



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:07 PM BST

PDB ID : 3JBT
EMDB ID: : EMD-6480
Title : Atomic structure of the Apaf-1 apoptosome
Authors : Zhou, M.; Li, Y.; Hu, Q.; Bai, X.; Huang, W.; Yan, C.; Scheres, S.H.W.; Shi, Y.
Deposited on : 2015-10-15
Resolution : 3.80 Å(reported)
Based on PDB ID : 3J2T, 4RSZ

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>

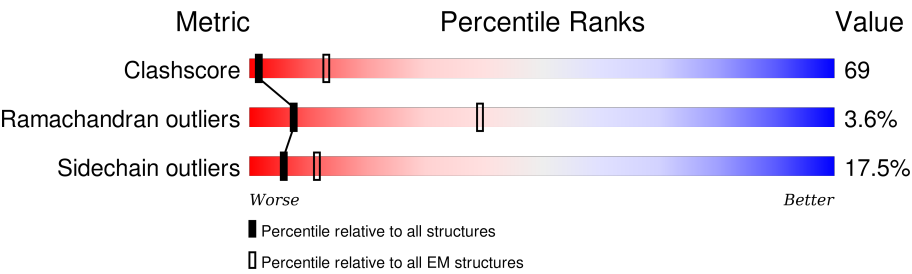
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 3.80 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	1260	32% 45% 13% • 9%
1	C	1260	31% 45% 13% • 9%
1	E	1260	32% 45% 13% • 9%
1	G	1260	32% 45% 13% • 9%
1	I	1260	32% 45% 13% • 9%
1	K	1260	32% 45% 13% • 9%
1	M	1260	32% 45% 13% • 9%
2	B	105	82% 15% ••
2	D	105	82% 15% ••

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Mol	Chain	Length	Quality of chain
2	F	105	<div><div></div><div>82%</div><div>15%</div><div>..</div></div>
2	H	105	<div><div></div><div>82%</div><div>15%</div><div>..</div></div>
2	J	105	<div><div></div><div>83%</div><div>14%</div><div>..</div></div>
2	L	105	<div><div></div><div>82%</div><div>15%</div><div>..</div></div>
2	N	105	<div><div></div><div>82%</div><div>16%</div><div>..</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 70252 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	C	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	G	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	I	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	K	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	M	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	LEU	-	EXPRESSION TAG	UNP O14727
A	1250	GLU	-	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
A	1258	HIS	-	EXPRESSION TAG	UNP O14727
A	1259	HIS	-	EXPRESSION TAG	UNP O14727
A	1260	HIS	-	EXPRESSION TAG	UNP O14727
C	1249	LEU	-	EXPRESSION TAG	UNP O14727
C	1250	GLU	-	EXPRESSION TAG	UNP O14727
C	1251	HIS	-	EXPRESSION TAG	UNP O14727
C	1252	HIS	-	EXPRESSION TAG	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	1258	HIS	-	EXPRESSION TAG	UNP O14727
C	1259	HIS	-	EXPRESSION TAG	UNP O14727
C	1260	HIS	-	EXPRESSION TAG	UNP O14727
E	1249	LEU	-	EXPRESSION TAG	UNP O14727
E	1250	GLU	-	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
E	1258	HIS	-	EXPRESSION TAG	UNP O14727
E	1259	HIS	-	EXPRESSION TAG	UNP O14727
E	1260	HIS	-	EXPRESSION TAG	UNP O14727
G	1249	LEU	-	EXPRESSION TAG	UNP O14727
G	1250	GLU	-	EXPRESSION TAG	UNP O14727
G	1251	HIS	-	EXPRESSION TAG	UNP O14727
G	1252	HIS	-	EXPRESSION TAG	UNP O14727
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
G	1258	HIS	-	EXPRESSION TAG	UNP O14727
G	1259	HIS	-	EXPRESSION TAG	UNP O14727
G	1260	HIS	-	EXPRESSION TAG	UNP O14727
I	1249	LEU	-	EXPRESSION TAG	UNP O14727
I	1250	GLU	-	EXPRESSION TAG	UNP O14727
I	1251	HIS	-	EXPRESSION TAG	UNP O14727
I	1252	HIS	-	EXPRESSION TAG	UNP O14727
I	1253	HIS	-	EXPRESSION TAG	UNP O14727
I	1254	HIS	-	EXPRESSION TAG	UNP O14727
I	1255	HIS	-	EXPRESSION TAG	UNP O14727
I	1256	HIS	-	EXPRESSION TAG	UNP O14727
I	1257	HIS	-	EXPRESSION TAG	UNP O14727
I	1258	HIS	-	EXPRESSION TAG	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1259	HIS	-	EXPRESSION TAG	UNP O14727
I	1260	HIS	-	EXPRESSION TAG	UNP O14727
K	1249	LEU	-	EXPRESSION TAG	UNP O14727
K	1250	GLU	-	EXPRESSION TAG	UNP O14727
K	1251	HIS	-	EXPRESSION TAG	UNP O14727
K	1252	HIS	-	EXPRESSION TAG	UNP O14727
K	1253	HIS	-	EXPRESSION TAG	UNP O14727
K	1254	HIS	-	EXPRESSION TAG	UNP O14727
K	1255	HIS	-	EXPRESSION TAG	UNP O14727
K	1256	HIS	-	EXPRESSION TAG	UNP O14727
K	1257	HIS	-	EXPRESSION TAG	UNP O14727
K	1258	HIS	-	EXPRESSION TAG	UNP O14727
K	1259	HIS	-	EXPRESSION TAG	UNP O14727
K	1260	HIS	-	EXPRESSION TAG	UNP O14727
M	1249	LEU	-	EXPRESSION TAG	UNP O14727
M	1250	GLU	-	EXPRESSION TAG	UNP O14727
M	1251	HIS	-	EXPRESSION TAG	UNP O14727
M	1252	HIS	-	EXPRESSION TAG	UNP O14727
M	1253	HIS	-	EXPRESSION TAG	UNP O14727
M	1254	HIS	-	EXPRESSION TAG	UNP O14727
M	1255	HIS	-	EXPRESSION TAG	UNP O14727
M	1256	HIS	-	EXPRESSION TAG	UNP O14727
M	1257	HIS	-	EXPRESSION TAG	UNP O14727
M	1258	HIS	-	EXPRESSION TAG	UNP O14727
M	1259	HIS	-	EXPRESSION TAG	UNP O14727
M	1260	HIS	-	EXPRESSION TAG	UNP O14727

