



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:17 PM BST

PDB ID : 5ANY
EMDB ID: : EMD-3144
Title : Electron cryo-microscopy of chikungunya virus in complex with neutralizing antibody Fab CHK265
Authors : Fox, J.M.; Long, F.; Edeling, M.A.; Lin, H.; Duijl-Richter, M.; Fong, R.H.; Kahle, K.M.; Smit, J.M.; Jin, J.; Simmons, G.; Doranz, B.J.; Crowe, J.E.; Fremont, D.H.; Rossmann, M.G.; Diamond, M.S.
Deposited on : 2015-09-08
Resolution : 16.90 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 : unknown
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

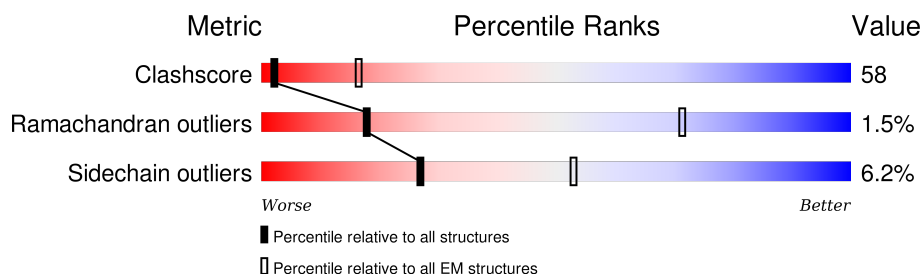
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 16.90 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	451	75% 11% • 13%
1	C	451	76% 10% • 13%
1	E	451	76% 10% • 13%
1	G	451	78% 8% • 13%
2	B	354	66% 26% • • 5%
2	D	354	65% 27% • • 5%
2	F	354	65% 27% • • 5%
2	H	354	66% 26% • • 5%
3	I	218	60% 36% • •

