wwPDB EM Map/Model Validation Report (i)

Sep 27, 2016 – 02:58 PM EDT

PDB ID	:	5KHU
EMDB ID:	:	EMD-4021
Title	:	Model of human Anaphase-promoting complex/Cyclosome (APC15 deletion mutant), in complex with the Mitotic checkpoint complex (APC/C-CDC20-MCC) based on cryo EM data at 4.8 Angstrom resolution
Authors	:	Yamaguchi, M.; VanderLinden, R.; Dube, P.; Stark, H.; Schulman, B.
Deposited on	:	2016-06-15
Resolution	:	4.80 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

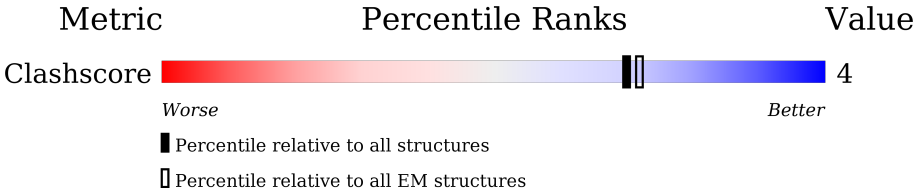
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.80 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

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	1944	70% · 29%
2	B	84	17% · 81%
3	C	597	77% 22%
3	P	597	74% 26%
4	E	110	51% 49%
5	F	824	57% 43%
5	H	824	58% 42%
6	G	85	29% 71%
6	W	85	29% 71%
7	I	808	87% 13%
8	J	620	81% 19%
8	K	620	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	L	185	89% 9%
10	M	74	58% 42%
11	N	822	74% 24%
12	O	755	81% 19%
13	Q	1050	20% 79%
14	R	499	74% 24%
14	S	499	65% 33%
15	T	205	89% 11%
16	U	9	100%
17	X	565	70% 30%
17	Y	565	76% 24%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 8453 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	1374	Total	C	0	1374
			1374	1374		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLU	SER	engineered mutation	UNP Q9H1A4
A	286	GLU	SER	engineered mutation	UNP Q9H1A4
A	291	GLU	THR	engineered mutation	UNP Q9H1A4
A	313	GLU	SER	engineered mutation	UNP Q9H1A4
A	316	GLU	THR	engineered mutation	UNP Q9H1A4
A	317	GLU	SER	engineered mutation	UNP Q9H1A4
A	334	GLU	SER	engineered mutation	UNP Q9H1A4
A	341	GLU	SER	engineered mutation	UNP Q9H1A4
A	343	GLU	SER	engineered mutation	UNP Q9H1A4
A	355	GLU	SER	engineered mutation	UNP Q9H1A4
A	362	GLU	SER	engineered mutation	UNP Q9H1A4
A	372	GLU	SER	engineered mutation	UNP Q9H1A4
A	377	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	THR	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	671	GLN	ASN	conflict	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	916	GLU	SER	engineered mutation	UNP Q9H1A4
A	1347	GLU	SER	engineered mutation	UNP Q9H1A4

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	B	16	Total C 16 16	0	16

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	C	463	Total C 463 463	0	463
3	P	442	Total C 442 442	0	442

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	542	GLU	THR	engineered mutation	UNP Q9UJX2
C	562	GLU	THR	engineered mutation	UNP Q9UJX2
C	582	GLU	THR	engineered mutation	UNP Q9UJX2
C	588	GLU	SER	engineered mutation	UNP Q9UJX2
C	596	GLU	THR	engineered mutation	UNP Q9UJX2
P	542	GLU	THR	engineered mutation	UNP Q9UJX2
P	562	GLU	THR	engineered mutation	UNP Q9UJX2
P	582	GLU	THR	engineered mutation	UNP Q9UJX2
P	588	GLU	SER	engineered mutation	UNP Q9UJX2
P	596	GLU	THR	engineered mutation	UNP Q9UJX2

- Molecule 4 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	E	56	Total C 56 56	0	56

- Molecule 5 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	F	473	Total C 473 473	0	473
5	H	479	Total C 479 479	0	479

