wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:56 PM BST

PDB ID	:	3J2T
EMDB ID:	:	EMD-5186
Title	:	An improved model of the human apoptosome
Authors	:	Yuan, S.; Topf, M.; Akey, C.W.
Deposited on	:	2012-12-23
Resolution	:	9.50 Å(reported)
Based on PDB ID	:	2B4Z, 3SFZ, 1Z6T

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

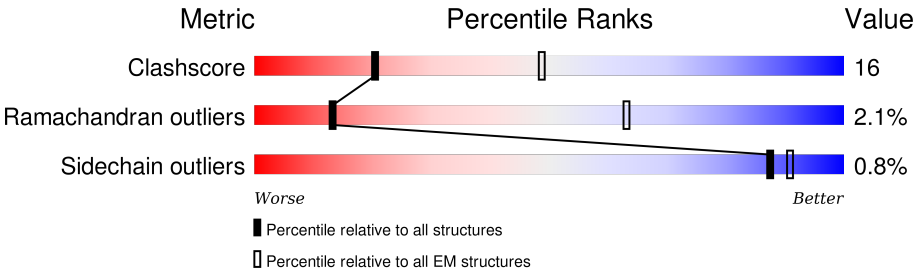
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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	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	1263	81% 9% • 9%
1	B	1263	80% 9% • 9%
1	C	1263	81% 9% • 9%
1	D	1263	80% 9% • 9%
1	E	1263	80% 9% • 9%
1	F	1263	81% 8% • 9%
1	G	1263	81% 8% • 9%
2	H	104	81% 17% ••
2	I	104	81% 17% ••