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Mol	Chain	Length	Quality of chain
3	J	218	<div><div></div><div>58%37%<div><div></div><div></div></div></div></div>
3	K	218	<div><div></div><div>60%36%<div><div></div><div></div></div></div></div>
3	L	218	<div><div></div><div>59%37%<div><div></div><div></div></div></div></div>
4	M	214	<div><div></div><div>40%45%13%<div><div></div><div></div></div></div></div>
4	N	214	<div><div></div><div>38%47%13%<div><div></div><div></div></div></div></div>
4	O	214	<div><div></div><div>40%46%12%<div><div></div><div></div></div></div></div>
4	P	214	<div><div></div><div>40%46%12%<div><div></div><div></div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35620 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 E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		
1	C	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		
1	E	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		
1	G	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	414	PRO	-	EXPRESSION TAG	UNP Q1H8W5
A	415	PHE	-	EXPRESSION TAG	UNP Q1H8W5
A	416	GLU	-	EXPRESSION TAG	UNP Q1H8W5
A	417	ASP	-	EXPRESSION TAG	UNP Q1H8W5
A	418	ASP	-	EXPRESSION TAG	UNP Q1H8W5
A	419	ASP	-	EXPRESSION TAG	UNP Q1H8W5
A	420	ASP	-	EXPRESSION TAG	UNP Q1H8W5
A	421	LYS	-	EXPRESSION TAG	UNP Q1H8W5
A	422	ALA	-	EXPRESSION TAG	UNP Q1H8W5
A	423	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	424	TRP	-	EXPRESSION TAG	UNP Q1H8W5
A	425	SER	-	EXPRESSION TAG	UNP Q1H8W5
A	426	HIS	-	EXPRESSION TAG	UNP Q1H8W5
A	427	PRO	-	EXPRESSION TAG	UNP Q1H8W5
A	428	GLN	-	EXPRESSION TAG	UNP Q1H8W5
A	429	PHE	-	EXPRESSION TAG	UNP Q1H8W5
A	430	GLU	-	EXPRESSION TAG	UNP Q1H8W5
A	431	LYS	-	EXPRESSION TAG	UNP Q1H8W5
A	432	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	433	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	434	GLY	-	EXPRESSION TAG	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	435	SER	-	EXPRESSION TAG	UNP Q1H8W5
A	436	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	437	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	438	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	439	SER	-	EXPRESSION TAG	UNP Q1H8W5
A	440	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	441	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	442	GLY	-	EXPRESSION TAG	UNP Q1H8W5
A	443	SER	-	EXPRESSION TAG	UNP Q1H8W5
A	444	TRP	-	EXPRESSION TAG	UNP Q1H8W5
A	445	SER	-	EXPRESSION TAG	UNP Q1H8W5
A	446	HIS	-	EXPRESSION TAG	UNP Q1H8W5
A	447	PRO	-	EXPRESSION TAG	UNP Q1H8W5
A	448	GLN	-	EXPRESSION TAG	UNP Q1H8W5
A	449	PHE	-	EXPRESSION TAG	UNP Q1H8W5
A	450	GLU	-	EXPRESSION TAG	UNP Q1H8W5
A	451	LYS	-	EXPRESSION TAG	UNP Q1H8W5
C	413	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	414	PRO	-	EXPRESSION TAG	UNP Q1H8W5
C	415	PHE	-	EXPRESSION TAG	UNP Q1H8W5
C	416	GLU	-	EXPRESSION TAG	UNP Q1H8W5
C	417	ASP	-	EXPRESSION TAG	UNP Q1H8W5
C	418	ASP	-	EXPRESSION TAG	UNP Q1H8W5
C	419	ASP	-	EXPRESSION TAG	UNP Q1H8W5
C	420	ASP	-	EXPRESSION TAG	UNP Q1H8W5
C	421	LYS	-	EXPRESSION TAG	UNP Q1H8W5
C	422	ALA	-	EXPRESSION TAG	UNP Q1H8W5
C	423	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	424	TRP	-	EXPRESSION TAG	UNP Q1H8W5
C	425	SER	-	EXPRESSION TAG	UNP Q1H8W5
C	426	HIS	-	EXPRESSION TAG	UNP Q1H8W5
C	427	PRO	-	EXPRESSION TAG	UNP Q1H8W5
C	428	GLN	-	EXPRESSION TAG	UNP Q1H8W5
C	429	PHE	-	EXPRESSION TAG	UNP Q1H8W5
C	430	GLU	-	EXPRESSION TAG	UNP Q1H8W5
C	431	LYS	-	EXPRESSION TAG	UNP Q1H8W5
C	432	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	433	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	434	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	435	SER	-	EXPRESSION TAG	UNP Q1H8W5
C	436	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	437	GLY	-	EXPRESSION TAG	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	438	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	439	SER	-	EXPRESSION TAG	UNP Q1H8W5