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	200	GLU	THR	engineered mutation	UNP P30260
F	205	GLU	THR	engineered mutation	UNP P30260
F	220	GLU	SER	engineered mutation	UNP P30260
F	241	GLU	SER	engineered mutation	UNP P30260
F	276	GLU	SER	engineered mutation	UNP P30260
F	320	GLU	SER	engineered mutation	UNP P30260
F	336	GLU	SER	engineered mutation	UNP P30260
F	339	GLU	SER	engineered mutation	UNP P30260
F	386	GLU	SER	engineered mutation	UNP P30260
F	387	GLU	SER	engineered mutation	UNP P30260
F	393	GLU	SER	engineered mutation	UNP P30260
F	426	GLU	SER	engineered mutation	UNP P30260
F	435	GLU	SER	engineered mutation	UNP P30260
F	446	GLU	THR	engineered mutation	UNP P30260
H	200	GLU	THR	engineered mutation	UNP P30260
H	205	GLU	THR	engineered mutation	UNP P30260
H	220	GLU	SER	engineered mutation	UNP P30260
H	241	GLU	SER	engineered mutation	UNP P30260
H	276	GLU	SER	engineered mutation	UNP P30260
H	320	GLU	SER	engineered mutation	UNP P30260
H	336	GLU	SER	engineered mutation	UNP P30260
H	339	GLU	SER	engineered mutation	UNP P30260
H	386	GLU	SER	engineered mutation	UNP P30260
H	387	GLU	SER	engineered mutation	UNP P30260
H	393	GLU	SER	engineered mutation	UNP P30260
H	426	GLU	SER	engineered mutation	UNP P30260
H	435	GLU	SER	engineered mutation	UNP P30260
H	446	GLU	THR	engineered mutation	UNP P30260

- Molecule 6 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	G	25	Total C 25 25	0	25
6	W	25	Total C 25 25	0	25

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	51	GLU	SER	engineered mutation	UNP Q8NHZ8
G	52	GLU	SER	engineered mutation	UNP Q8NHZ8
G	82	GLU	SER	engineered mutation	UNP Q8NHZ8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
W	51	GLU	SER	engineered mutation	UNP Q8NHZ8
W	52	GLU	SER	engineered mutation	UNP Q8NHZ8
W	82	GLU	SER	engineered mutation	UNP Q8NHZ8

- Molecule 7 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	I	706	Total C 706 706	0	706

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	777	GLU	SER	engineered mutation	UNP Q9UJX5
I	779	GLU	SER	engineered mutation	UNP Q9UJX5

- Molecule 8 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	J	504	Total C 504 504	0	504
8	K	493	Total C 493 493	0	493

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	112	GLU	SER	engineered mutation	UNP Q13042
J	560	GLU	SER	engineered mutation	UNP Q13042
J	581	GLU	THR	engineered mutation	UNP Q13042
J	585	GLU	THR	engineered mutation	UNP Q13042
J	586	GLU	SER	engineered mutation	UNP Q13042
K	112	GLU	SER	engineered mutation	UNP Q13042
K	560	GLU	SER	engineered mutation	UNP Q13042
K	581	GLU	THR	engineered mutation	UNP Q13042
K	585	GLU	THR	engineered mutation	UNP Q13042
K	586	GLU	SER	engineered mutation	UNP Q13042

- Molecule 9 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	L	169	Total C 169 169	0	169

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLU	THR	engineered mutation	UNP Q9UM13

- Molecule 10 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	M	43	Total C 43 43	0	43

- Molecule 11 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	N	627	Total C 627 627	0	627

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	218	GLU	SER	engineered mutation	UNP Q9UJX6
N	314	GLU	SER	engineered mutation	UNP Q9UJX6
N	470	GLU	SER	engineered mutation	UNP Q9UJX6
N	534	GLU	SER	engineered mutation	UNP Q9UJX6
N	811	GLU	SER	engineered mutation	UNP Q9UJX6

- Molecule 12 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	O	608	Total C 608 608	0	608

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	178	GLU	THR	engineered mutation	UNP Q9UJX4
O	179	GLU	SER	engineered mutation	UNP Q9UJX4
O	195	GLU	SER	engineered mutation	UNP Q9UJX4
O	202	GLU	SER	engineered mutation	UNP Q9UJX4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	221	GLU	SER	engineered mutation	UNP Q9UJX4
O	232	GLU	THR	engineered mutation	UNP Q9UJX4
O	364	GLU	SER	engineered mutation	UNP Q9UJX4