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Mol	Chain	Length	Quality of chain
2	J	104	
2	K	104	
2	L	104	
2	M	104	
2	N	104	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 70189 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	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	B	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	C	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	D	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	E	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	F	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	G	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP O14727
A	-4	HIS	-	EXPRESSION TAG	UNP O14727
A	-3	HIS	-	EXPRESSION TAG	UNP O14727
A	-2	HIS	-	EXPRESSION TAG	UNP O14727
A	-1	HIS	-	EXPRESSION TAG	UNP O14727
A	0	HIS	-	EXPRESSION TAG	UNP O14727
A	1249	HIS	-	EXPRESSION TAG	UNP O14727
A	1250	HIS	-	EXPRESSION TAG	UNP O14727
A	1251	HIS	-	EXPRESSION TAG	UNP O14727
A	1252	HIS	-	EXPRESSION TAG	UNP O14727
A	1253	HIS	-	EXPRESSION TAG	UNP O14727
A	1254	HIS	-	EXPRESSION TAG	UNP O14727
A	1255	HIS	-	EXPRESSION TAG	UNP O14727
A	1256	HIS	-	EXPRESSION TAG	UNP O14727
A	1257	HIS	-	EXPRESSION TAG	UNP O14727
B	-5	HIS	-	EXPRESSION TAG	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP O14727
B	-3	HIS	-	EXPRESSION TAG	UNP O14727
B	-2	HIS	-	EXPRESSION TAG	UNP O14727
B	-1	HIS	-	EXPRESSION TAG	UNP O14727
B	0	HIS	-	EXPRESSION TAG	UNP O14727
B	1249	HIS	-	EXPRESSION TAG	UNP O14727
B	1250	HIS	-	EXPRESSION TAG	UNP O14727
B	1251	HIS	-	EXPRESSION TAG	UNP O14727
B	1252	HIS	-	EXPRESSION TAG	UNP O14727
B	1253	HIS	-	EXPRESSION TAG	UNP O14727
B	1254	HIS	-	EXPRESSION TAG	UNP O14727
B	1255	HIS	-	EXPRESSION TAG	UNP O14727
B	1256	HIS	-	EXPRESSION TAG	UNP O14727
B	1257	HIS	-	EXPRESSION TAG	UNP O14727
C	-5	HIS	-	EXPRESSION TAG	UNP O14727
C	-4	HIS	-	EXPRESSION TAG	UNP O14727
C	-3	HIS	-	EXPRESSION TAG	UNP O14727
C	-2	HIS	-	EXPRESSION TAG	UNP O14727
C	-1	HIS	-	EXPRESSION TAG	UNP O14727
C	0	HIS	-	EXPRESSION TAG	UNP O14727
C	1249	HIS	-	EXPRESSION TAG	UNP O14727
C	1250	HIS	-	EXPRESSION TAG	UNP O14727
C	1251	HIS	-	EXPRESSION TAG	UNP O14727
C	1252	HIS	-	EXPRESSION TAG	UNP O14727
C	1253	HIS	-	EXPRESSION TAG	UNP O14727
C	1254	HIS	-	EXPRESSION TAG	UNP O14727
C	1255	HIS	-	EXPRESSION TAG	UNP O14727
C	1256	HIS	-	EXPRESSION TAG	UNP O14727
C	1257	HIS	-	EXPRESSION TAG	UNP O14727
D	-5	HIS	-	EXPRESSION TAG	UNP O14727
D	-4	HIS	-	EXPRESSION TAG	UNP O14727
D	-3	HIS	-	EXPRESSION TAG	UNP O14727
D	-2	HIS	-	EXPRESSION TAG	UNP O14727
D	-1	HIS	-	EXPRESSION TAG	UNP O14727
D	0	HIS	-	EXPRESSION TAG	UNP O14727
D	1249	HIS	-	EXPRESSION TAG	UNP O14727
D	1250	HIS	-	EXPRESSION TAG	UNP O14727
D	1251	HIS	-	EXPRESSION TAG	UNP O14727
D	1252	HIS	-	EXPRESSION TAG	UNP O14727
D	1253	HIS	-	EXPRESSION TAG	UNP O14727
D	1254	HIS	-	EXPRESSION TAG	UNP O14727
D	1255	HIS	-	EXPRESSION TAG	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1256	HIS	-	EXPRESSION TAG	UNP O14727
D	1257	HIS	-	EXPRESSION TAG	UNP O14727
E	-5	HIS	-	EXPRESSION TAG	UNP O14727
E	-4	HIS	-	EXPRESSION TAG	UNP O14727
E	-3	HIS	-	EXPRESSION TAG	UNP O14727
E	-2	HIS	-	EXPRESSION TAG	UNP O14727
E	-1	HIS	-	EXPRESSION TAG	UNP O14727
E	0	HIS	-	EXPRESSION TAG	UNP O14727
E	1249	HIS	-	EXPRESSION TAG	UNP O14727
E	1250	HIS	-	EXPRESSION TAG	UNP O14727
E	1251	HIS	-	EXPRESSION TAG	UNP O14727
E	1252	HIS	-	EXPRESSION TAG	UNP O14727
E	1253	HIS	-	EXPRESSION TAG	UNP O14727
E	1254	HIS	-	EXPRESSION TAG	UNP O14727
E	1255	HIS	-	EXPRESSION TAG	UNP O14727
E	1256	HIS	-	EXPRESSION TAG	UNP O14727
E	1257	HIS	-	EXPRESSION TAG	UNP O14727
F	-5	HIS	-	EXPRESSION TAG	UNP O14727
F	-4	HIS	-	EXPRESSION TAG	UNP O14727
F	-3	HIS	-	EXPRESSION TAG	UNP O14727
F	-2	HIS	-	EXPRESSION TAG	UNP O14727
F	-1	HIS	-	EXPRESSION TAG	UNP O14727
F	0	HIS	-	EXPRESSION TAG	UNP O14727
F	1249	HIS	-	EXPRESSION TAG	UNP O14727
F	1250	HIS	-	EXPRESSION TAG	UNP O14727
F	1251	HIS	-	EXPRESSION TAG	UNP O14727
F	1252	HIS	-	EXPRESSION TAG	UNP O14727
F	1253	HIS	-	EXPRESSION TAG	UNP O14727
F	1254	HIS	-	EXPRESSION TAG	UNP O14727
F	1255	HIS	-	EXPRESSION TAG	UNP O14727
F	1256	HIS	-	EXPRESSION TAG	UNP O14727
F	1257	HIS	-	EXPRESSION TAG	UNP O14727
G	-5	HIS	-	EXPRESSION TAG	UNP O14727
G	-4	HIS	-	EXPRESSION TAG	UNP O14727
G	-3	HIS	-	EXPRESSION TAG	UNP O14727
G	-2	HIS	-	EXPRESSION TAG	UNP O14727
G	-1	HIS	-	EXPRESSION TAG	UNP O14727
G	0	HIS	-	EXPRESSION TAG	UNP O14727
G	1249	HIS	-	EXPRESSION TAG	UNP O14727
G	1250	HIS	-	EXPRESSION TAG	UNP O14727
G	1251	HIS	-	EXPRESSION TAG	UNP O14727
G	1252	HIS	-	EXPRESSION TAG	UNP O14727

