wwPDB EM Map/Model Validation Report (i)

Oct 18, 2016 – 11:30 AM EDT

PDB ID	:	5JUY
EMDB ID:	:	EMD-8178
Title	:	Active human apoptosome with procaspase-9
Authors	:	Cheng, T.C.; Hong, C.; Akey, I.V.; Yuan, S.; Akey, C.W.
Deposited on	:	2016-05-10
Resolution	:	4.10 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

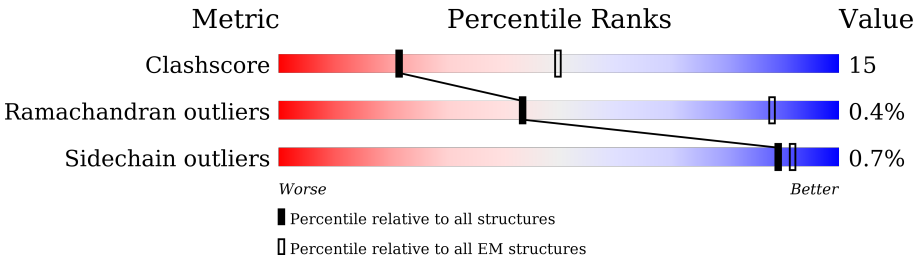
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.10 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1248	65% 26% • 9%
1	B	1248	72% 26% ••
1	C	1248	65% 26% • 9%
1	D	1248	72% 27% ••
1	E	1248	72% 27% ••
1	F	1248	65% 26% • 9%
1	G	1248	72% 26% ••
2	H	104	57% 43%
2	I	104	56% 44%

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Mol	Chain	Length	Quality of chain
2	J	104	58% 42%
2	K	104	58% 42%
2	L	104	58% 42%
2	M	104	59% 41%
2	N	104	60% 40%
3	O	95	76% 20% •
3	P	95	76% 19% 5%
3	Q	95	77% 19% •
3	R	95	77% 19% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 76058 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 Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	B	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	C	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	D	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	E	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	F	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	G	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		

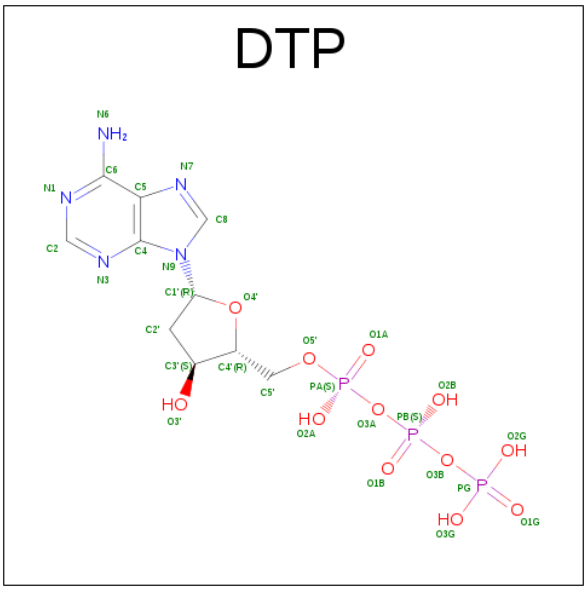
- Molecule 2 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	I	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	J	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	K	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	L	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	M	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	N	104	Total	C	N	O	S	0	0
			814	517	143	150	4		

- Molecule 3 is a protein called Caspase-9.

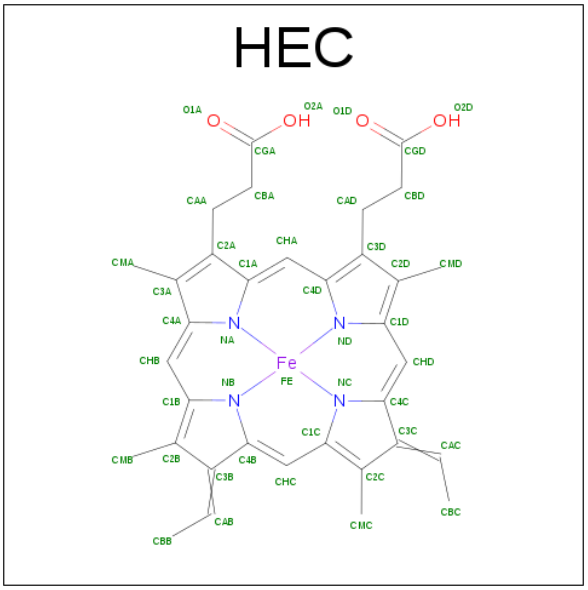
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	P	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	Q	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	R	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	F	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	G	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