- Molecule 2 is a protein called Cytochrome c.

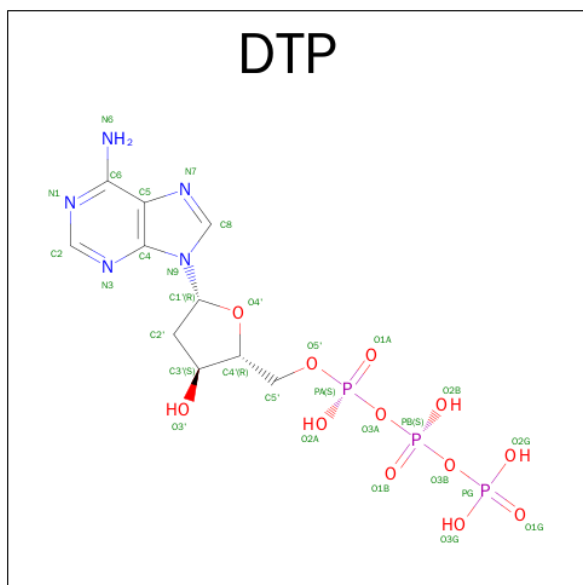
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	D	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	F	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	H	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	J	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	L	104	Total 823	C 524	N 144	O 151	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	104	Total	C	N	O	S	0	0
			823	524	144	151	4		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	G	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	I	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	K	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	M	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

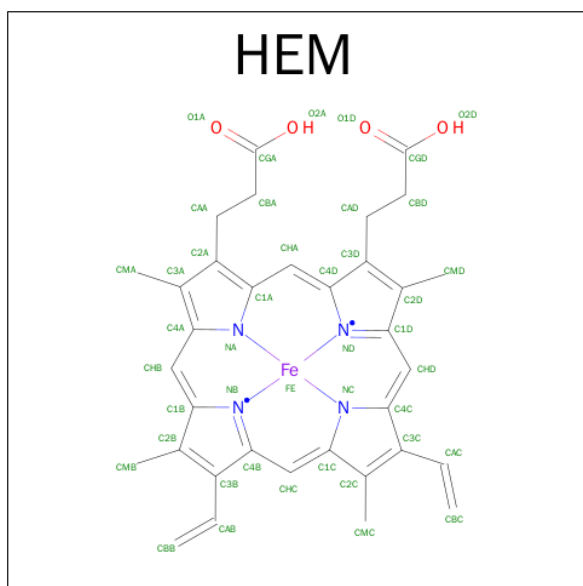
Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
4	K	1	Total Mg 1 1	0
4	E	1	Total Mg 1 1	0
4	I	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	A	1	Total Mg 1 1	0
4	M	1	Total Mg 1 1	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