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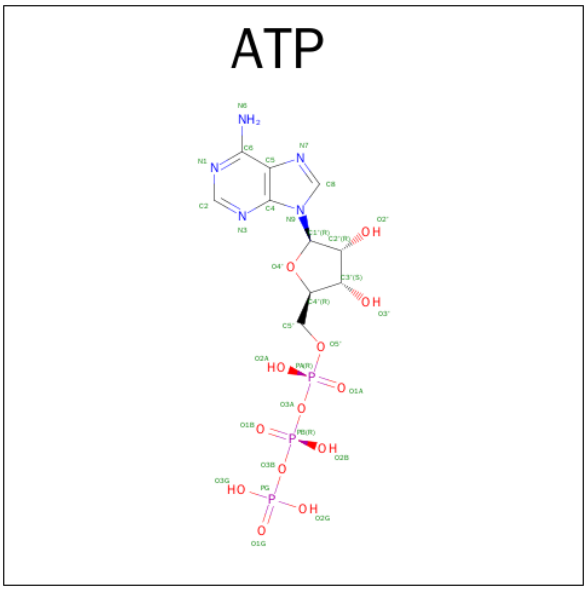
Chain	Residue	Modelled	Actual	Comment	Reference
G	1253	HIS	-	EXPRESSION TAG	UNP O14727
G	1254	HIS	-	EXPRESSION TAG	UNP O14727
G	1255	HIS	-	EXPRESSION TAG	UNP O14727
G	1256	HIS	-	EXPRESSION TAG	UNP O14727
G	1257	HIS	-	EXPRESSION TAG	UNP O14727

- Molecule 2 is a protein called Cytochrome c.

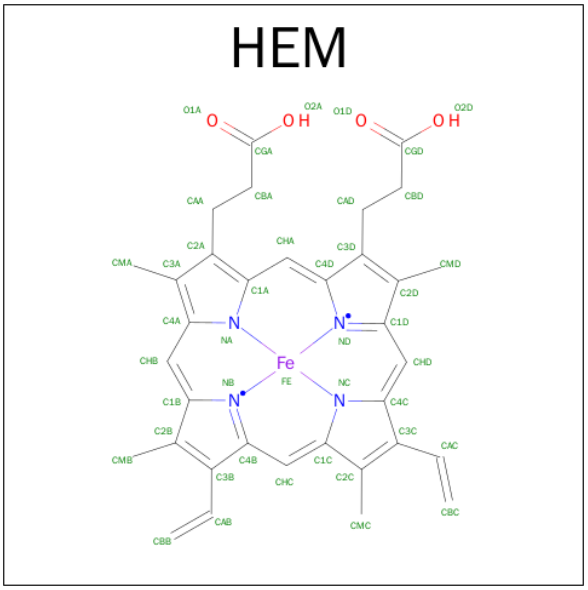
Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	I	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	J	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	K	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	L	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	M	104	Total	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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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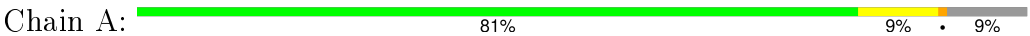
Mol	Chain	Residues	Atoms					AltConf
4	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
4	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
4	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

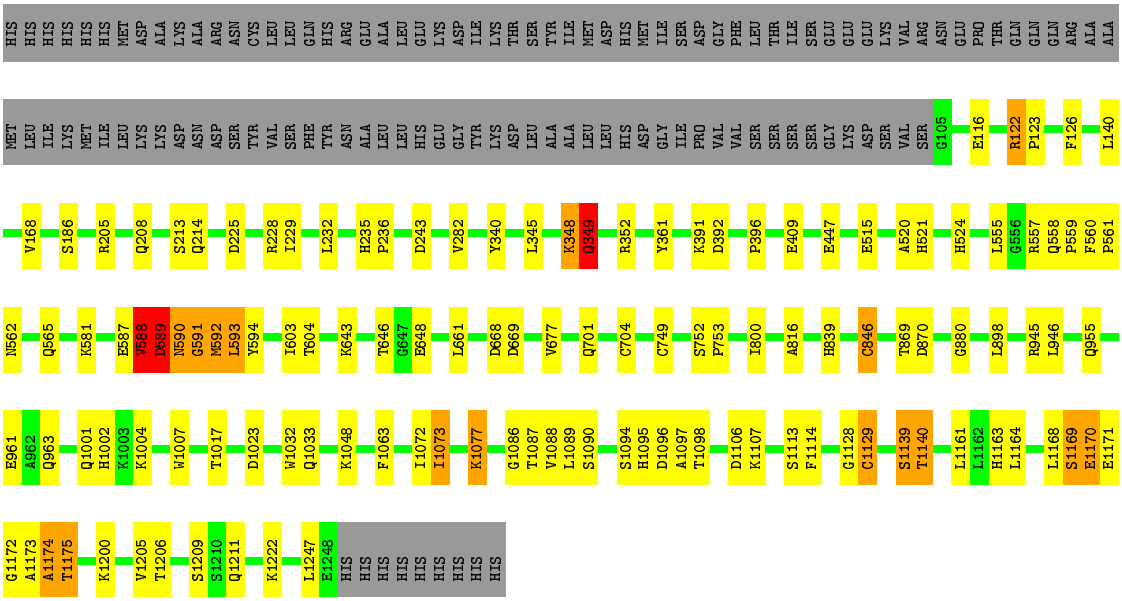
3 Residue-property plots (i)