C	440	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	441	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	442	GLY	-	EXPRESSION TAG	UNP Q1H8W5
C	443	SER	-	EXPRESSION TAG	UNP Q1H8W5
C	444	TRP	-	EXPRESSION TAG	UNP Q1H8W5
C	445	SER	-	EXPRESSION TAG	UNP Q1H8W5
C	446	HIS	-	EXPRESSION TAG	UNP Q1H8W5
C	447	PRO	-	EXPRESSION TAG	UNP Q1H8W5
C	448	GLN	-	EXPRESSION TAG	UNP Q1H8W5
C	449	PHE	-	EXPRESSION TAG	UNP Q1H8W5
C	450	GLU	-	EXPRESSION TAG	UNP Q1H8W5
C	451	LYS	-	EXPRESSION TAG	UNP Q1H8W5
E	413	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	414	PRO	-	EXPRESSION TAG	UNP Q1H8W5
E	415	PHE	-	EXPRESSION TAG	UNP Q1H8W5
E	416	GLU	-	EXPRESSION TAG	UNP Q1H8W5
E	417	ASP	-	EXPRESSION TAG	UNP Q1H8W5
E	418	ASP	-	EXPRESSION TAG	UNP Q1H8W5
E	419	ASP	-	EXPRESSION TAG	UNP Q1H8W5
E	420	ASP	-	EXPRESSION TAG	UNP Q1H8W5
E	421	LYS	-	EXPRESSION TAG	UNP Q1H8W5
E	422	ALA	-	EXPRESSION TAG	UNP Q1H8W5
E	423	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	424	TRP	-	EXPRESSION TAG	UNP Q1H8W5
E	425	SER	-	EXPRESSION TAG	UNP Q1H8W5
E	426	HIS	-	EXPRESSION TAG	UNP Q1H8W5
E	427	PRO	-	EXPRESSION TAG	UNP Q1H8W5
E	428	GLN	-	EXPRESSION TAG	UNP Q1H8W5
E	429	PHE	-	EXPRESSION TAG	UNP Q1H8W5
E	430	GLU	-	EXPRESSION TAG	UNP Q1H8W5
E	431	LYS	-	EXPRESSION TAG	UNP Q1H8W5
E	432	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	433	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	434	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	435	SER	-	EXPRESSION TAG	UNP Q1H8W5
E	436	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	437	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	438	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	439	SER	-	EXPRESSION TAG	UNP Q1H8W5
E	440	GLY	-	EXPRESSION TAG	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	441	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	442	GLY	-	EXPRESSION TAG	UNP Q1H8W5
E	443	SER	-	EXPRESSION TAG	UNP Q1H8W5
E	444	TRP	-	EXPRESSION TAG	UNP Q1H8W5
E	445	SER	-	EXPRESSION TAG	UNP Q1H8W5
E	446	HIS	-	EXPRESSION TAG	UNP Q1H8W5
E	447	PRO	-	EXPRESSION TAG	UNP Q1H8W5
E	448	GLN	-	EXPRESSION TAG	UNP Q1H8W5
E	449	PHE	-	EXPRESSION TAG	UNP Q1H8W5
E	450	GLU	-	EXPRESSION TAG	UNP Q1H8W5
E	451	LYS	-	EXPRESSION TAG	UNP Q1H8W5
G	413	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	414	PRO	-	EXPRESSION TAG	UNP Q1H8W5
G	415	PHE	-	EXPRESSION TAG	UNP Q1H8W5
G	416	GLU	-	EXPRESSION TAG	UNP Q1H8W5
G	417	ASP	-	EXPRESSION TAG	UNP Q1H8W5
G	418	ASP	-	EXPRESSION TAG	UNP Q1H8W5
G	419	ASP	-	EXPRESSION TAG	UNP Q1H8W5
G	420	ASP	-	EXPRESSION TAG	UNP Q1H8W5
G	421	LYS	-	EXPRESSION TAG	UNP Q1H8W5
G	422	ALA	-	EXPRESSION TAG	UNP Q1H8W5
G	423	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	424	TRP	-	EXPRESSION TAG	UNP Q1H8W5
G	425	SER	-	EXPRESSION TAG	UNP Q1H8W5
G	426	HIS	-	EXPRESSION TAG	UNP Q1H8W5
G	427	PRO	-	EXPRESSION TAG	UNP Q1H8W5
G	428	GLN	-	EXPRESSION TAG	UNP Q1H8W5
G	429	PHE	-	EXPRESSION TAG	UNP Q1H8W5
G	430	GLU	-	EXPRESSION TAG	UNP Q1H8W5
G	431	LYS	-	EXPRESSION TAG	UNP Q1H8W5
G	432	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	433	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	434	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	435	SER	-	EXPRESSION TAG	UNP Q1H8W5
G	436	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	437	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	438	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	439	SER	-	EXPRESSION TAG	UNP Q1H8W5
G	440	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	441	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	442	GLY	-	EXPRESSION TAG	UNP Q1H8W5
G	443	SER	-	EXPRESSION TAG	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	444	TRP	-	EXPRESSION TAG	UNP Q1H8W5
G	445	SER	-	EXPRESSION TAG	UNP Q1H8W5
G	446	HIS	-	EXPRESSION TAG	UNP Q1H8W5
G	447	PRO	-	EXPRESSION TAG	UNP Q1H8W5
G	448	GLN	-	EXPRESSION TAG	UNP Q1H8W5
G	449	PHE	-	EXPRESSION TAG	UNP Q1H8W5
G	450	GLU	-	EXPRESSION TAG	UNP Q1H8W5
G	451	LYS	-	EXPRESSION TAG	UNP Q1H8W5