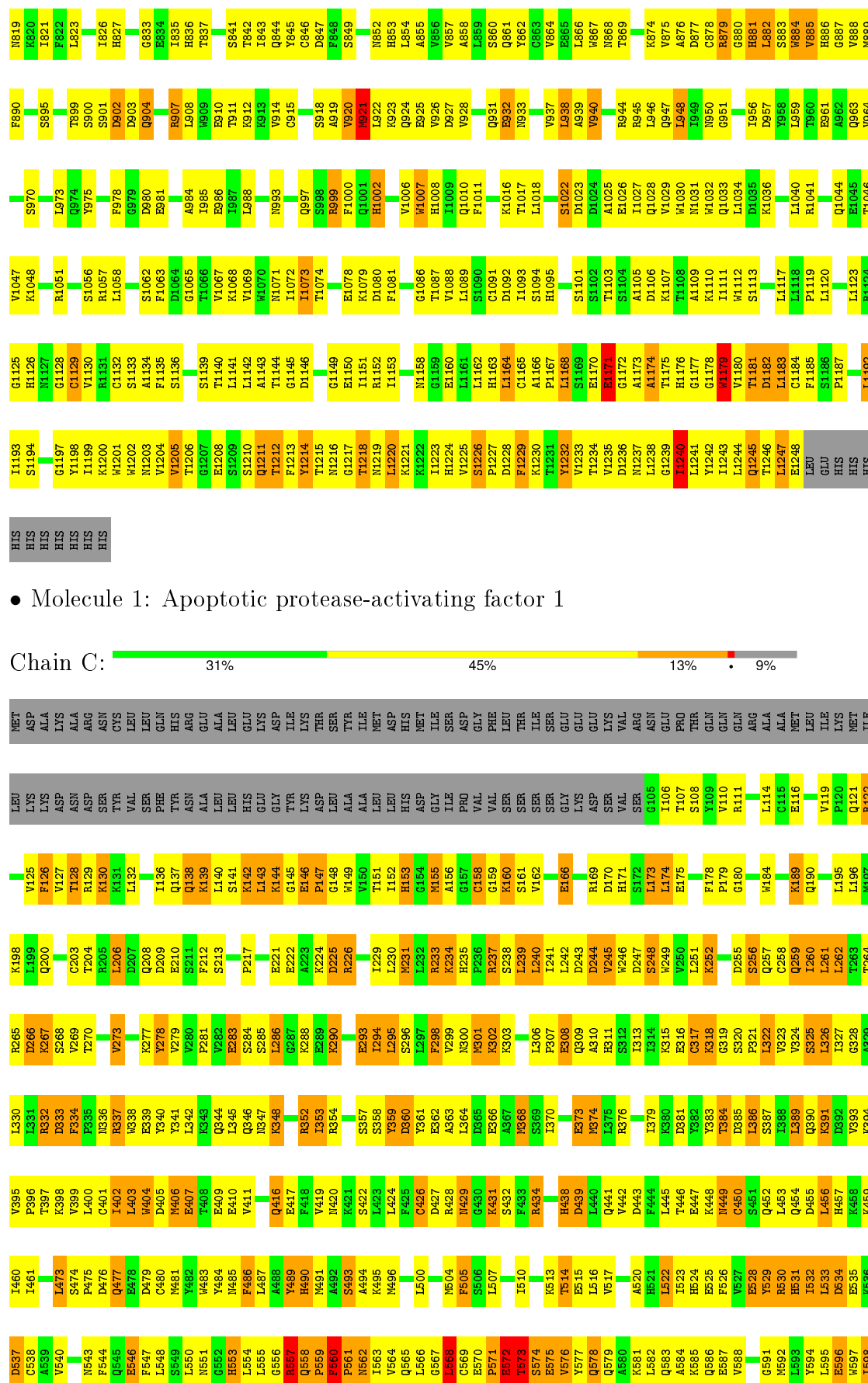


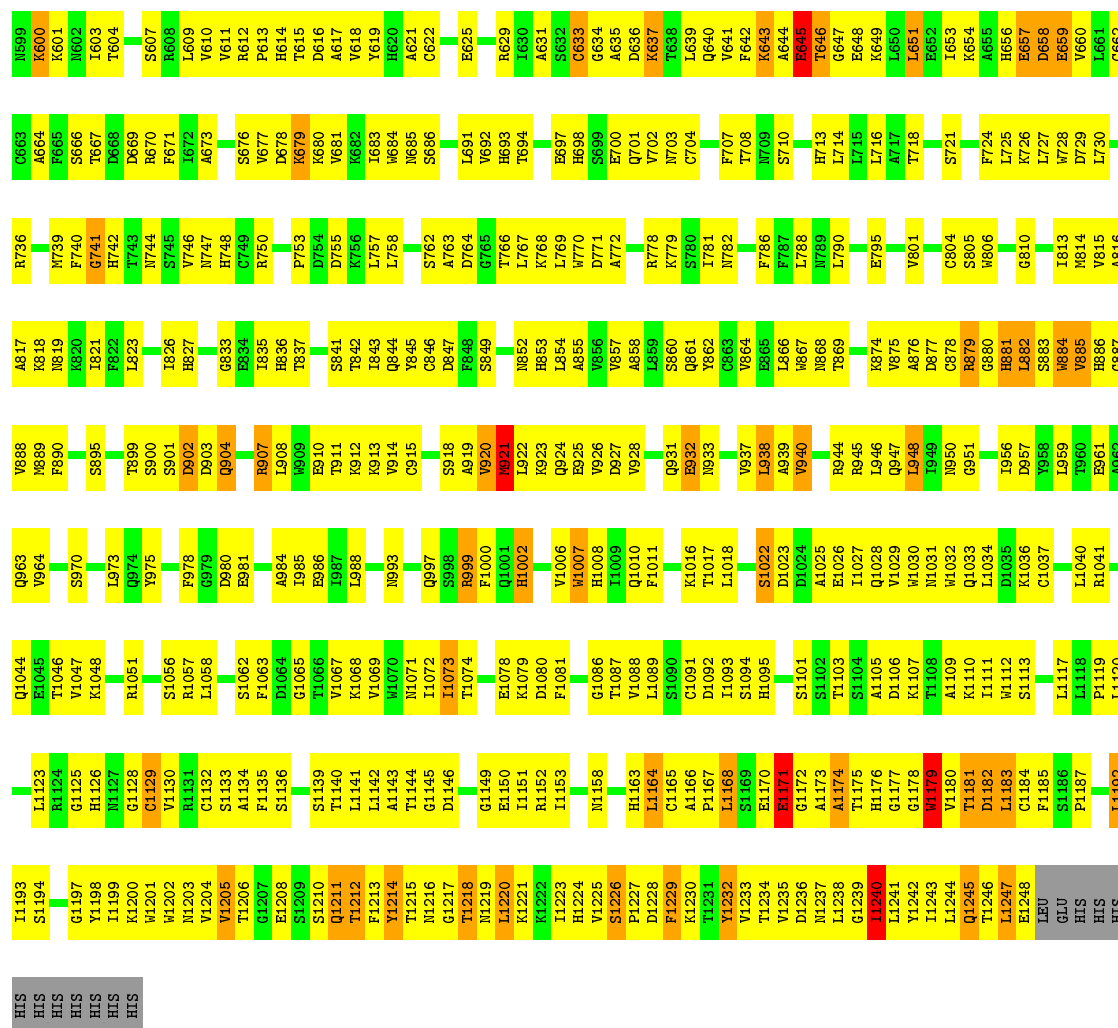
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	H	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	J	1	Total 43	C 34	Fe 1	N 4	O 4	0