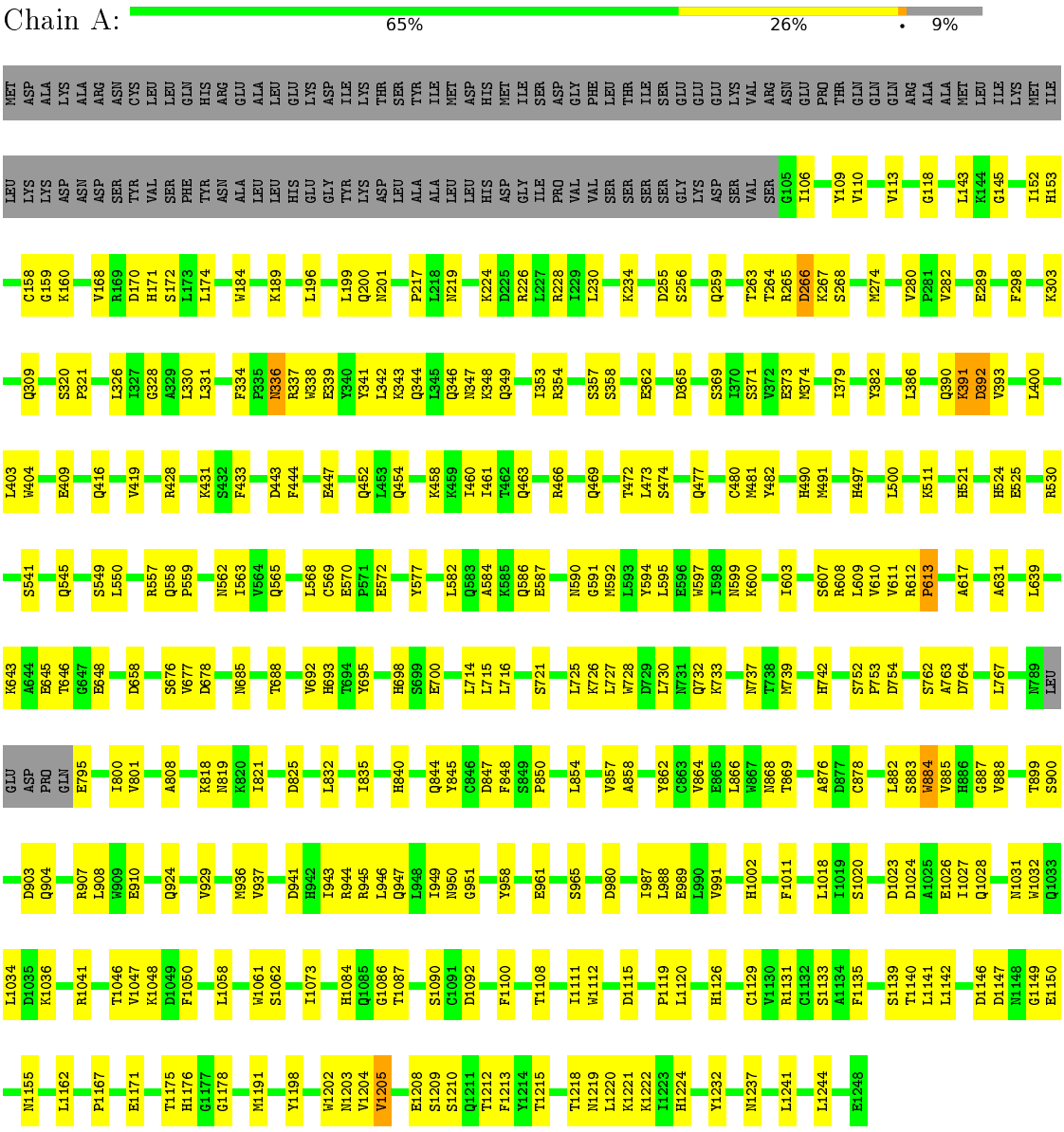
Mol	Chain	Residues	Atoms					AltConf
5	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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.

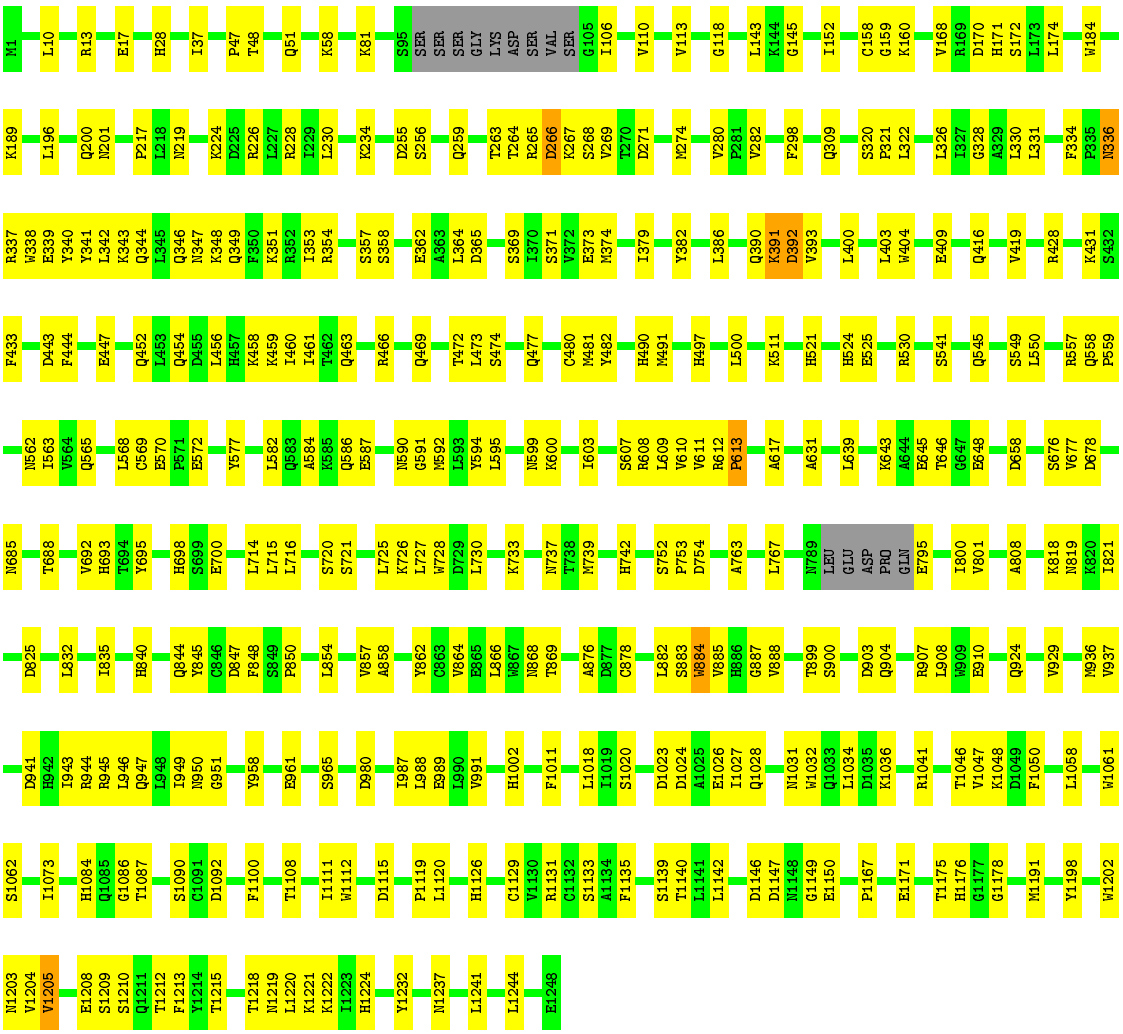
- Molecule 1: Apoptotic protease-activating factor 1