- Molecule 13 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	Q	219	Total C 219 219	0	219

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	367	GLU	SER	engineered mutation	UNP O60566
Q	435	GLU	SER	engineered mutation	UNP O60566
Q	543	GLU	SER	engineered mutation	UNP O60566
Q	600	GLU	THR	engineered mutation	UNP O60566
Q	665	GLU	SER	engineered mutation	UNP O60566
Q	670	GLU	SER	engineered mutation	UNP O60566
Q	720	GLU	SER	engineered mutation	UNP O60566
Q	1043	GLU	SER	engineered mutation	UNP O60566

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	R	378	Total C 378 378	0	378
14	S	333	Total C 333 333	0	333

- Molecule 15 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	T	183	Total C 183 183	0	183

- Molecule 16 is a protein called unknown.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	U	9	Total C 9 9	0	9

- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	X	396	Total C 396 396	0	396
17	Y	432	Total C 432 432	0	432

There are 10 discrepancies between the modelled and reference sequences:

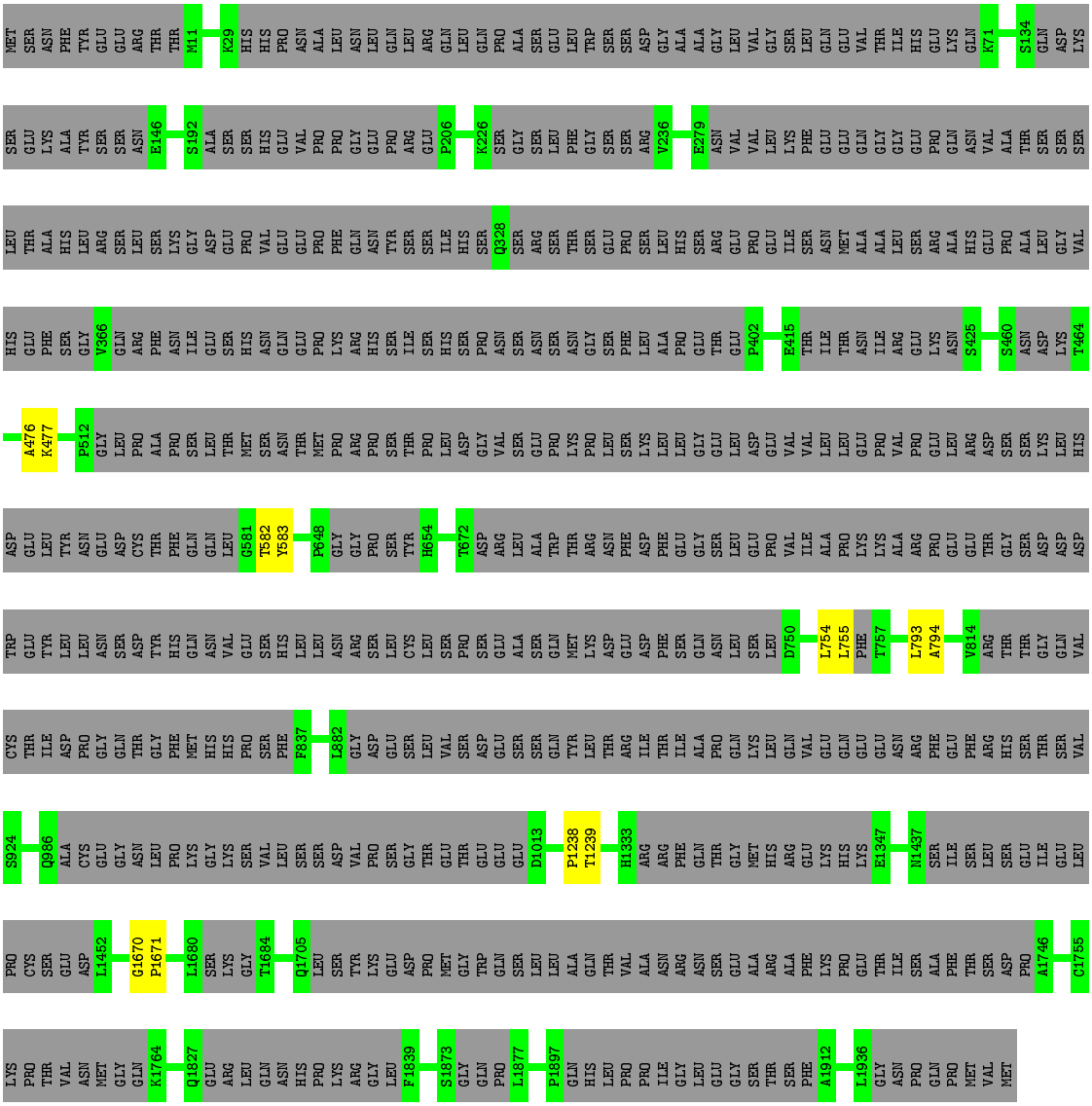
Chain	Residue	Modelled	Actual	Comment	Reference
X	119	GLU	SER	engineered mutation	UNP Q9UJX3
X	120	GLU	THR	engineered mutation	UNP Q9UJX3
X	123	GLU	SER	engineered mutation	UNP Q9UJX3
X	125	GLU	SER	engineered mutation	UNP Q9UJX3
X	126	GLU	THR	engineered mutation	UNP Q9UJX3
Y	119	GLU	SER	engineered mutation	UNP Q9UJX3
Y	120	GLU	THR	engineered mutation	UNP Q9UJX3
Y	123	GLU	SER	engineered mutation	UNP Q9UJX3
Y	125	GLU	SER	engineered mutation	UNP Q9UJX3
Y	126	GLU	THR	engineered mutation	UNP Q9UJX3