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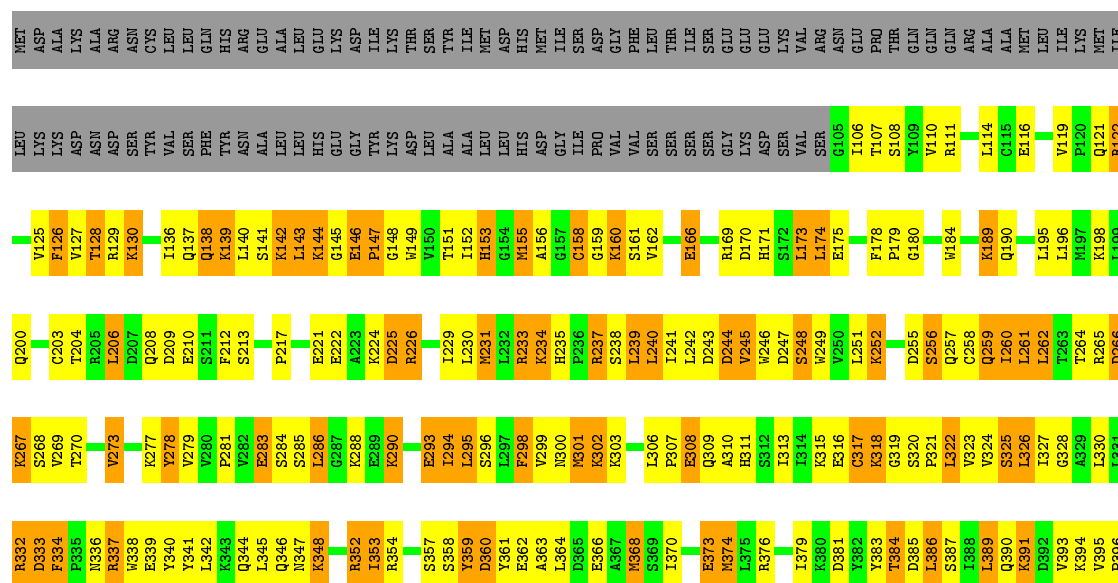
Mol	Chain	Residues	Atoms					AltConf
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