Chain A:



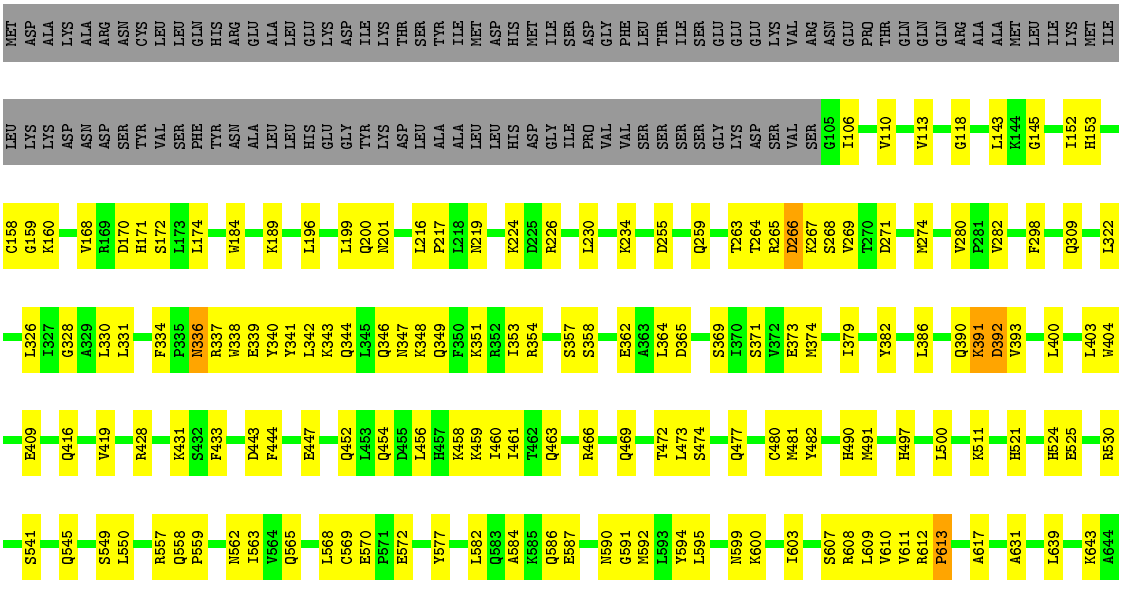
- Molecule 1: Apoptotic protease-activating factor 1

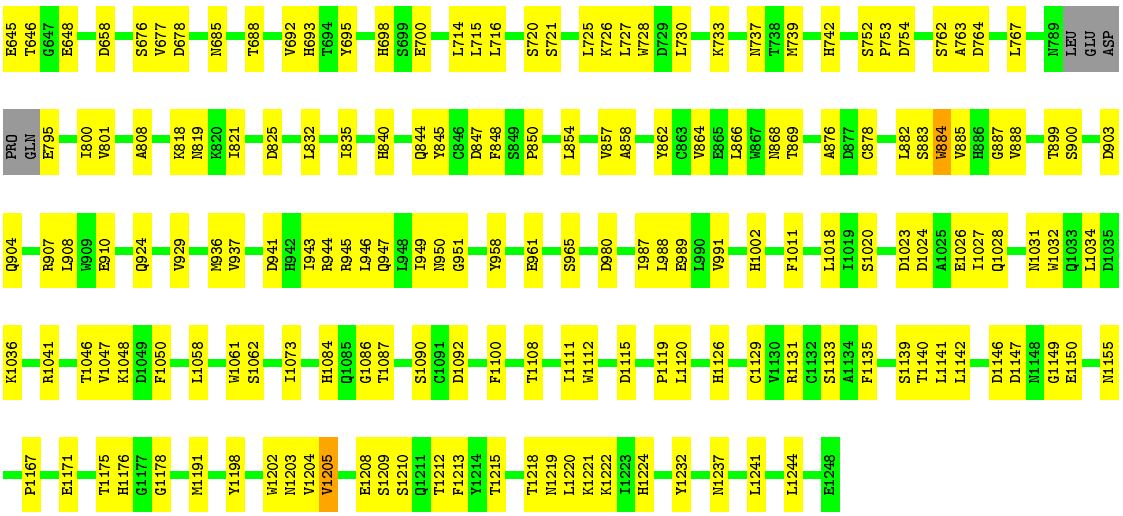
Chain B:



• Molecule 1: Apoptotic protease-activating factor 1

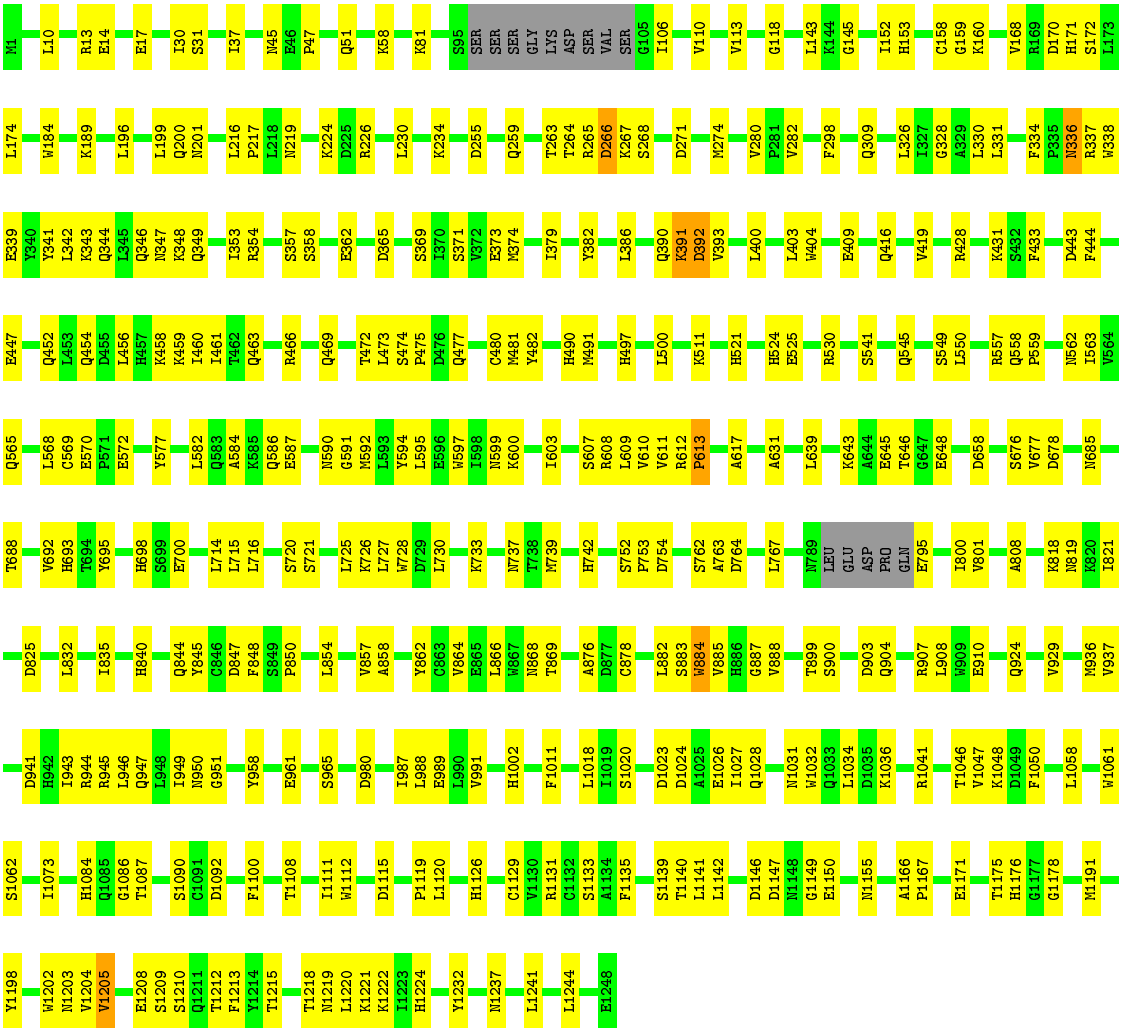
Chain C:





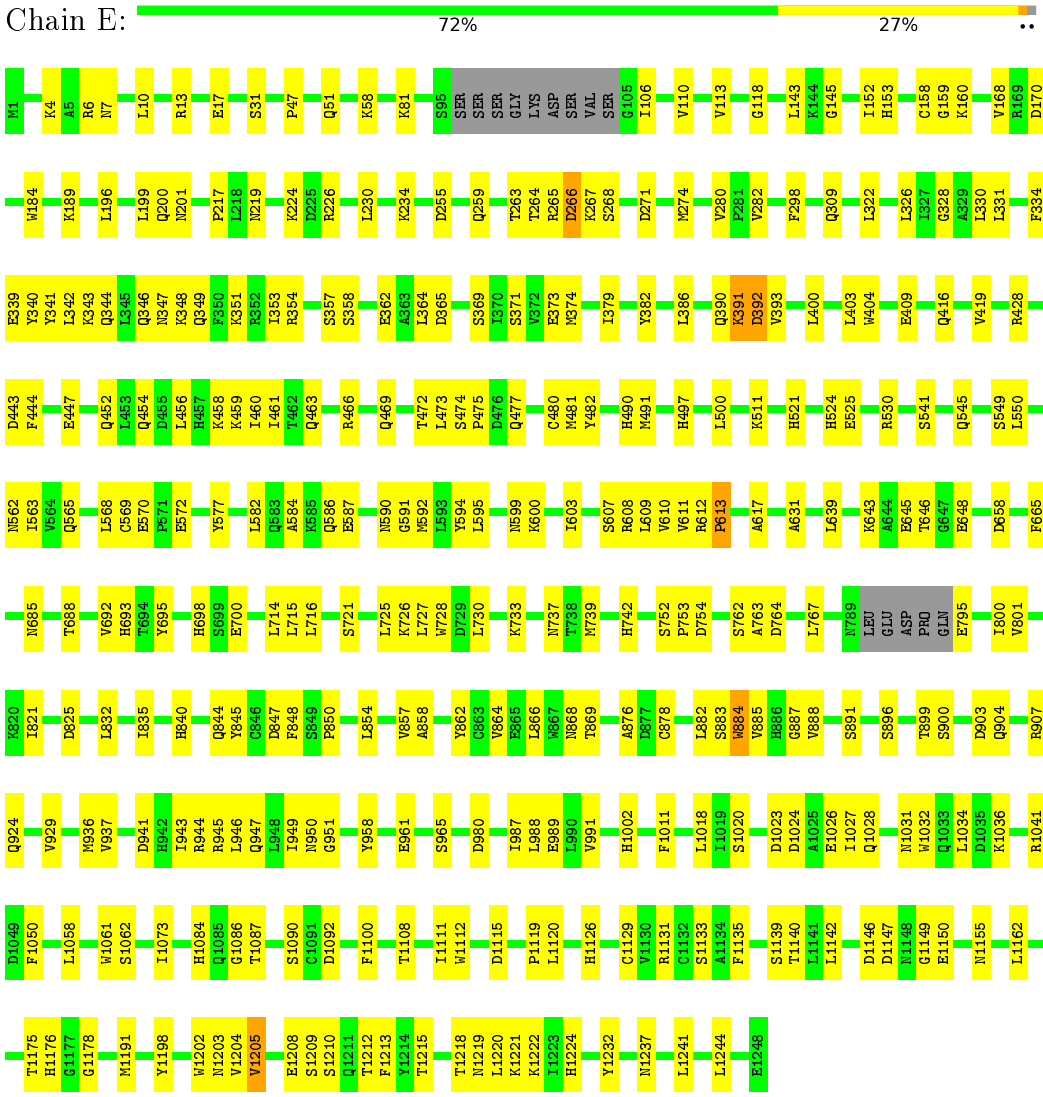
- Molecule 1: Apoptotic protease-activating factor 1

Chain D:



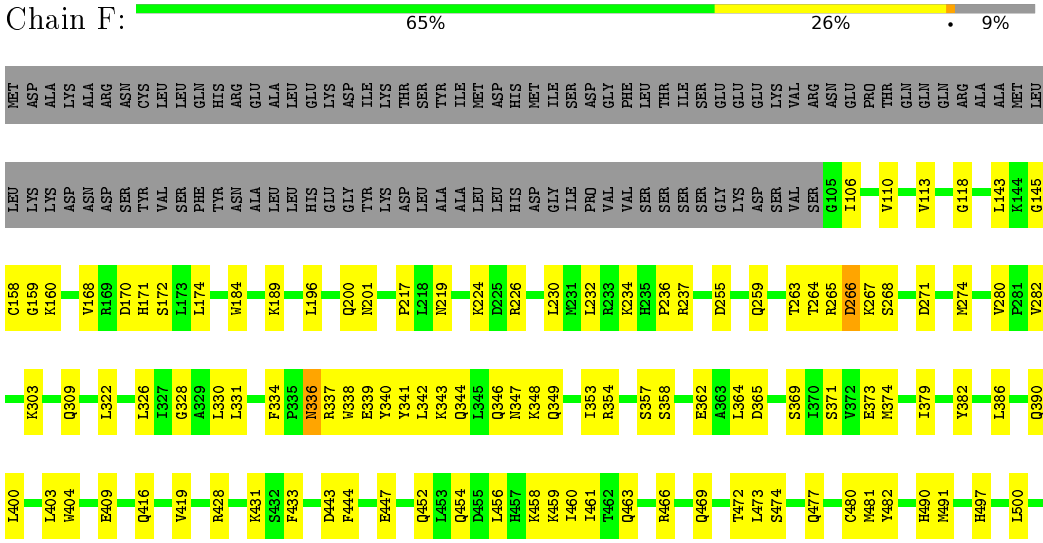
- Molecule 1: Apoptotic protease-activating factor 1

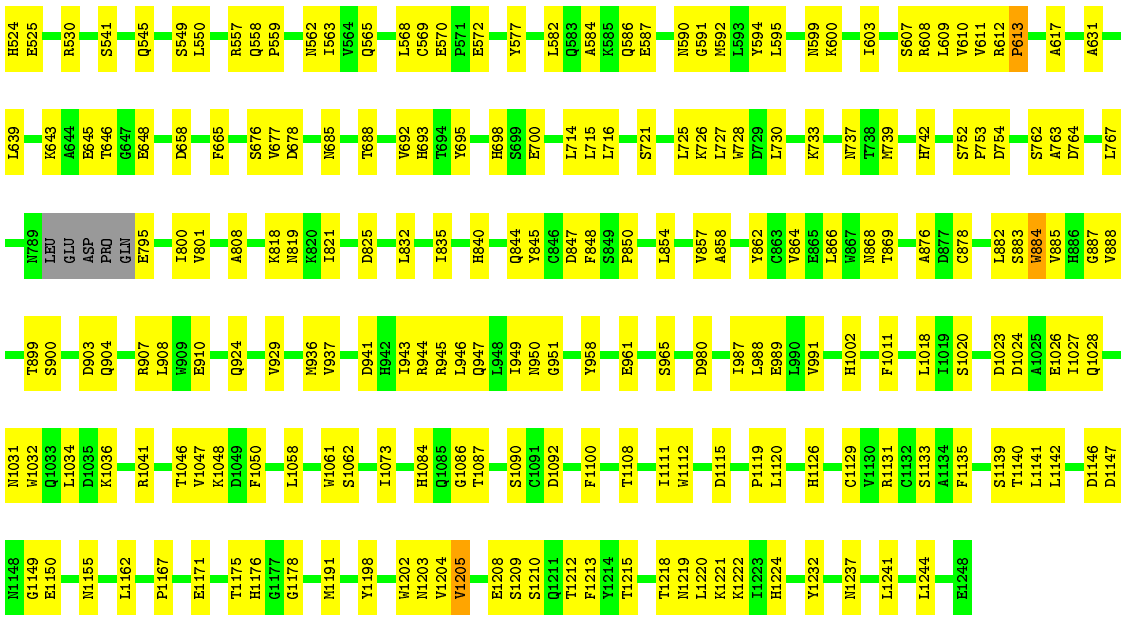
Chain E:



• Molecule 1: Apoptotic protease-activating factor 1

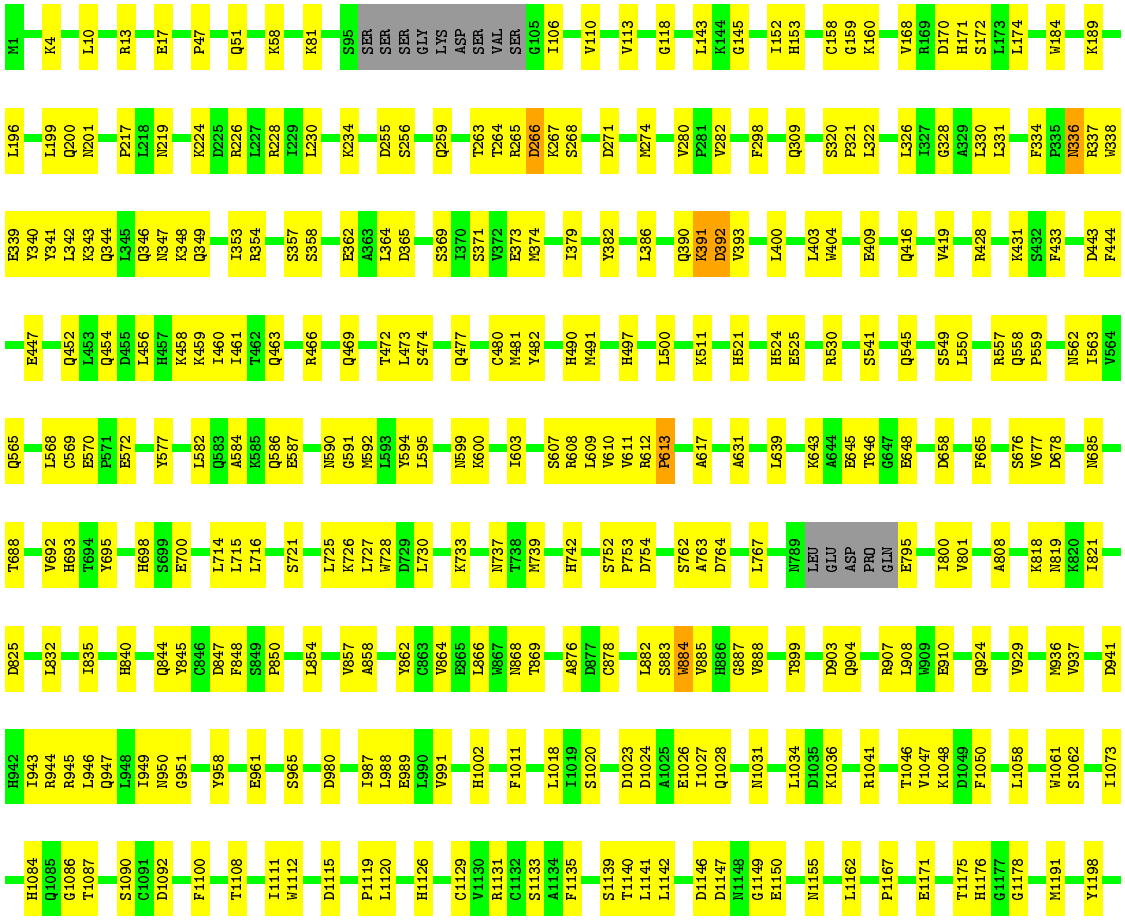
Chain F:

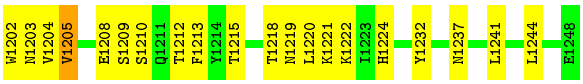




• Molecule 1: Apoptotic protease-activating factor 1

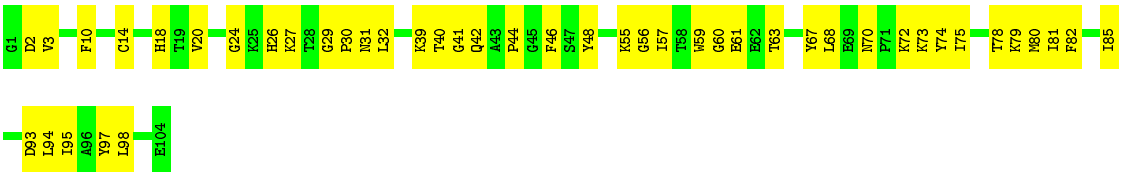
Chain G:





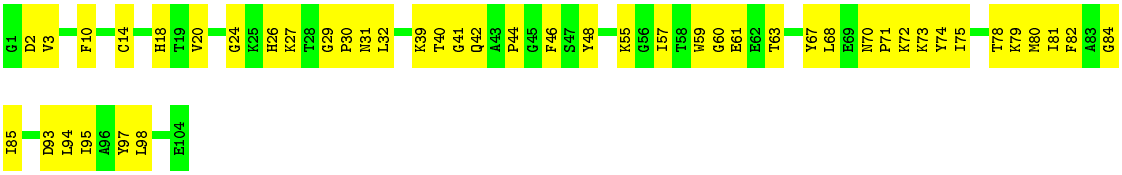
- Molecule 2: Cytochrome c

Chain H:



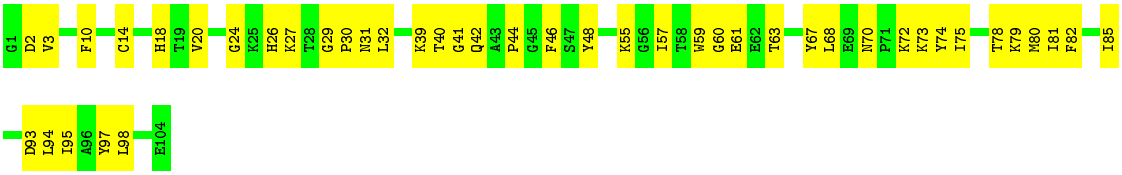
- Molecule 2: Cytochrome c

Chain I:



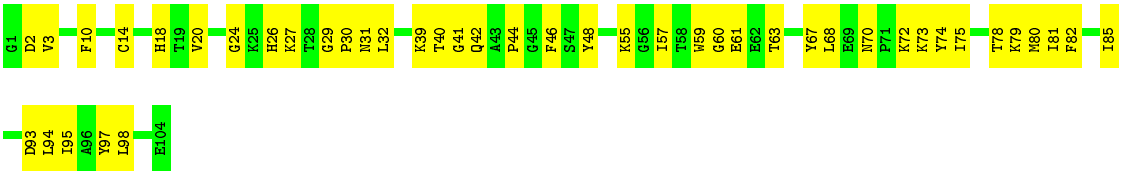
- Molecule 2: Cytochrome c

Chain J:



- Molecule 2: Cytochrome c

Chain K:

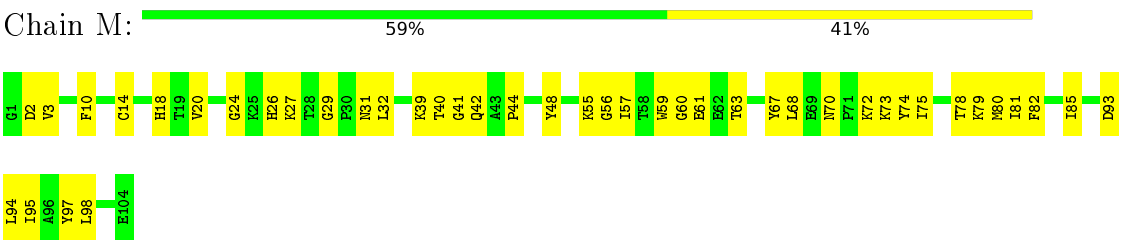


- Molecule 2: Cytochrome c

Chain L:

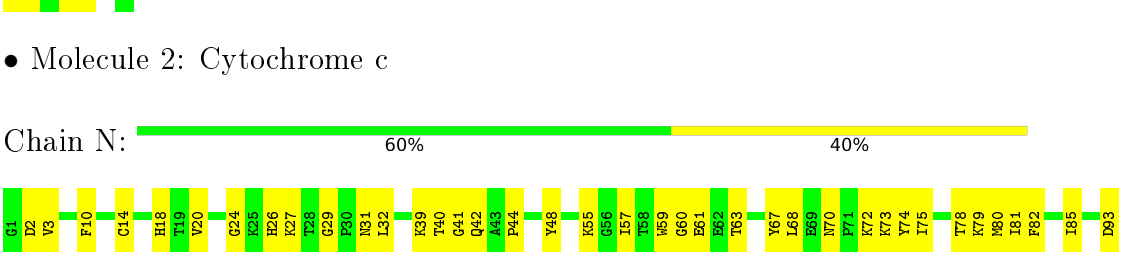
• Molecule 2: Cytochrome c

Chain M:



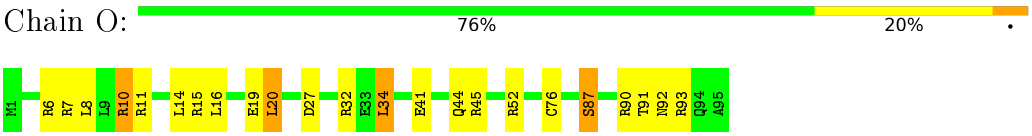
• Molecule 2: Cytochrome c

Chain N:



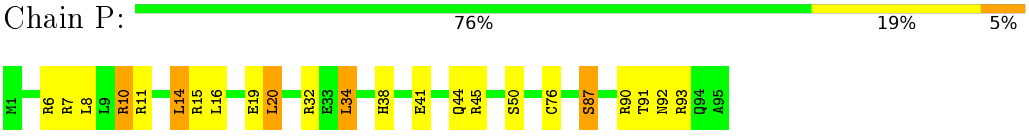
• Molecule 3: Caspase-9

Chain O:



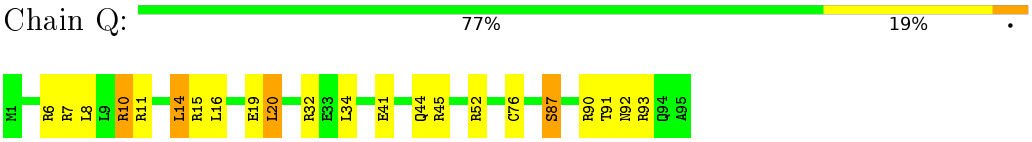
• Molecule 3: Caspase-9

Chain P:



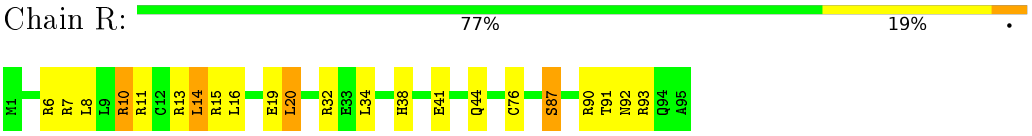
• Molecule 3: Caspase-9

Chain Q:



• Molecule 3: Caspase-9

Chain R:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	92867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.33	1/9295 (0.0%)	0.46	0/12575
1	B	0.37	1/10068 (0.0%)	0.47	0/13613
1	C	0.33	1/9295 (0.0%)	0.46	0/12575
1	D	0.36	1/10068 (0.0%)	0.47	0/13613
1	E	0.36	1/10068 (0.0%)	0.47	0/13613
1	F	0.33	1/9295 (0.0%)	0.47	0/12575
1	G	0.37	1/10068 (0.0%)	0.47	0/13613
2	H	0.25	0/830	0.42	0/1105
2	I	0.25	0/830	0.42	0/1105
2	J	0.25	0/830	0.42	0/1105
2	K	0.25	0/830	0.42	0/1105
2	L	0.25	0/830	0.42	0/1105
2	M	0.25	0/830	0.42	0/1105
2	N	0.25	0/830	0.42	0/1105
3	O	0.60	0/784	0.61	0/1051
3	P	0.60	0/784	0.61	0/1051
3	Q	0.60	0/784	0.61	0/1051
3	R	0.60	0/784	0.61	0/1051
All	All	0.36	7/77103 (0.0%)	0.47	0/104116

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	168	VAL	C-N	6.96	1.50	1.34
1	B	168	VAL	C-N	6.94	1.50	1.34
1	A	168	VAL	C-N	6.94	1.50	1.34
1	E	168	VAL	C-N	6.94	1.50	1.34
1	D	168	VAL	C-N	6.93	1.50	1.34

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASN	Peptide
1	B	336	ASN	Peptide
1	C	336	ASN	Peptide
1	D	336	ASN	Peptide
1	E	336	ASN	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	A	9099	0	8967	296	0
1	B	9861	0	9736	300	0
1	C	9099	0	8968	293	0
1	D	9861	0	9736	310	0
1	E	9861	0	9736	313	0
1	F	9099	0	8968	300	0
1	G	9861	0	9736	300	0
2	H	814	0	833	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	814	0	833	58	0
2	J	814	0	833	59	0
2	K	814	0	833	57	0
2	L	814	0	833	58	0
2	M	814	0	833	59	0
2	N	814	0	833	56	0
3	O	777	0	787	21	0
3	P	777	0	787	28	0
3	Q	777	0	786	39	0
3	R	777	0	787	29	0
4	A	30	0	9	3	0
4	B	30	0	9	3	0
4	C	30	0	9	3	0
4	D	30	0	9	3	0
4	E	30	0	9	3	0
4	F	30	0	9	3	0
4	G	30	0	9	3	0
5	H	43	0	32	4	0
5	I	43	0	32	4	0
5	J	43	0	32	4	0
5	K	43	0	32	4	0
5	L	43	0	32	4	0
5	M	43	0	32	4	0
5	N	43	0	32	4	0
All	All	76058	0	75112	2327	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 15.