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

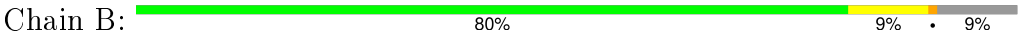
Chain A:

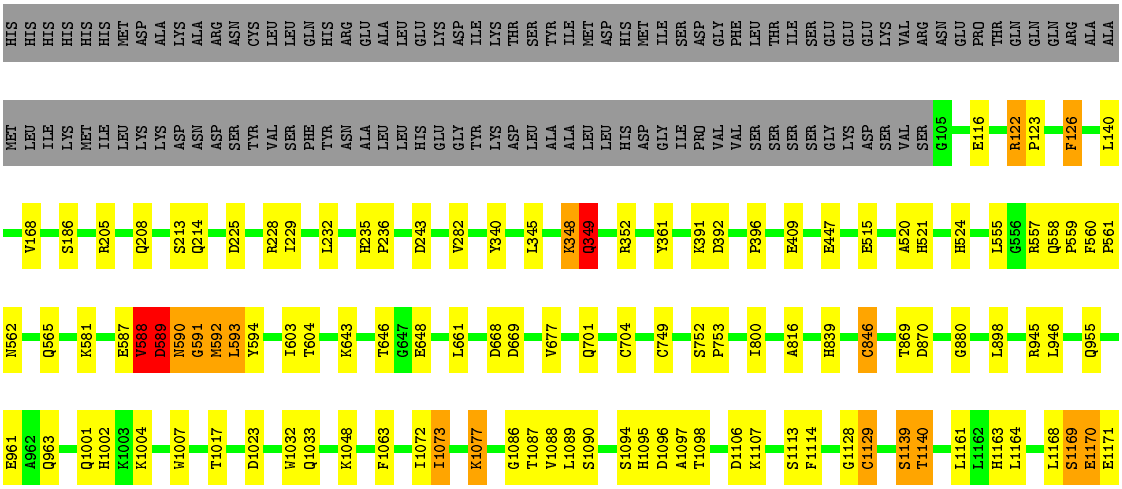




- Molecule 1: Apoptotic protease-activating factor 1

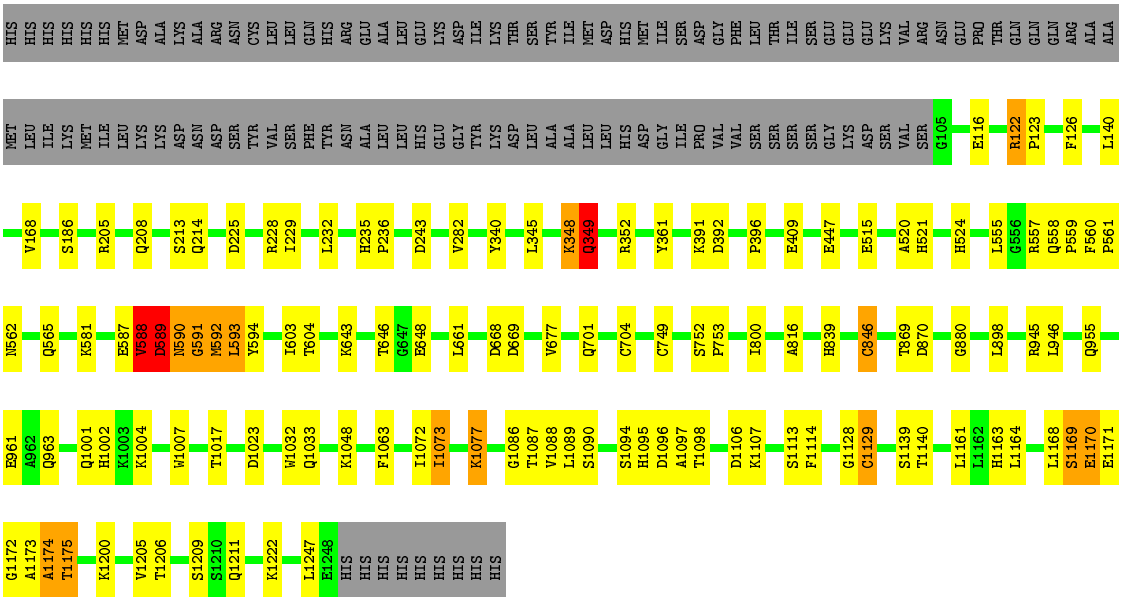
Chain B:





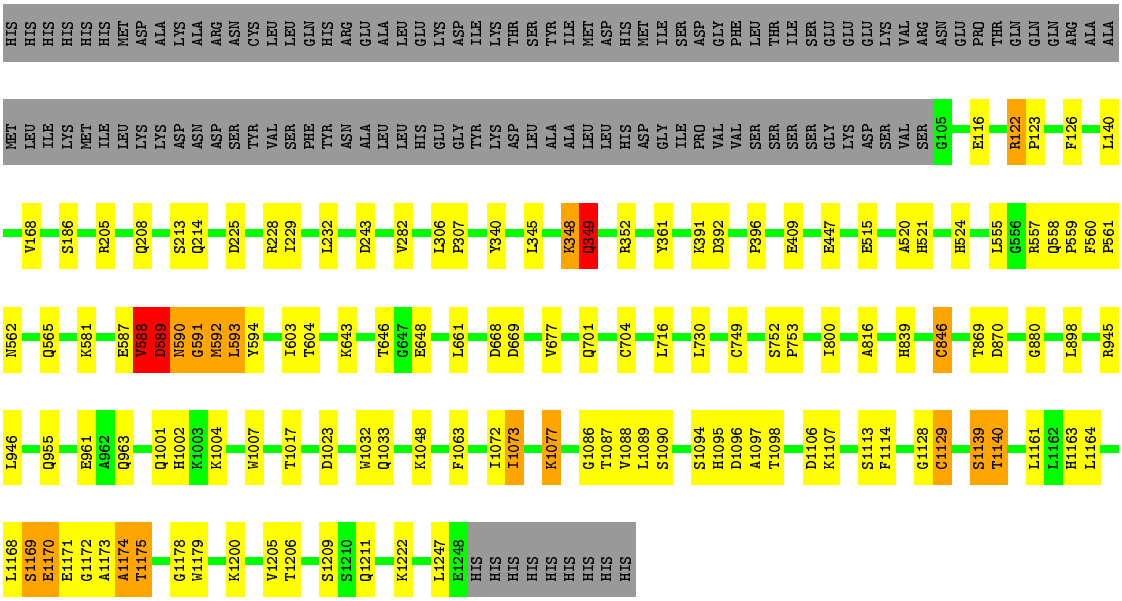
• Molecule 1: Apoptotic protease-activating factor 1

Chain C:



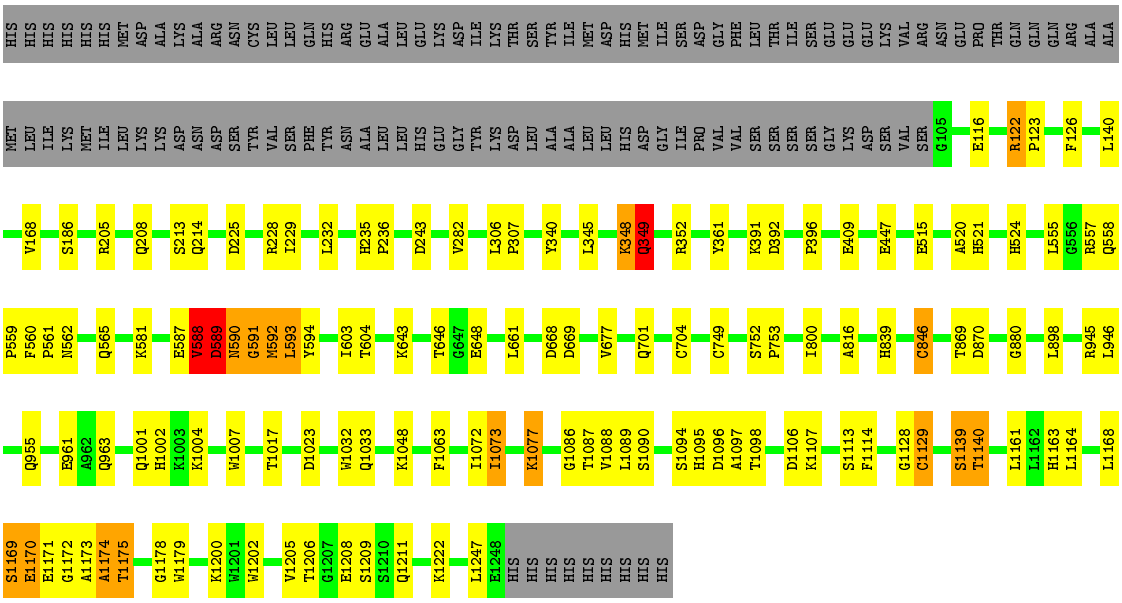
• Molecule 1: Apoptotic protease-activating factor 1

Chain D:



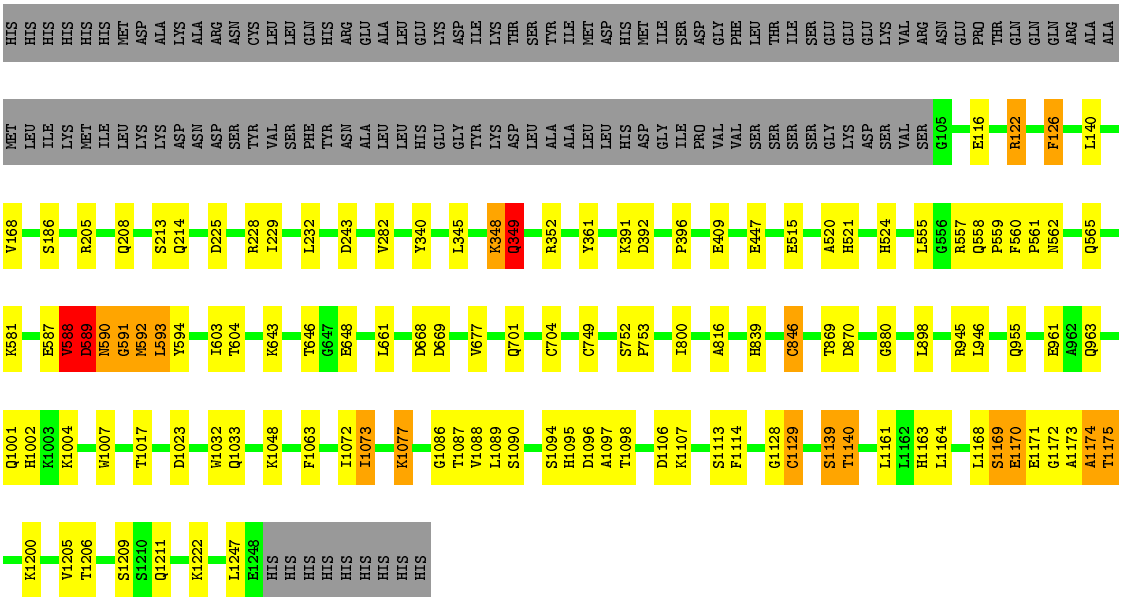
• Molecule 1: Apoptotic protease-activating factor 1

Chain E:



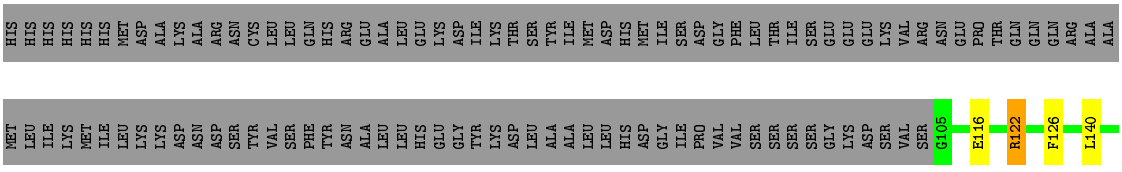
• Molecule 1: Apoptotic protease-activating factor 1

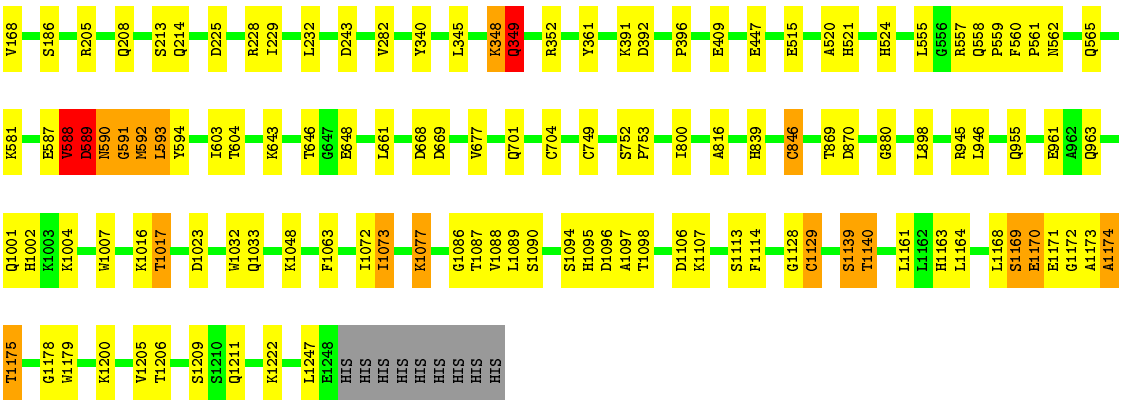
Chain F:



• Molecule 1: Apoptotic protease-activating factor 1

Chain G:





- Molecule 2: Cytochrome c

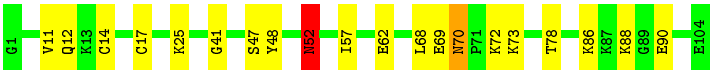
Chain H:

- Molecule 2: Cytochrome c

Chain I:

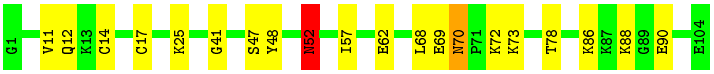
- Molecule 2: Cytochrome c

Chain J:



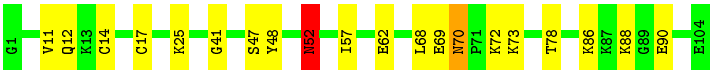
- Molecule 2: Cytochrome c

Chain K:



- Molecule 2: Cytochrome c

Chain L:



- Molecule 2: Cytochrome c

Chain M:

- Molecule 2: Cytochrome c

Chain N:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	34000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction was done on each particle image based on summed power spectra from each micrograph.	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	62000	Depositor
Image detector	Kodak SO163 film	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	B	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	C	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	D	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	E	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	F	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	G	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
2	H	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	I	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	J	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	K	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	L	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	M	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	N	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
All	All	0.85	35/71169 (0.0%)	0.83	77/96187 (0.1%)

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
2	H	0	1
2	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1
2	K	0	1
2	L	0	1
2	M	0	1
2	N	0	1
All	All	0	21

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	52	ASN	CG-OD1	15.38	1.57	1.24
2	M	52	ASN	CG-OD1	15.37	1.57	1.24
2	L	52	ASN	CG-OD1	15.37	1.57	1.24
2	H	52	ASN	CG-OD1	15.36	1.57	1.24
2	J	52	ASN	CG-OD1	15.35	1.57	1.24

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	11	VAL	CG1-CB-CG2	-15.51	86.09	110.90
2	M	11	VAL	CG1-CB-CG2	-15.49	86.11	110.90
2	H	11	VAL	CG1-CB-CG2	-15.49	86.12	110.90
2	N	11	VAL	CG1-CB-CG2	-15.49	86.12	110.90
2	K	11	VAL	CG1-CB-CG2	-15.48	86.14	110.90

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	TYR	Mainchain
1	A	588	VAL	Mainchain
1	B	361	TYR	Mainchain
1	B	588	VAL	Mainchain
1	C	361	TYR	Mainchain

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	9139	0	8998	336	0
1	B	9139	0	8998	330	0
1	C	9139	0	8998	333	0
1	D	9139	0	8998	337	0
1	E	9139	0	8998	336	0
1	F	9139	0	8998	338	0
1	G	9139	0	8998	337	0
2	H	814	0	833	92	0
2	I	814	0	833	90	0
2	J	814	0	833	90	0
2	K	814	0	833	88	0
2	L	814	0	833	88	0
2	M	814	0	833	91	0
2	N	814	0	833	91	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
3	E	31	0	12	1	0
3	F	31	0	12	2	0
3	G	31	0	12	1	0
4	H	43	0	30	7	0
4	I	43	0	30	10	0
4	J	43	0	30	7	0
4	K	43	0	30	6	0
4	L	43	0	30	6	0
4	M	43	0	30	8	0
4	N	43	0	30	7	0
All	All	70189	0	69111	2213	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 16.

The worst 5 of 2213 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:E:1063:PHE:CE2	2:L:86:LYS:HG3	1.14	1.66
1:D:1063:PHE:CE2	2:K:86:LYS:HG3	1.14	1.65
1:F:1063:PHE:CE2	2:M:86:LYS:HG3	1.14	1.64
1:A:1063:PHE:CE2	2:H:86:LYS:HG3	1.14	1.62
1:B:1063:PHE:CE2	2:I:86:LYS:HG3	1.14	1.61

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	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	8 48
1	B	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	8 48
1	C	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	8 48
1	D	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	8 48
1	E	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	8 48
1	F	1142/1263 (90%)	1049 (92%)	67 (6%)	26 (2%)	8 48
1	G	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	8 48
2	H	102/104 (98%)	99 (97%)	3 (3%)	0	100 100
2	I	102/104 (98%)	99 (97%)	3 (3%)	0	100 100
2	J	102/104 (98%)	99 (97%)	3 (3%)	0	100 100
2	K	102/104 (98%)	99 (97%)	3 (3%)	0	100 100
2	L	102/104 (98%)	99 (97%)	3 (3%)	0	100 100
2	M	102/104 (98%)	99 (97%)	3 (3%)	0	100 100
2	N	102/104 (98%)	99 (97%)	3 (3%)	0	100 100
All	All	8708/9569 (91%)	8030 (92%)	496 (6%)	182 (2%)	13 50

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	LYS
1	A	349	GLN
1	A	591	GLY
1	A	592	MET
1	A	839	HIS