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

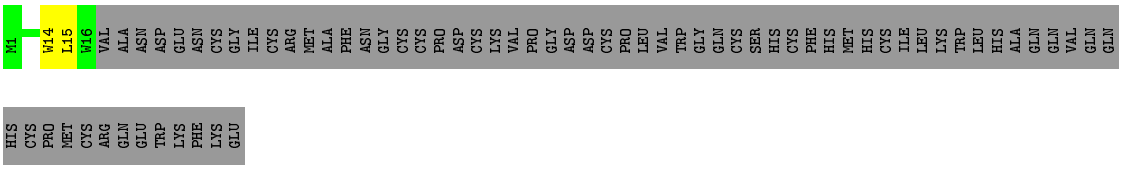
- Molecule 1: Anaphase-promoting complex subunit 1

Chain A:



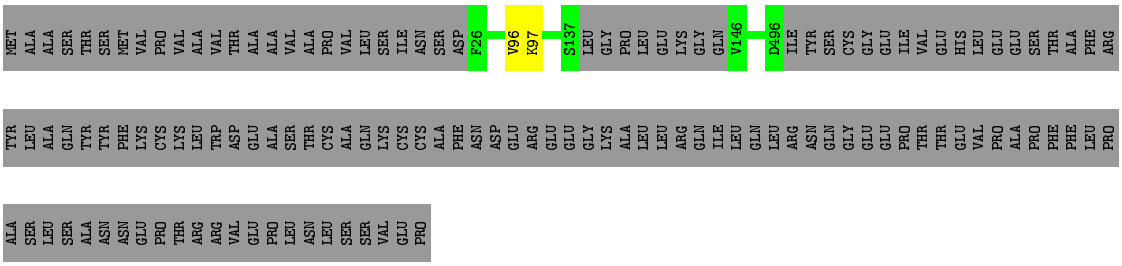
- Molecule 2: Anaphase-promoting complex subunit 11

Chain B:



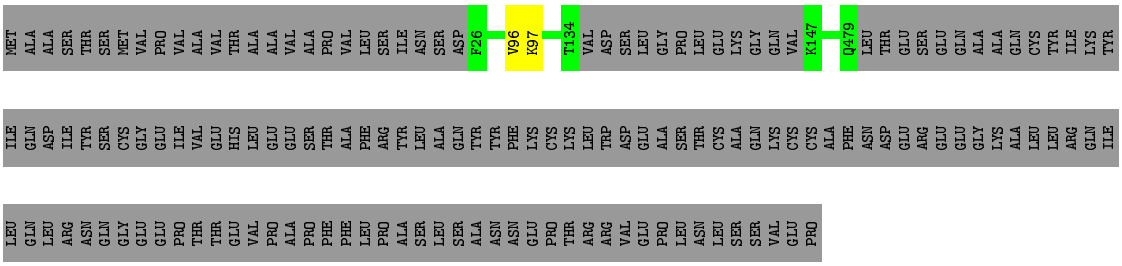
• Molecule 3: Cell division cycle protein 23 homolog