- Molecule 2 is a protein called E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		
2	D	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		
2	F	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		
2	H	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		

- Molecule 3 is a protein called FAB CHK265.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	J	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	K	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	L	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		

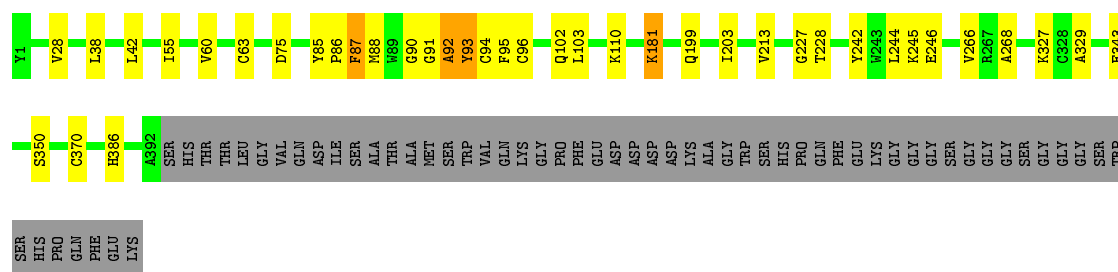
- Molecule 4 is a protein called FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	211	Total	C	N	O	S	0	0
			1598	999	270	322	7		
4	N	211	Total	C	N	O	S	0	0
			1598	999	270	322	7		
4	O	211	Total	C	N	O	S	0	0
			1598	999	270	322	7		

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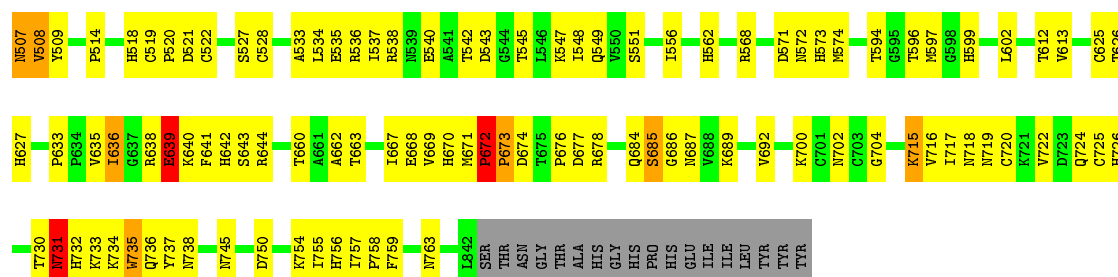
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	211	1598	999	270	322	7	0	0