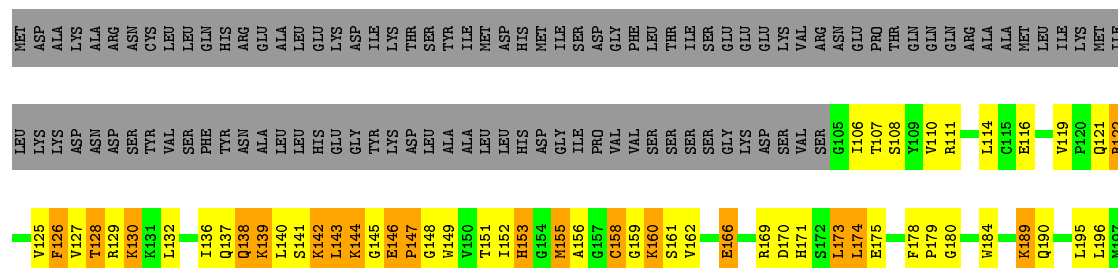




• Molecule 1: Apoptotic protease-activating factor 1

Chain E: 32% 45% 13% 9%



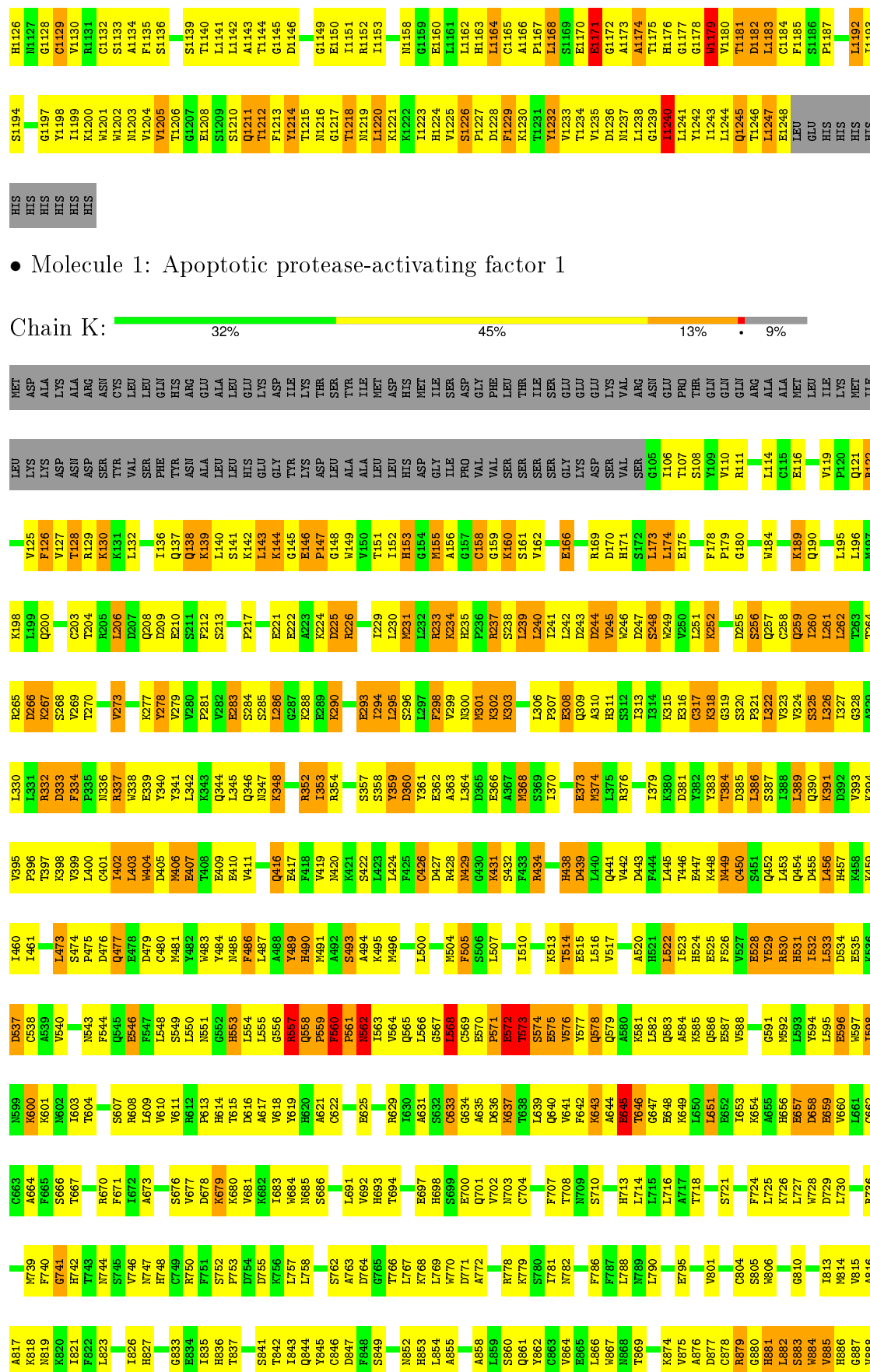


HIS	L1182	L1123	E1045	Q963	V888	A817	M739	A664	R600	C538	L460	V395	L330	R265	K198
HIS	L1193	G1124	T1046	V964	M889	K818	M739	F665	R601	A539	L461	P396	L331	D266	L199
HIS	S1194	G1125	K1048	S970	F890	M819	F740	S666	R602	V540	L473	K397	R332	K267	Q200
HIS						R320	G741	T667	T604	N543	D476	L400	F334	V269	C203
HIS						R821	H742	D668	S607	F544	Q477	C401	P336	T270	T204
HIS						F822	H743	R670	R603	Q545	Q477	L402	R337	V273	R205
HIS						L823	S745	F671	L609	E546	D476	L403	R338		L206
HIS						T826	V746	I672	V610	F547	D479	L404	F339	K277	Q208
HIS						R827	H747	A673	V611	L548	C480	W405	F340	D209	D209
HIS						G833	G749	S676	R612	S549	Y481	M406	Y341	V279	E210
HIS						R834	G750	V677	R613	L550	Y483	M407	L342	V280	S211
HIS						I835	F751	D678	H614	G552	Y484	T408	K343	P281	F212
HIS						R836	S752	K679	T615	R553	M485	E409	Q344	V282	F213
HIS						T837	F753	K680	D616	R554	M486	E410	L345	E282	S213
HIS						S841	D754	V681	A621	L555	L487	Q346	Q346	S284	
HIS						T842	G755	K682	V618	G556	L488	N347	L347	S285	
HIS						I843	K756	I683	V619	R557	Y489	Q416	K348	L286	E221
HIS						Q844	L757	V684	H620	Q558	H490	E417	R352	G287	A222
HIS						C846	L758	S686	C622	P559	M491	V419	I353	E289	K224
HIS						D847	S762			P561	S493	M420	R354	K290	D225
HIS						F848	A763	L691	E625	N562	A494	K421		L286	R226
HIS						S849	D764	H693	R629	I563	K495	S422	S357	E293	T229
HIS							G765	T694	R630	V564	M496	L453	S358	I294	L230
