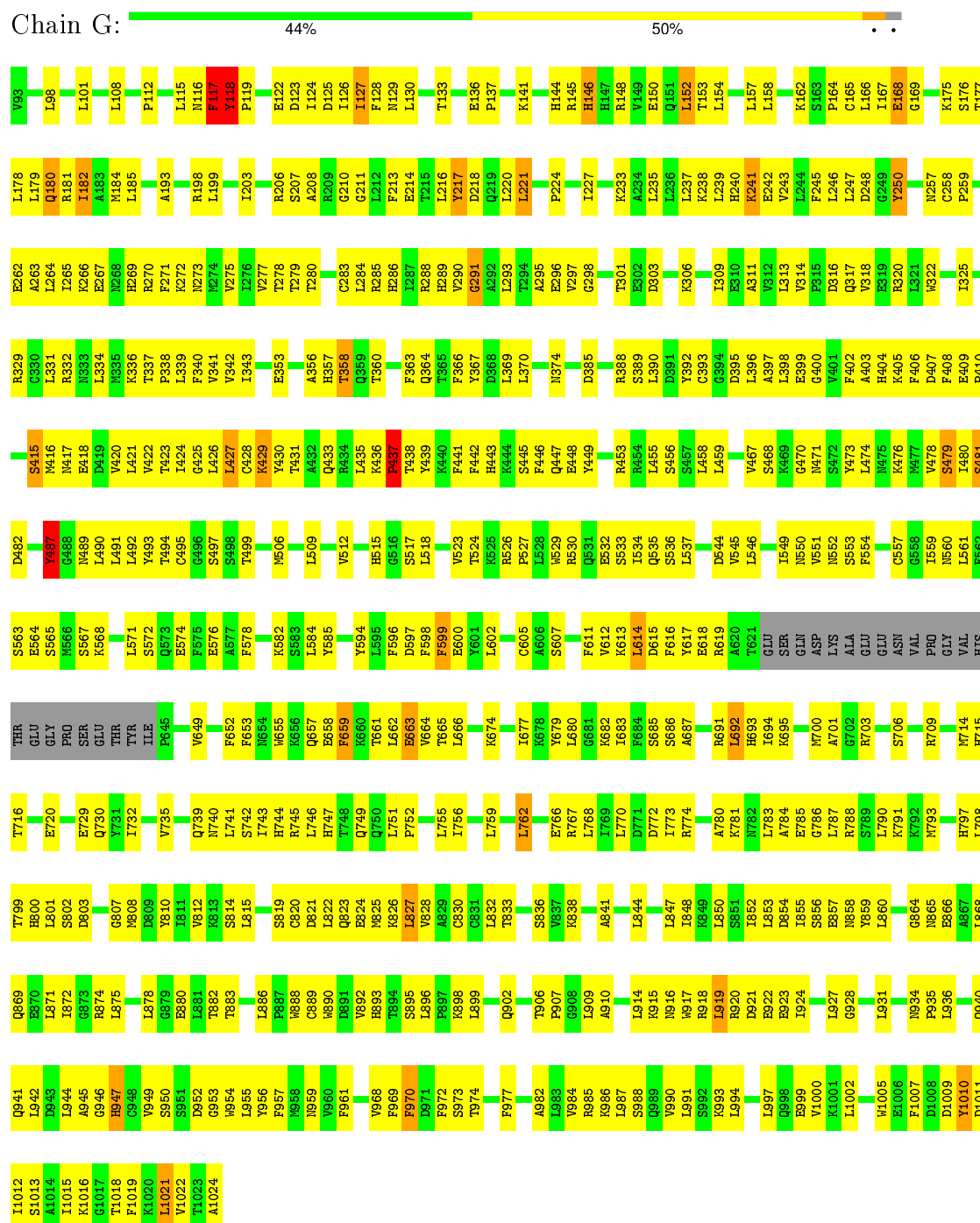


• Molecule 1: NLR family CARD domain-containing protein 4

Chain F: 44% 50%



- Molecule 1: NLR family CARD domain-containing protein 4



- Molecule 1: NLR family CARD domain-containing protein 4





E1006	N934	G864	R792		VAL	I559	V478
F1007	P935	N865	R793	R709	PRQ	N560	S479
D1008	L936	E866	L796	M714	GLY	L561	I480
D1009		E867	L797	H715	VAL	F562	S481
D1010	Q940	L868	H798	T716	HIS	S563	D482
I1012	Q941	Q869	T799		THR	E564	
S1013	L942	E870	H800	E720	GLU	S565	V483
A1014	D943	L871	L801		GLY	F566	G486
I1015	L944	I872	S802	E729	PRQ	S567	I489
K1016	A945	G873	D803	E729	SER	K568	L490
	G946	R874		Y731	GLU	Q730	L491
T1018	H947	L875	G807	I732	THR	L571	L492
F1019	G948		N808		TVR	S572	Y493
K1020	V949	L878	D809	V735	ILE	Q573	T494
L1021	S950	G879	Y810			E574	C495
V1022	S951	E880	J811	Q739		F575	G496
T1023	D952	L881	N812	N740		E576	S497
A1024	G953	T882	K813	L741		A577	S498
	N954	T883	S814	S742		F578	T499
	L955		L815	I743			
	Y956	L886		H744		K582	M506
	F957	N887	S819	R745		S583	L509
N958		N888	C920	L746		Y585	
N959		C889	D821	H747			
V960		N890	L822	T748		Y594	V512
F961		D891	Q823	Q749		L595	H515
	V968	V892	E824	Q750		F596	S516
F969		H893	N825	L751		D597	S517
F970		T894	K826	P752		F598	L518
D971		S895	L827			F599	
F972		L896	N828	L755		E600	V523
S973		F897	A829	I756		L601	T524
T974		L899	C830			L602	K525
			L832	L759		N604	R526
		Q902	T833			P527	P528
				L762		Q605	L528
A982		T906	S836	E766		A606	N529
L983		P907	T837	R767		S607	R530
V984		G908	K838	L768		F611	E532
R985		L909		I769		V612	S533
K986		A910	A841	L770		K613	I534
L987			L844	D771		L614	Q535
		L914		D772		D615	S536
V990		K915	L847	I773		F616	L537
L991		N916	I848	R774		Y617	D544
K993		W917	K849	A760		E618	V545
L994		L918	L850	K781		R619	L546
T995		R920	S851	N782		A620	
L996		D921	I852	L783		GLU	T649