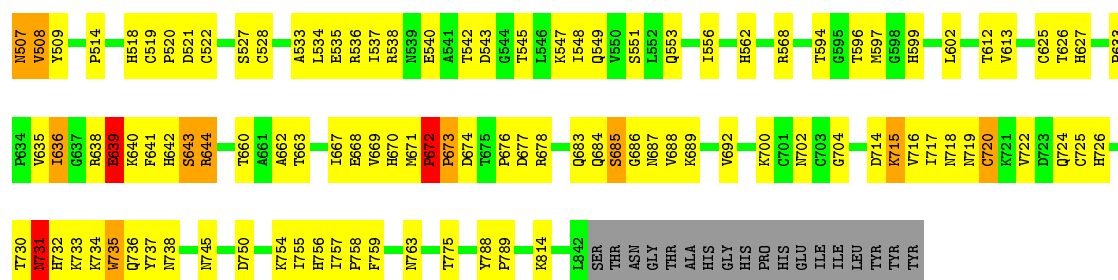
- Molecule 2: E2

Chain B: 66% 26% • • 5%



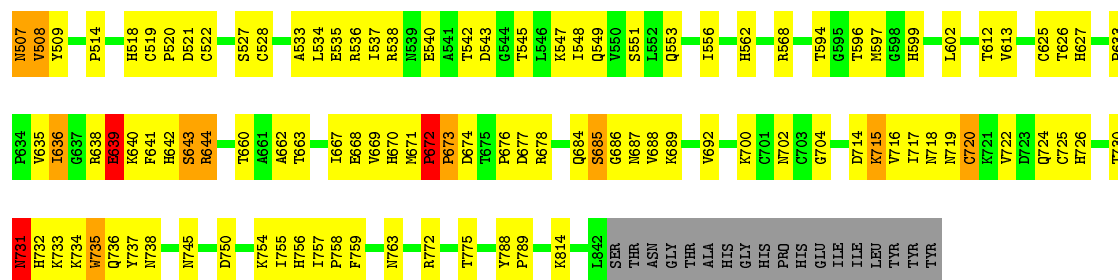
- Molecule 2: E2

Chain D: 65% 27% • • 5%



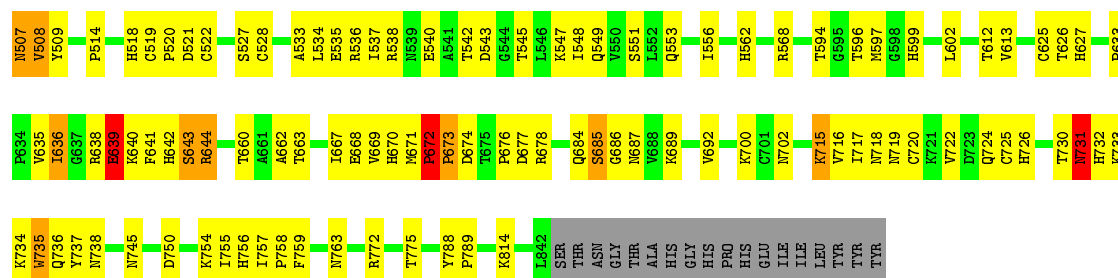
- Molecule 2: E2

Chain F: 65% 27% • • 5%



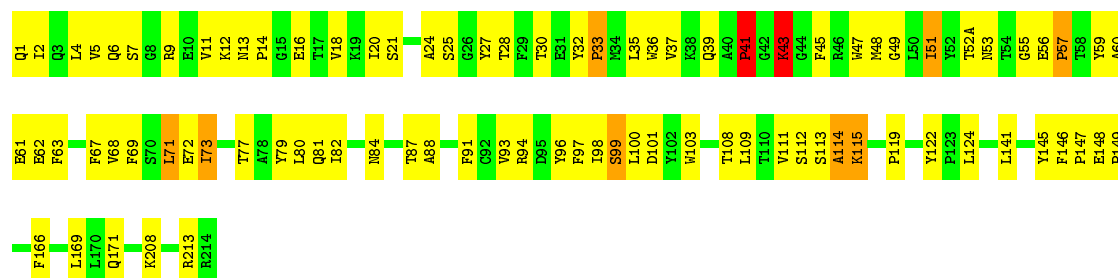
- Molecule 2: E2

Chain H: 66% 26% • • 5%



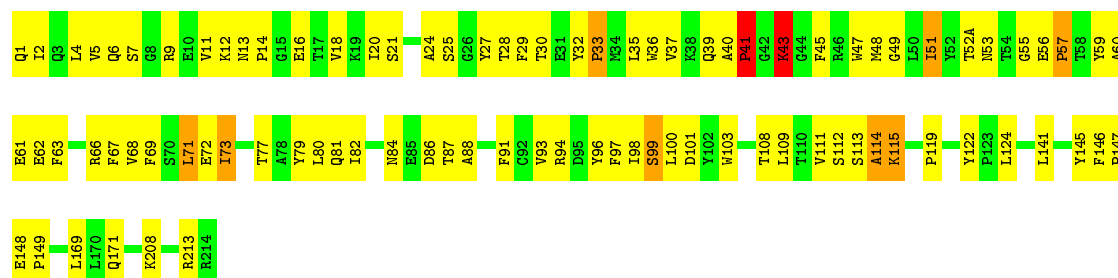