HIS						N852	T766		R631	Q565	L500	F425	P359	L295	W231
HIS						R853	L767		A631	L566		F426	D360	S296	
HIS						L854	K768		G533	C567		D427	F362	L297	L232
HIS						A855	V770		G534	C569		R428	A363	V299	K234
HIS						V856	D771		A635	E570		M429	L364	I300	H235
HIS						R857	A772		D636	E571		Q301	D365	K301	F236
HIS						A858	A772		V702	E572		K432	A367	K302	R237
HIS						S860	R778		T638	E573		S431	E366	S238	
HIS						Q861	K779		L639	S574		F433	K368	L239	L240
HIS						V862	S780		Q640	E575		R434	I370	L241	
HIS						C863	I781		V641	V576		H438	E373	P307	T241
HIS						V864	M782		F642	Y577		D439	Q309	Q309	D243
HIS						R865	M786		R643	Q578		L440	L375	H311	V245
HIS						L866	F787		A644	A579		Q441	R376	R312	D246
HIS						W867	L788		T646	K581		V442	I313	I313	D247
HIS						T869	M789		G647	L582		D443	I314	I314	S248
HIS						K874	E795		R649	Q583		F444	I379	I379	W249
HIS						V875	M801		L651	A584		T446	D381	E316	V250
HIS						A876	V801		L652	Q586		E447	F382	C317	L251
HIS						D877	S721		P653	E587		K448	Y383	K318	K252
HIS						C878			L654	V588		M449	T384	G319	
HIS						R879	C804		R655			C450	D385	S320	D255
HIS						G880	S905		A656	G591		S451	L386	P321	S256
HIS						R881	M806		T657	M592		L445	S387	L322	Q257
HIS						L882	T610		D658	L593		L453	F388	V323	C258
HIS						S883	G810		L727	Y594		Q454	F389	V324	Q259
HIS						W884			V660	L595		D455	Q390	S325	L260
HIS						R886	T613		L661	E596		L456	K391	L326	L261
HIS						G887	V814		C662	W597		H457	D392	I327	L262
HIS							V815		L662	K598		K458	V393	G328	T263
HIS							A816		C663	M599		K459	K394	A329	T264