L997		E922	L853	A784		SER	N550
Q998		E923	D854	E785		GLN	V551
E999		I924	I855	G786		ASP	N552
V1000			S856	L787		LYS	S553
K1001		L927	E857	R788		ALA	F554
L1002		G928	N858	S789		GLU	
			Y859	L790		GLU	C557
		W1005	L860	K791		ASN	S558

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	75114	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Wiener-type filter	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	21000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	0.37	0/7412	0.93	18/10004 (0.2%)
1	B	0.37	0/7412	0.93	18/10004 (0.2%)
1	C	0.37	0/7412	0.93	18/10004 (0.2%)
1	D	0.37	0/7412	0.93	18/10004 (0.2%)
1	E	0.37	0/7412	0.93	18/10004 (0.2%)
1	F	0.37	0/7412	0.93	18/10004 (0.2%)
1	G	0.37	0/7412	0.93	17/10004 (0.2%)
1	H	0.37	0/7412	0.93	18/10004 (0.2%)
1	I	0.37	0/7412	0.93	17/10004 (0.2%)
1	J	0.37	0/7412	0.93	18/10004 (0.2%)
1	K	0.37	0/7412	0.93	18/10004 (0.2%)
All	All	0.37	0/81532	0.93	196/110044 (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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
All	All	0	22

There are no bond length outliers.

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	280	THR	N-CA-C	-8.11	89.11	111.00
1	G	280	THR	N-CA-C	-8.11	89.11	111.00
1	K	280	THR	N-CA-C	-8.10	89.12	111.00
1	B	280	THR	N-CA-C	-8.10	89.12	111.00
1	C	280	THR	N-CA-C	-8.10	89.13	111.00

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	PHE	Peptide
1	A	441	PHE	Peptide
1	B	117	PHE	Peptide
1	K	117	PHE	Peptide
1	K	441	PHE	Peptide

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	7284	0	7329	442	0
1	B	7284	0	7329	440	0
1	C	7284	0	7329	440	0
1	D	7284	0	7329	442	0
1	E	7284	0	7329	437	0
1	F	7284	0	7329	442	0
1	G	7284	0	7329	436	0
1	H	7284	0	7329	444	0
1	I	7284	0	7329	442	0
1	J	7284	0	7329	457	0
1	K	7284	0	7329	454	0
All	All	80124	0	80619	4740	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 29.