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	1027/1134 (91%)	1020 (99%)	7 (1%)	88	94
1	B	1027/1134 (91%)	1020 (99%)	7 (1%)	88	94
1	C	1027/1134 (91%)	1020 (99%)	7 (1%)	88	94
1	D	1027/1134 (91%)	1020 (99%)	7 (1%)	88	94
1	E	1027/1134 (91%)	1020 (99%)	7 (1%)	88	94
1	F	1027/1134 (91%)	1020 (99%)	7 (1%)	88	94
1	G	1027/1134 (91%)	1020 (99%)	7 (1%)	88	94
2	H	84/84 (100%)	82 (98%)	2 (2%)	57	82
2	I	84/84 (100%)	82 (98%)	2 (2%)	57	82
2	J	84/84 (100%)	82 (98%)	2 (2%)	57	82
2	K	84/84 (100%)	82 (98%)	2 (2%)	57	82
2	L	84/84 (100%)	82 (98%)	2 (2%)	57	82
2	M	84/84 (100%)	82 (98%)	2 (2%)	57	82
2	N	84/84 (100%)	82 (98%)	2 (2%)	57	82
All	All	7777/8526 (91%)	7714 (99%)	63 (1%)	87	94

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	122	ARG
1	F	122	ARG
2	L	70	ASN
1	E	140	LEU
1	E	589	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	441	GLN

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Mol	Chain	Res	Type
1	G	565	GLN
2	M	54	ASN
1	F	565	GLN
1	F	693	HIS

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	$\#\|Z\| > 2$
3	ATP	A	1301	-	26,33,33	1.10	2 (7%)	26,52,52	1.89	3 (11%)
3	ATP	B	1301	-	26,33,33	1.10	2 (7%)	26,52,52	1.89	3 (11%)
3	ATP	C	1301	-	26,33,33	1.10	2 (7%)	26,52,52	1.89	3 (11%)
3	ATP	D	1301	-	26,33,33	1.10	2 (7%)	26,52,52	1.88	3 (11%)
3	ATP	E	1301	-	26,33,33	1.10	2 (7%)	26,52,52	1.89	3 (11%)
3	ATP	F	1301	-	26,33,33	1.10	2 (7%)	26,52,52	1.89	3 (11%)
3	ATP	G	1301	-	26,33,33	1.10	2 (7%)	26,52,52	1.89	3 (11%)
4	HEM	H	500	2	24,50,50	1.65	4 (16%)	16,82,82	2.86	8 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HEM	I	500	2	24,50,50	1.65	4 (16%)	16,82,82	2.86	8 (50%)
4	HEM	J	500	2	24,50,50	1.65	4 (16%)	16,82,82	2.86	8 (50%)
4	HEM	K	500	2	24,50,50	1.65	4 (16%)	16,82,82	2.87	8 (50%)
4	HEM	L	500	2	24,50,50	1.65	4 (16%)	16,82,82	2.86	8 (50%)
4	HEM	M	500	2	24,50,50	1.65	4 (16%)	16,82,82	2.86	8 (50%)
4	HEM	N	500	2	24,50,50	1.65	4 (16%)	16,82,82	2.87	8 (50%)

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
3	ATP	A	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	B	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	C	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	D	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	E	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	F	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	G	1301	-	-	0/18/38/38	0/3/3/3
4	HEM	H	500	2	-	0/6/54/54	0/0/8/8
4	HEM	I	500	2	-	0/6/54/54	0/0/8/8
4	HEM	J	500	2	-	0/6/54/54	0/0/8/8
4	HEM	K	500	2	-	0/6/54/54	0/0/8/8
4	HEM	L	500	2	-	0/6/54/54	0/0/8/8
4	HEM	M	500	2	-	0/6/54/54	0/0/8/8
4	HEM	N	500	2	-	0/6/54/54	0/0/8/8

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	500	HEM	C3C-CAC	-4.78	1.37	1.47
4	H	500	HEM	C3C-CAC	-4.77	1.37	1.47
4	N	500	HEM	C3C-CAC	-4.76	1.37	1.47
4	I	500	HEM	C3C-CAC	-4.76	1.37	1.47
4	L	500	HEM	C3C-CAC	-4.76	1.37	1.47

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1301	ATP	N3-C2-N1	-7.58	122.91	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1301	ATP	N3-C2-N1	-7.58	122.92	128.87
3	F	1301	ATP	N3-C2-N1	-7.56	122.93	128.87
3	C	1301	ATP	N3-C2-N1	-7.55	122.94	128.87
3	B	1301	ATP	N3-C2-N1	-7.54	122.95	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	ATP	1	0
3	B	1301	ATP	2	0
3	C	1301	ATP	1	0
3	D	1301	ATP	1	0
3	E	1301	ATP	1	0
3	F	1301	ATP	2	0
3	G	1301	ATP	1	0
4	H	500	HEM	7	0
4	I	500	HEM	10	0
4	J	500	HEM	7	0
4	K	500	HEM	6	0
4	L	500	HEM	6	0
4	M	500	HEM	8	0
4	N	500	HEM	7	0

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.