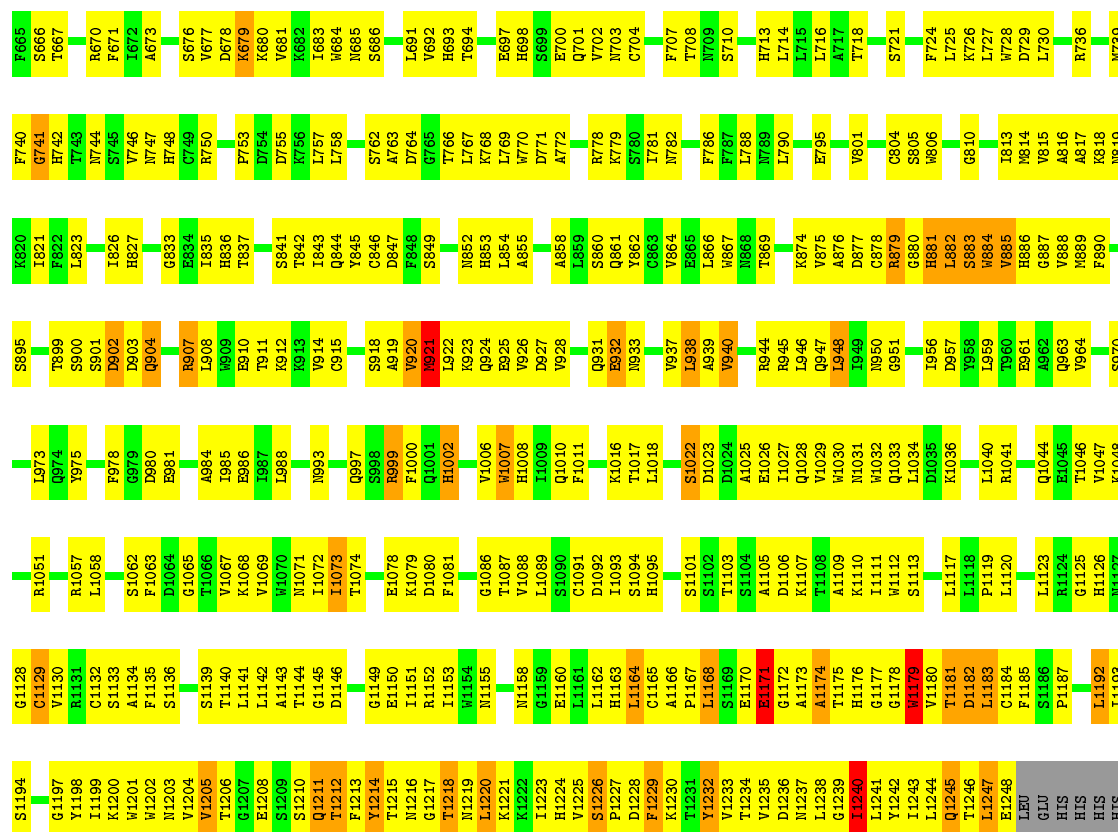
- Molecule 1: Apoptotic protease-activating factor 1

Category	Percentage
Category 1 (Green)	32%
Category 2 (Yellow)	45%
Category 3 (Orange)	13%
Category 4 (Grey)	9%



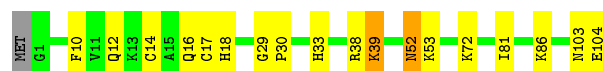


- Molecule 1: Apoptotic protease-activating factor 1



- Molecule 2: Cytochrome c

Chain B: 82% 15% ..



- Molecule 2: Cytochrome c

Chain D: 82% 15% ..




- Molecule 2: Cytochrome c

Chain F: 82% 15% ..




- Molecule 2: Cytochrome c

Chain H:  82% 15% ..




- Molecule 2: Cytochrome c

Chain J:  83% 14% ..




- Molecule 2: Cytochrome c

Chain L:  82% 15% ..



- Molecule 2: Cytochrome c

Chain N:  82% 16% ..



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	134919	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	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: HEM, MG, DTP

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	0.30	0/9337	0.51	2/12636 (0.0%)
1	C	0.30	0/9337	0.51	2/12636 (0.0%)
1	E	0.30	0/9337	0.51	2/12636 (0.0%)
1	G	0.30	0/9337	0.51	2/12636 (0.0%)
1	I	0.30	0/9337	0.51	2/12636 (0.0%)
1	K	0.30	0/9337	0.51	2/12636 (0.0%)
1	M	0.30	0/9337	0.51	2/12636 (0.0%)
2	B	0.65	0/839	0.73	0/1118
2	D	0.65	0/839	0.73	0/1118
2	F	0.65	0/839	0.73	0/1118
2	H	0.65	0/839	0.73	0/1118
2	J	0.65	0/839	0.73	0/1118
2	L	0.65	0/839	0.73	0/1118
2	N	0.65	0/839	0.73	0/1118
All	All	0.34	0/71232	0.53	14/96278 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	880	GLY	N-CA-C	5.73	127.43	113.10
1	I	880	GLY	N-CA-C	5.73	127.43	113.10
1	K	880	GLY	N-CA-C	5.73	127.43	113.10
1	M	880	GLY	N-CA-C	5.73	127.42	113.10
1	E	880	GLY	N-CA-C	5.72	127.41	113.10