The worst 5 of 4740 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)
1:K:125:ASP:H	1:J:433:GLN:HG2	1.28	0.95
1:A:433:GLN:HG2	1:B:125:ASP:H	1.33	0.94
1:F:433:GLN:HG2	1:G:125:ASP:H	1.33	0.93
1:G:433:GLN:HG2	1:H:125:ASP:H	1.33	0.93
1:D:433:GLN:HG2	1:E:125:ASP:H	1.34	0.93

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	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
1	B	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
1	C	904/932 (97%)	822 (91%)	66 (7%)	16 (2%)	11	55
1	D	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
1	E	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
1	F	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
1	G	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
1	H	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
1	I	904/932 (97%)	822 (91%)	66 (7%)	16 (2%)	11	55
1	J	904/932 (97%)	822 (91%)	66 (7%)	16 (2%)	11	55
1	K	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	11	55
All	All	9944/10252 (97%)	9050 (91%)	718 (7%)	176 (2%)	15	55

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	146	HIS
1	K	241	LYS
1	K	272	LYS
1	K	442	PHE
1	K	481	SER

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	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	B	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	C	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	D	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	E	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	F	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	G	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	H	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	I	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	J	810/830 (98%)	784 (97%)	26 (3%)	46	77
1	K	810/830 (98%)	784 (97%)	26 (3%)	46	77
All	All	8910/9130 (98%)	8624 (97%)	286 (3%)	50	77

5 of 286 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1021	LEU
1	F	182	ILE
1	J	182	ILE
1	E	168	GLU
1	E	576	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	257	ASN
1	F	257	ASN
1	J	146	HIS
1	E	693	HIS
1	F	433	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.16	1 (12%)
1	SEP	B	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.15	1 (12%)
1	SEP	C	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.16	1 (12%)
1	SEP	D	533	1	7,9,10	1.69	1 (14%)	8,12,14	1.15	1 (12%)
1	SEP	E	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.16	1 (12%)
1	SEP	F	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.15	1 (12%)
1	SEP	G	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.15	1 (12%)
1	SEP	H	533	1	7,9,10	1.69	1 (14%)	8,12,14	1.15	1 (12%)
1	SEP	I	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.16	1 (12%)
1	SEP	J	533	1	7,9,10	1.69	1 (14%)	8,12,14	1.16	1 (12%)
1	SEP	K	533	1	7,9,10	1.70	1 (14%)	8,12,14	1.15	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	533	1	-	0/5/8/10	0/0/0/0
1	SEP	B	533	1	-	0/5/8/10	0/0/0/0
1	SEP	C	533	1	-	0/5/8/10	0/0/0/0
1	SEP	D	533	1	-	0/5/8/10	0/0/0/0
1	SEP	E	533	1	-	0/5/8/10	0/0/0/0
1	SEP	F	533	1	-	0/5/8/10	0/0/0/0
1	SEP	G	533	1	-	0/5/8/10	0/0/0/0
1	SEP	H	533	1	-	0/5/8/10	0/0/0/0
1	SEP	I	533	1	-	0/5/8/10	0/0/0/0
1	SEP	J	533	1	-	0/5/8/10	0/0/0/0
1	SEP	K	533	1	-	0/5/8/10	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	533	SEP	P-O1P	3.35	1.61	1.50
1	J	533	SEP	P-O1P	3.35	1.61	1.50
1	H	533	SEP	P-O1P	3.35	1.61	1.50
1	E	533	SEP	P-O1P	3.36	1.61	1.50
1	I	533	SEP	P-O1P	3.37	1.61	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	SEP	O-C-CA	-2.07	120.16	125.72
1	A	533	SEP	O-C-CA	-2.07	120.18	125.72
1	K	533	SEP	O-C-CA	-2.06	120.18	125.72
1	J	533	SEP	O-C-CA	-2.06	120.19	125.72
1	I	533	SEP	O-C-CA	-2.06	120.19	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	533	SEP	2	0
1	B	533	SEP	2	0
1	C	533	SEP	2	0
1	D	533	SEP	2	0
1	E	533	SEP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	533	SEP	3	0
1	G	533	SEP	2	0
1	H	533	SEP	2	0
1	I	533	SEP	2	0
1	J	533	SEP	2	0
1	K	533	SEP	2	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.