• Molecule 3: FAB CHK265

Chain I: 60% 36%



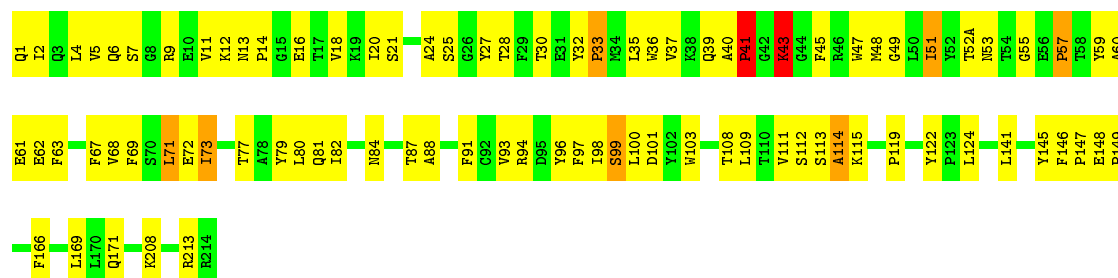
• Molecule 3: FAB CHK265

Chain J: 58% 37%



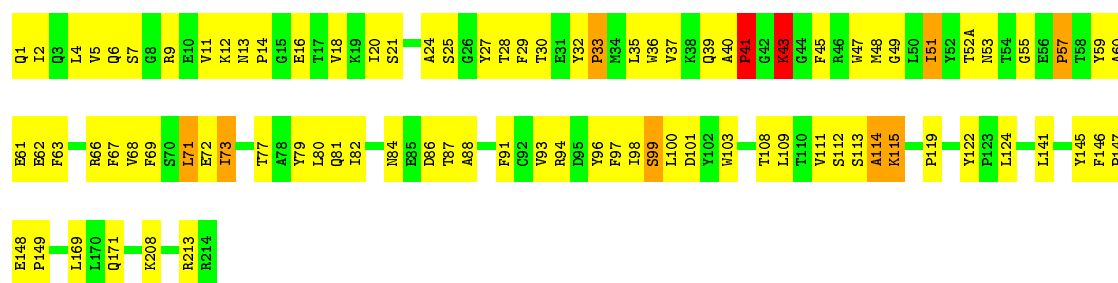
• Molecule 3: FAB CHK265

Chain K: 60% 36%



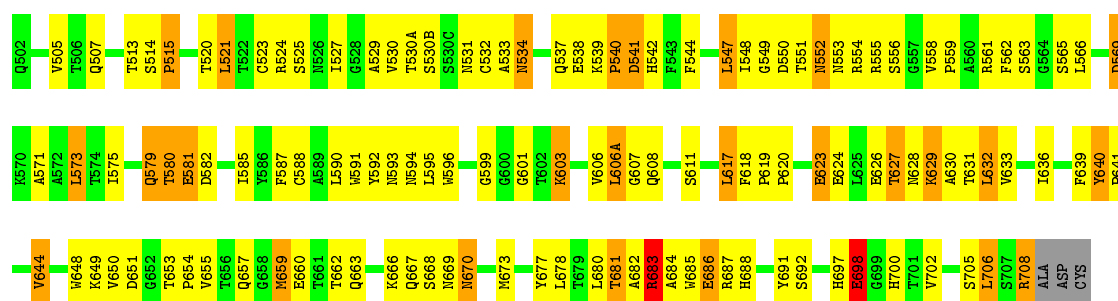
• Molecule 3: FAB CHK265

Chain L: 59% 37%



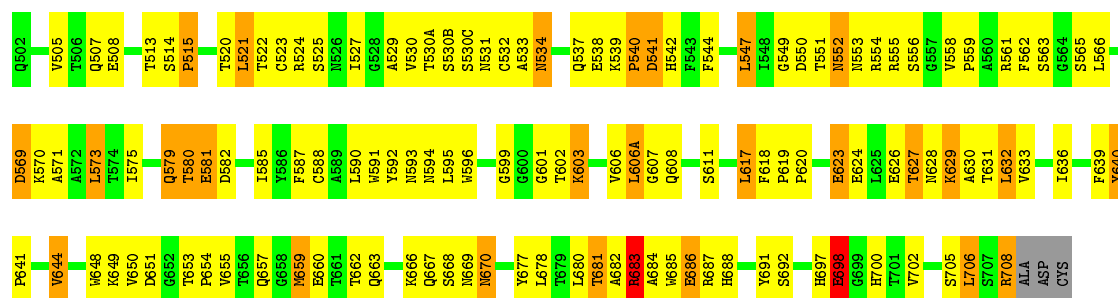
- Molecule 4: FAB

Chain M: 40% 45% 13% ..