The worst 5 of 2327 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)
3:Q:52:ARG:HD3	3:R:38:HIS:CE1	1.20	1.66
3:Q:52:ARG:CD	3:R:38:HIS:CE1	2.01	1.40
1:E:884:TRP:CH2	2:L:79:LYS:HA	1.68	1.28
1:D:884:TRP:CH2	2:K:79:LYS:HA	1.68	1.28
1:G:884:TRP:CH2	2:N:79:LYS:HA	1.68	1.28

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	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	34	76
1	B	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	34	76
1	C	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	34	76
1	D	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	34	76
1	E	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	34	76
1	F	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	34	76
1	G	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	34	76
2	H	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	I	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	J	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	K	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	L	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	M	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	N	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
3	O	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	P	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	Q	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	R	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
All	All	9403/9844 (96%)	8741 (93%)	620 (7%)	42 (0%)	43	79

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1073	ILE
1	B	1073	ILE
1	C	1073	ILE
1	D	1073	ILE

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Mol	Chain	Res	Type
1	E	1073	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	1022/1119 (91%)	1019 (100%)	3 (0%)	94 96
1	B	1106/1119 (99%)	1101 (100%)	5 (0%)	92 96
1	C	1022/1119 (91%)	1019 (100%)	3 (0%)	94 96
1	D	1106/1119 (99%)	1101 (100%)	5 (0%)	92 96
1	E	1106/1119 (99%)	1101 (100%)	5 (0%)	92 96
1	F	1022/1119 (91%)	1019 (100%)	3 (0%)	94 96
1	G	1106/1119 (99%)	1101 (100%)	5 (0%)	92 96
2	H	84/84 (100%)	84 (100%)	0	100 100
2	I	84/84 (100%)	84 (100%)	0	100 100
2	J	84/84 (100%)	84 (100%)	0	100 100
2	K	84/84 (100%)	84 (100%)	0	100 100
2	L	84/84 (100%)	84 (100%)	0	100 100
2	M	84/84 (100%)	84 (100%)	0	100 100
2	N	84/84 (100%)	84 (100%)	0	100 100
3	O	84/84 (100%)	77 (92%)	7 (8%)	14 52
3	P	84/84 (100%)	77 (92%)	7 (8%)	14 52
3	Q	84/84 (100%)	77 (92%)	7 (8%)	14 52
3	R	84/84 (100%)	77 (92%)	7 (8%)	14 52
All	All	8414/8757 (96%)	8357 (99%)	57 (1%)	89 94

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	81	LYS

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Mol	Chain	Res	Type
3	O	20	LEU
3	R	20	LEU
1	G	391	LYS
1	G	884	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	819	ASN
1	E	712	HIS
2	N	70	ASN
1	D	924	GLN
1	E	45	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

14 ligands 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	$\#\|Z\|>2$
4	DTP	A	1301	-	25,32,32	3.23	7 (28%)	26,50,50	2.80	3 (11%)
4	DTP	B	1301	-	25,32,32	3.22	7 (28%)	26,50,50	2.80	3 (11%)
4	DTP	C	1301	-	25,32,32	3.23	7 (28%)	26,50,50	2.80	3 (11%)
4	DTP	D	1301	-	25,32,32	3.24	7 (28%)	26,50,50	2.81	3 (11%)
4	DTP	E	1301	-	25,32,32	3.23	7 (28%)	26,50,50	2.81	3 (11%)
4	DTP	F	1301	-	25,32,32	3.23	7 (28%)	26,50,50	2.79	3 (11%)
4	DTP	G	1301	-	25,32,32	3.23	7 (28%)	26,50,50	2.81	3 (11%)
5	HEC	H	500	-	24,50,50	2.45	6 (25%)	19,82,82	1.84	4 (21%)
5	HEC	I	500	-	24,50,50	2.45	6 (25%)	19,82,82	1.83	4 (21%)
5	HEC	J	500	-	24,50,50	2.45	6 (25%)	19,82,82	1.83	4 (21%)
5	HEC	K	500	-	24,50,50	2.46	6 (25%)	19,82,82	1.84	4 (21%)
5	HEC	L	500	-	24,50,50	2.45	6 (25%)	19,82,82	1.84	4 (21%)
5	HEC	M	500	-	24,50,50	2.45	6 (25%)	19,82,82	1.84	4 (21%)
5	HEC	N	500	-	24,50,50	2.45	6 (25%)	19,82,82	1.84	4 (21%)

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
4	DTP	A	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	B	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	C	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	D	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	E	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	F	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	G	1301	-	-	0/18/34/34	0/3/3/3
5	HEC	H	500	-	-	0/6/54/54	0/0/8/8
5	HEC	I	500	-	-	0/6/54/54	0/0/8/8
5	HEC	J	500	-	-	0/6/54/54	0/0/8/8
5	HEC	K	500	-	-	0/6/54/54	0/0/8/8
5	HEC	L	500	-	-	0/6/54/54	0/0/8/8
5	HEC	M	500	-	-	0/6/54/54	0/0/8/8
5	HEC	N	500	-	-	0/6/54/54	0/0/8/8

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	DTP	C2'-C3'	-11.56	1.21	1.52
4	G	1301	DTP	C2'-C3'	-11.55	1.21	1.52
4	F	1301	DTP	C2'-C3'	-11.55	1.21	1.52
4	A	1301	DTP	C2'-C3'	-11.54	1.21	1.52
4	E	1301	DTP	C2'-C3'	-11.54	1.21	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1301	DTP	N3-C2-N1	-11.29	120.00	128.87
4	G	1301	DTP	N3-C2-N1	-11.29	120.01	128.87
4	E	1301	DTP	N3-C2-N1	-11.28	120.01	128.87
4	C	1301	DTP	N3-C2-N1	-11.24	120.04	128.87
4	A	1301	DTP	N3-C2-N1	-11.24	120.04	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	DTP	3	0
4	B	1301	DTP	3	0
4	C	1301	DTP	3	0
4	D	1301	DTP	3	0
4	E	1301	DTP	3	0
4	F	1301	DTP	3	0
4	G	1301	DTP	3	0
5	H	500	HEC	4	0
5	I	500	HEC	4	0
5	J	500	HEC	4	0
5	K	500	HEC	4	0
5	L	500	HEC	4	0
5	M	500	HEC	4	0
5	N	500	HEC	4	0

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.