Chain C:



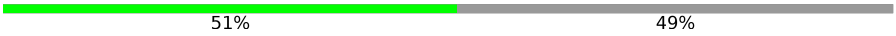
• Molecule 3: Cell division cycle protein 23 homolog

Chain P:



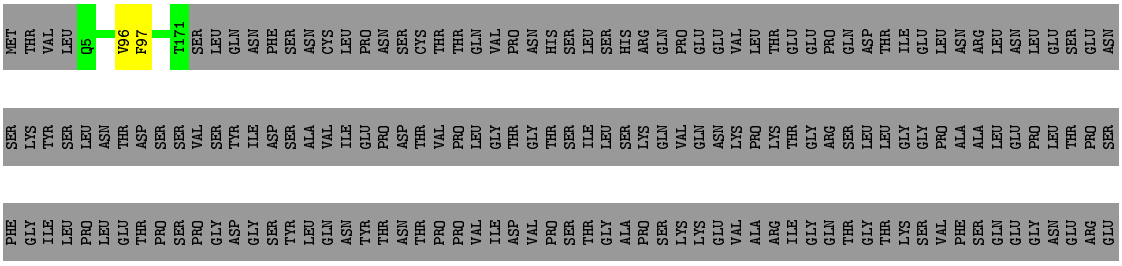
• Molecule 4: Anaphase-promoting complex subunit 16

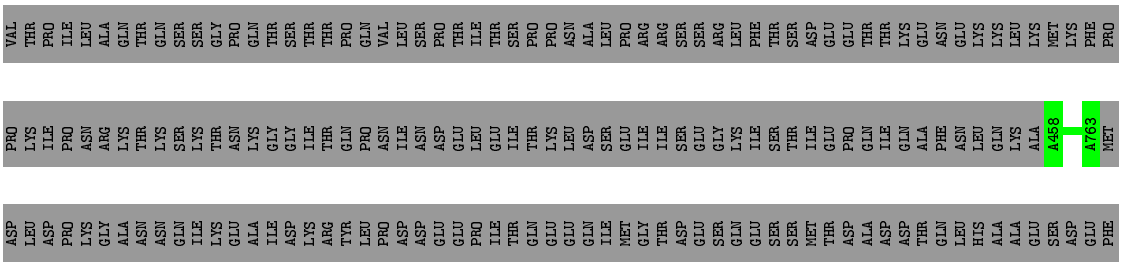
Chain E:



• Molecule 5: Cell division cycle protein 27 homolog

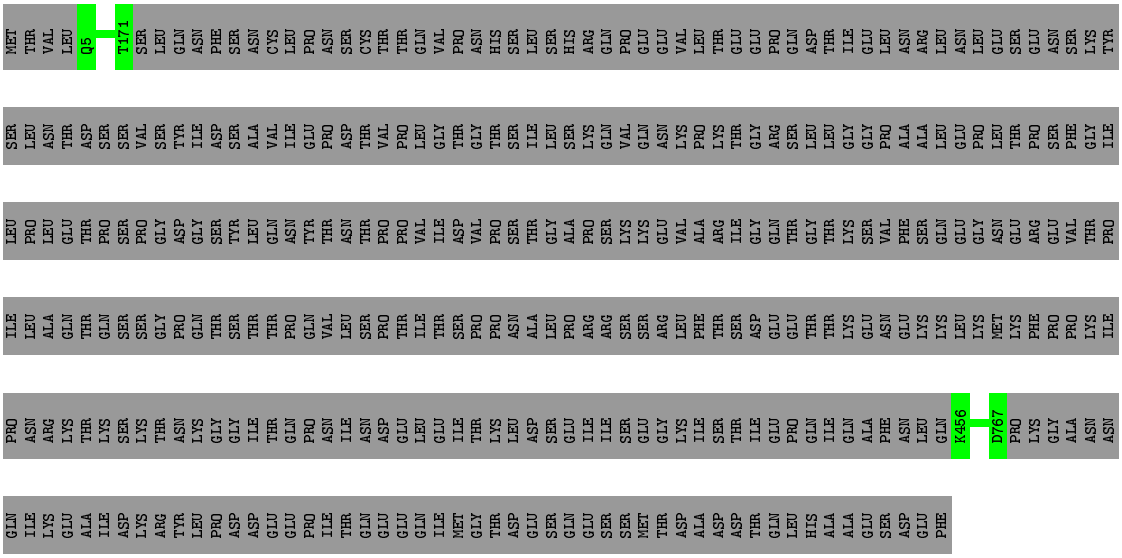
Chain F:





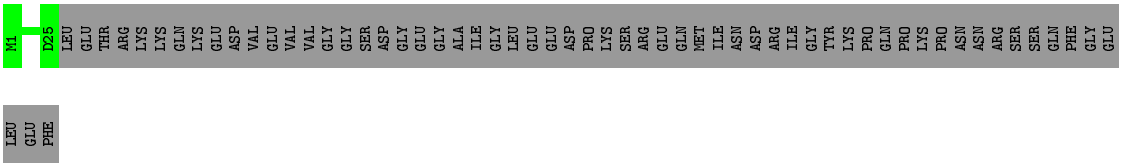
• Molecule 5: Cell division cycle protein 27 homolog

Chain H:



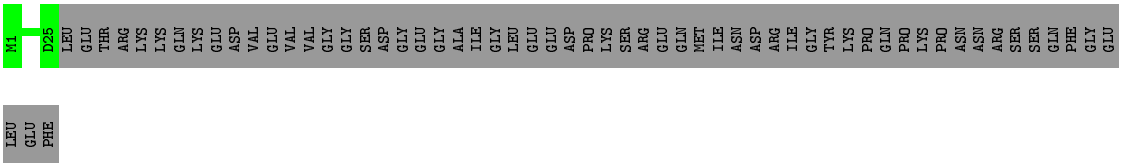
• Molecule 6: Anaphase-promoting complex subunit CDC26

Chain G:



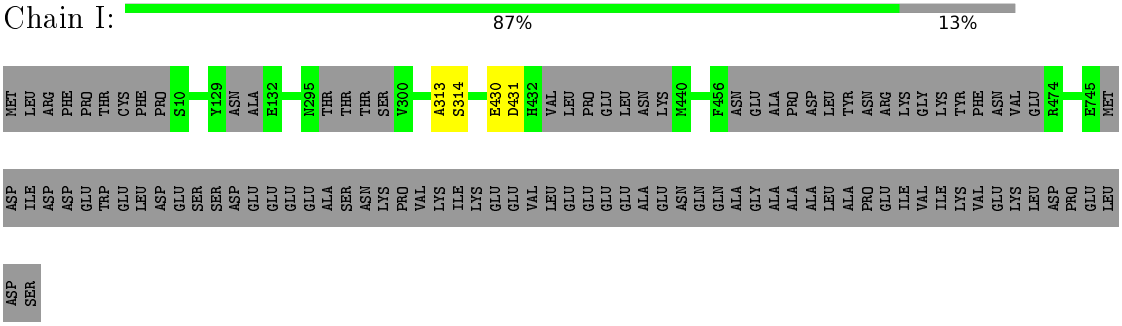
• Molecule 6: Anaphase-promoting complex subunit CDC26

Chain W:



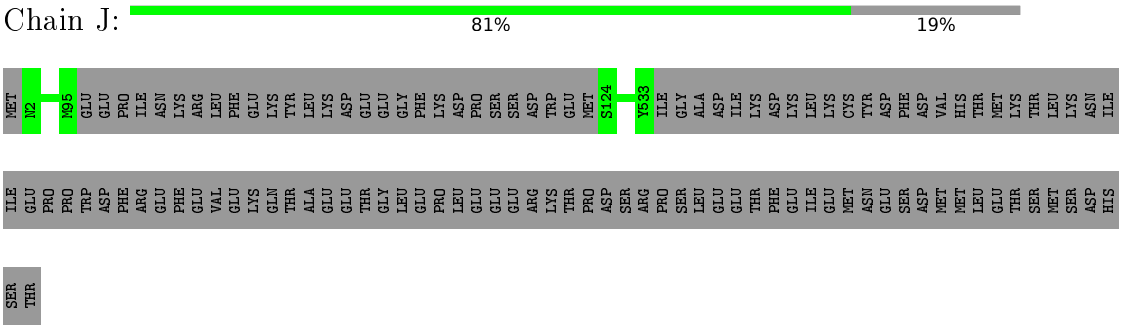
• Molecule 7: Anaphase-promoting complex subunit 4