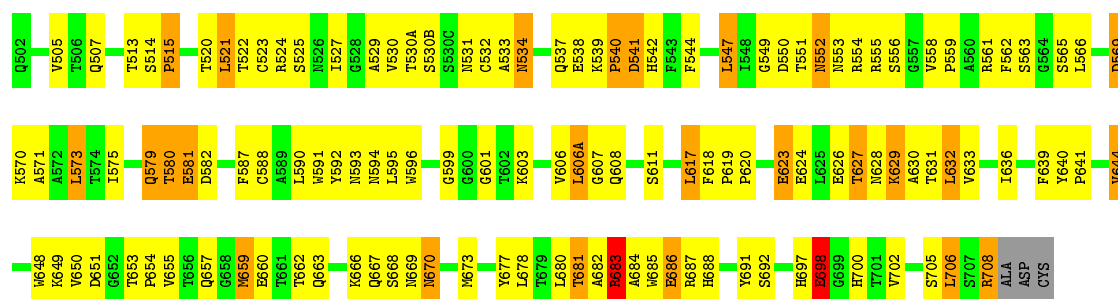
- Molecule 4: FAB

Chain N: 38% 47% 13% ..

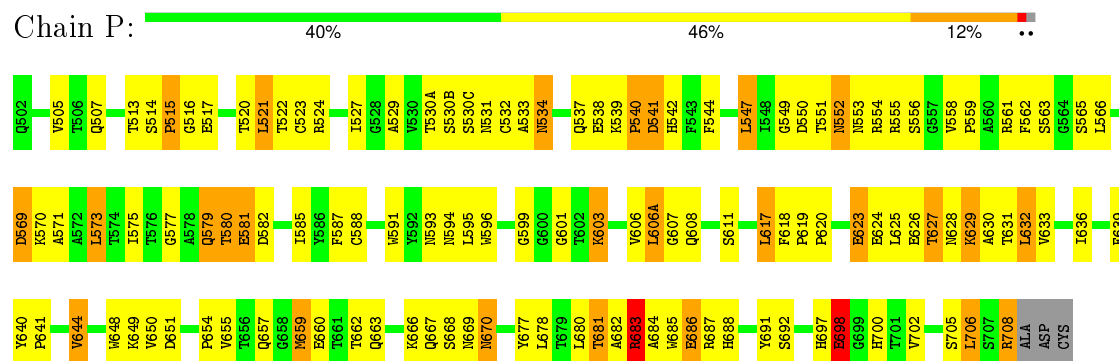


- Molecule 4: FAB

Chain O: 40% 46% 12% ..



- Molecule 4: FAB



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4K X 4K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.36	0/3063	0.54	0/4179
1	C	0.36	0/3063	0.54	0/4179
1	E	0.36	0/3063	0.54	0/4179
1	G	0.36	0/3063	0.54	0/4179
2	B	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
2	D	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
2	F	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
2	H	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
3	I	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	J	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	K	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	L	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
4	M	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
4	N	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
4	O	0.91	3/1634 (0.2%)	1.44	11/2232 (0.5%)
4	P	0.91	3/1634 (0.2%)	1.44	11/2232 (0.5%)
All	All	0.65	36/36528 (0.1%)	0.92	90/49820 (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
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
All	All	0	8

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	731	ASN	C-N	-26.23	0.73	1.34
2	H	731	ASN	C-N	-26.22	0.73	1.34
2	F	731	ASN	C-N	-26.19	0.73	1.34
2	B	731	ASN	C-N	-26.19	0.73	1.34
3	L	57	PRO	N-CD	17.40	1.72	1.47

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	731	ASN	O-C-N	-23.70	84.77	122.70
2	H	731	ASN	O-C-N	-23.70	84.77	122.70
2	B	731	ASN	O-C-N	-23.67	84.83	122.70
2	D	731	ASN	O-C-N	-23.62	84.90	122.70
2	B	672	PRO	O-C-N	-18.02	86.86	121.10