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	9139	0	9005	1372	0
1	C	9139	0	9005	1371	0
1	E	9139	0	9005	1360	0
1	G	9139	0	9005	1382	0
1	I	9139	0	9005	1358	0
1	K	9139	0	9005	1357	0
1	M	9139	0	9005	1366	0
2	B	823	0	849	31	0
2	D	823	0	849	33	0
2	F	823	0	849	30	0
2	H	823	0	849	34	0
2	J	823	0	849	32	0
2	L	823	0	849	33	0
2	N	823	0	849	31	0
3	A	30	0	12	6	0
3	C	30	0	12	6	0
3	E	30	0	12	6	0
3	G	30	0	12	6	0
3	I	30	0	12	7	0
3	K	30	0	12	6	0
3	M	30	0	12	6	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
5	B	43	0	30	15	0
5	D	43	0	30	16	0
5	F	43	0	30	14	0
5	H	43	0	30	16	0
5	J	43	0	30	15	0
5	L	43	0	30	15	0
5	N	43	0	30	13	0
All	All	70252	0	69272	9596	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 69.

The worst 5 of 9596 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:544:PHE:CE1	1:E:576:VAL:HG13	1.28	1.68
1:G:544:PHE:CE1	1:G:576:VAL:HG13	1.28	1.67
1:C:544:PHE:CE1	1:C:576:VAL:HG13	1.28	1.65
1:C:862:TYR:CD1	1:C:885:VAL:HG12	1.26	1.64
1:A:544:PHE:CE1	1:A:576:VAL:HG13	1.28	1.64

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	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	C	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	E	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	G	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	I	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	K	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	4	38
1	M	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	4	38
2	B	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	D	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	F	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	H	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	N	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
All	All	8708/9555 (91%)	7693 (88%)	698 (8%)	317 (4%)	7	41

5 of 317 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	557	ARG
1	A	560	PHE
1	A	562	ASN
1	A	645	GLU

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	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	C	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	E	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	G	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	I	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	K	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	M	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
2	B	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	D	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	F	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	H	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	J	86/87 (99%)	81 (94%)	5 (6%)	25	66
2	L	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	N	86/87 (99%)	80 (93%)	6 (7%)	19	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7791/8526 (91%)	6427 (82%)	1364 (18%)	6 17

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	243	ASP
1	G	1192	LEU
1	M	405	ASP
1	G	290	LYS
1	G	473	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	259	GLN
1	G	1245	GLN
1	M	490	HIS
1	G	416	GLN
1	G	583	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 for Mogul analysis.

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	DTP	A	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	B	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.64	2 (12%)
3	DTP	C	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	D	201	2	24,50,50	0.85	1 (4%)	16,82,82	1.64	2 (12%)
3	DTP	E	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	F	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.64	2 (12%)
3	DTP	G	1301	4	25,32,32	0.93	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	H	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.65	2 (12%)
3	DTP	I	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	J	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.65	2 (12%)
3	DTP	K	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	L	201	2	24,50,50	0.85	1 (4%)	16,82,82	1.65	2 (12%)
3	DTP	M	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	N	201	2	24,50,50	0.84	1 (4%)	16,82,82	1.65	2 (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
3	DTP	A	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	B	201	2	-	0/6/54/54	0/0/8/8
3	DTP	C	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	D	201	2	-	0/6/54/54	0/0/8/8
3	DTP	E	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	F	201	2	-	0/6/54/54	0/0/8/8
3	DTP	G	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	H	201	2	-	0/6/54/54	0/0/8/8
3	DTP	I	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	J	201	2	-	0/6/54/54	0/0/8/8
3	DTP	K	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	L	201	2	-	0/6/54/54	0/0/8/8
3	DTP	M	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	N	201	2	-	0/6/54/54	0/0/8/8

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	HEM	C3B-C2B	-2.82	1.36	1.40
5	J	201	HEM	C3B-C2B	-2.79	1.36	1.40
5	D	201	HEM	C3B-C2B	-2.79	1.36	1.40
5	H	201	HEM	C3B-C2B	-2.77	1.36	1.40
5	F	201	HEM	C3B-C2B	-2.76	1.36	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	DTP	N3-C2-N1	-6.59	123.70	128.87
3	A	1301	DTP	N3-C2-N1	-6.58	123.71	128.87
3	G	1301	DTP	N3-C2-N1	-6.57	123.71	128.87
3	E	1301	DTP	N3-C2-N1	-6.56	123.72	128.87
3	M	1301	DTP	N3-C2-N1	-6.56	123.72	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	DTP	6	0
5	B	201	HEM	15	0
3	C	1301	DTP	6	0
5	D	201	HEM	16	0
3	E	1301	DTP	6	0
5	F	201	HEM	14	0
3	G	1301	DTP	6	0
5	H	201	HEM	16	0
3	I	1301	DTP	7	0
5	J	201	HEM	15	0
3	K	1301	DTP	6	0
5	L	201	HEM	15	0
3	M	1301	DTP	6	0
5	N	201	HEM	13	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.