Chain I:



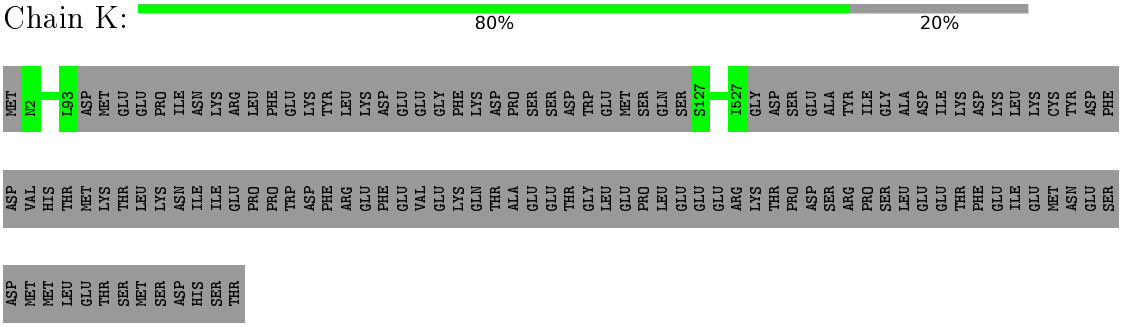
• Molecule 8: Cell division cycle protein 16 homolog

Chain J:



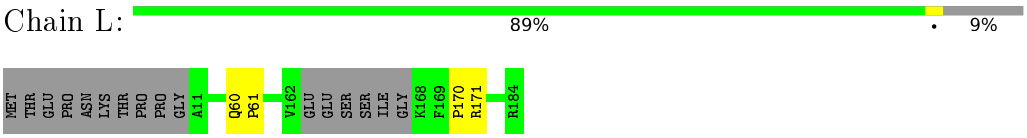
• Molecule 8: Cell division cycle protein 16 homolog

Chain K:



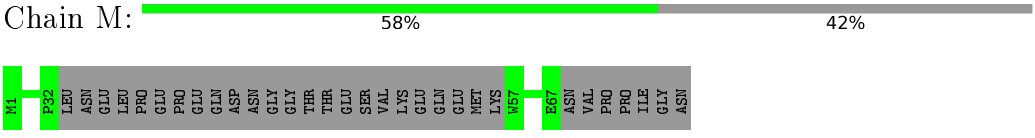
• Molecule 9: Anaphase-promoting complex subunit 10

Chain L:



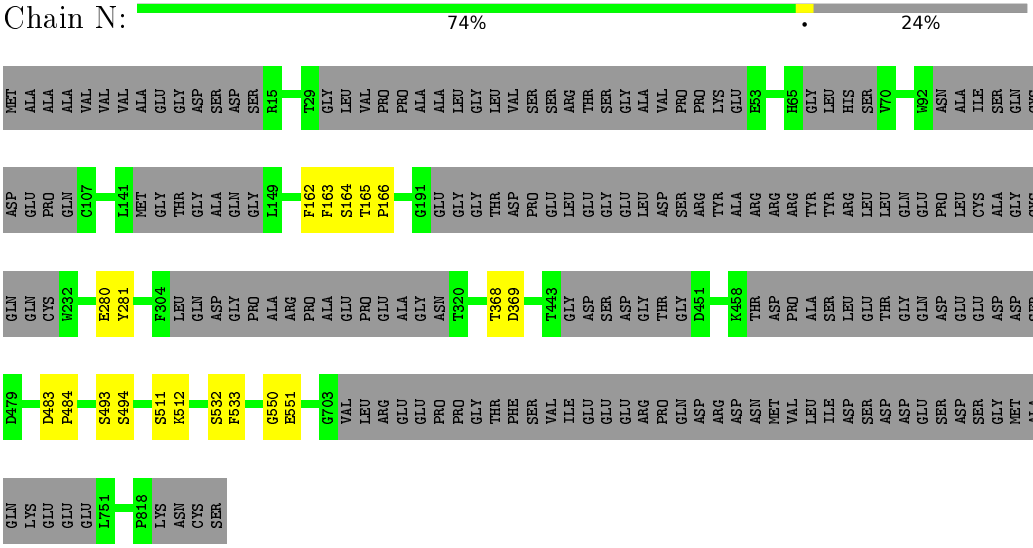
• Molecule 10: Anaphase-promoting complex subunit 13