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	672	PRO	Mainchain
2	B	731	ASN	Mainchain
2	D	672	PRO	Mainchain
2	D	731	ASN	Mainchain
2	F	672	PRO	Mainchain

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	2986	0	2889	188	0
1	C	2986	0	2889	146	0
1	E	2986	0	2885	156	0
1	G	2986	0	2889	102	0
2	B	2650	0	2542	648	0
2	D	2650	0	2537	669	0
2	F	2650	0	2536	638	0
2	H	2650	0	2541	672	0
3	I	1671	0	1641	225	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1671	0	1641	216	0
3	K	1671	0	1641	227	0
3	L	1671	0	1640	231	0
4	M	1598	0	1518	312	0
4	N	1598	0	1517	324	0
4	O	1598	0	1517	299	0
4	P	1598	0	1520	342	0
All	All	35620	0	34343	4086	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 58.

The worst 5 of 4086 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:C:93:TYR:CD1	2:D:676:PRO:HG3	1.19	1.71
1:E:93:TYR:CD1	2:F:676:PRO:HG3	1.19	1.69
3:K:114:ALA:HB3	3:K:146:PHE:CE2	1.17	1.69
3:L:114:ALA:HB3	3:L:146:PHE:CE2	1.17	1.68
3:L:32:TYR:HE1	3:L:96:TYR:CD1	1.00	1.67

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	390/451 (86%)	368 (94%)	19 (5%)	3 (1%)	24 69
1	C	390/451 (86%)	368 (94%)	19 (5%)	3 (1%)	24 69
1	E	390/451 (86%)	368 (94%)	19 (5%)	3 (1%)	24 69
1	G	390/451 (86%)	369 (95%)	18 (5%)	3 (1%)	24 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	9	50
2	D	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	9	50
2	F	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	9	50
2	H	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	9	50
3	I	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	8	48
3	J	216/218 (99%)	196 (91%)	14 (6%)	6 (3%)	6	44
3	K	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	8	48
3	L	216/218 (99%)	196 (91%)	14 (6%)	6 (3%)	6	44
4	M	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	19	65
4	N	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	19	65
4	O	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	19	65
4	P	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	19	65
All	All	4596/4948 (93%)	4213 (92%)	313 (7%)	70 (2%)	18	57

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	644	ARG
2	B	673	PRO
2	D	644	ARG
2	D	673	PRO
2	F	644	ARG

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	328/372 (88%)	316 (96%)	12 (4%)	41	73
1	C	328/372 (88%)	316 (96%)	12 (4%)	41	73
1	E	328/372 (88%)	316 (96%)	12 (4%)	41	73
1	G	328/372 (88%)	316 (96%)	12 (4%)	41	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	298/313 (95%)	287 (96%)	11 (4%)	41	73
2	D	298/313 (95%)	287 (96%)	11 (4%)	41	73
2	F	298/313 (95%)	287 (96%)	11 (4%)	41	73
2	H	298/313 (95%)	287 (96%)	11 (4%)	41	73
3	I	188/188 (100%)	178 (95%)	10 (5%)	28	64
3	J	188/188 (100%)	178 (95%)	10 (5%)	28	64
3	K	188/188 (100%)	178 (95%)	10 (5%)	28	64
3	L	188/188 (100%)	178 (95%)	10 (5%)	28	64
4	M	178/183 (97%)	149 (84%)	29 (16%)	3	20
4	N	178/183 (97%)	149 (84%)	29 (16%)	3	20
4	O	178/183 (97%)	149 (84%)	29 (16%)	3	20
4	P	178/183 (97%)	149 (84%)	29 (16%)	3	20
All	All	3968/4224 (94%)	3720 (94%)	248 (6%)	27	59

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	1	GLN
4	M	579	GLN
4	P	606(A)	LEU
3	K	28	THR
3	L	28	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	627	HIS
2	H	782	GLN
4	N	670	ASN
2	H	670	HIS
2	H	693	ASN

5.3.3 RNA ⓘ

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](#)

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.