Chain M:



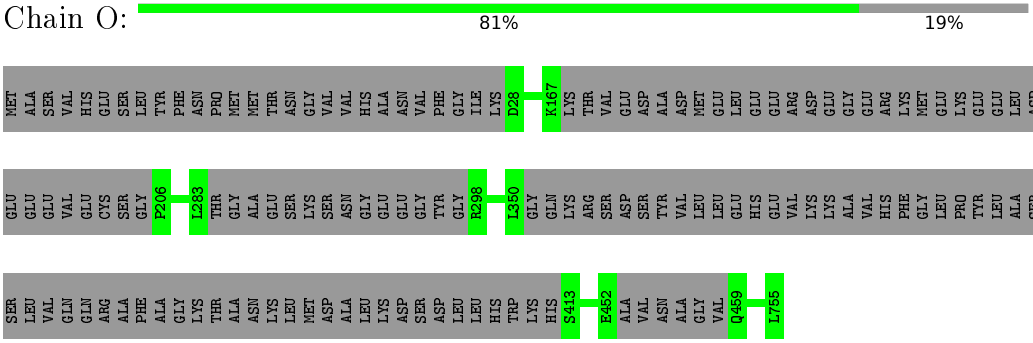
• Molecule 11: Anaphase-promoting complex subunit 2

Chain N:



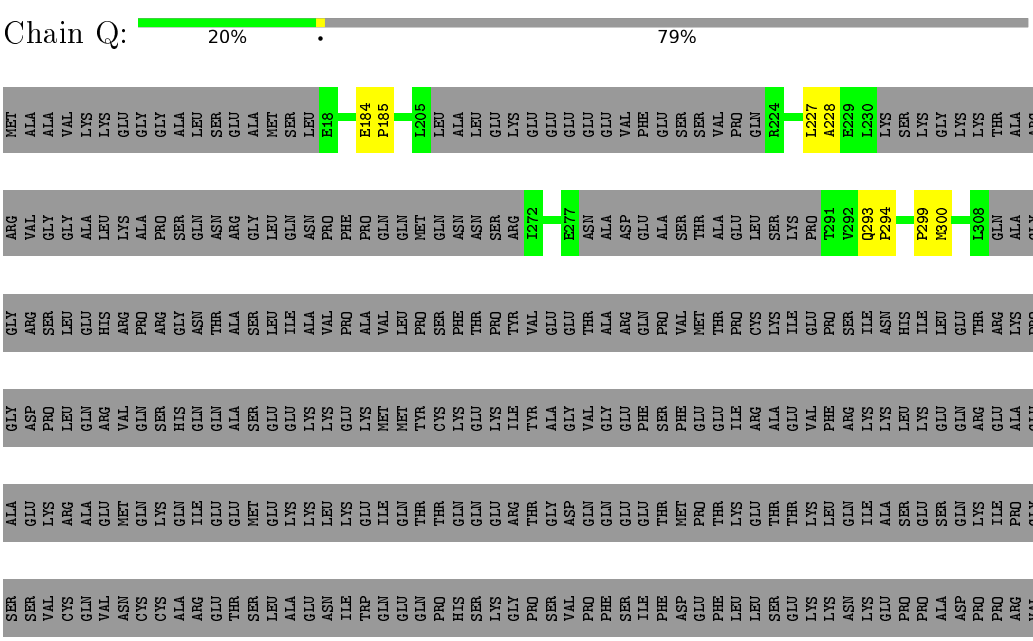
• Molecule 12: Anaphase-promoting complex subunit 5

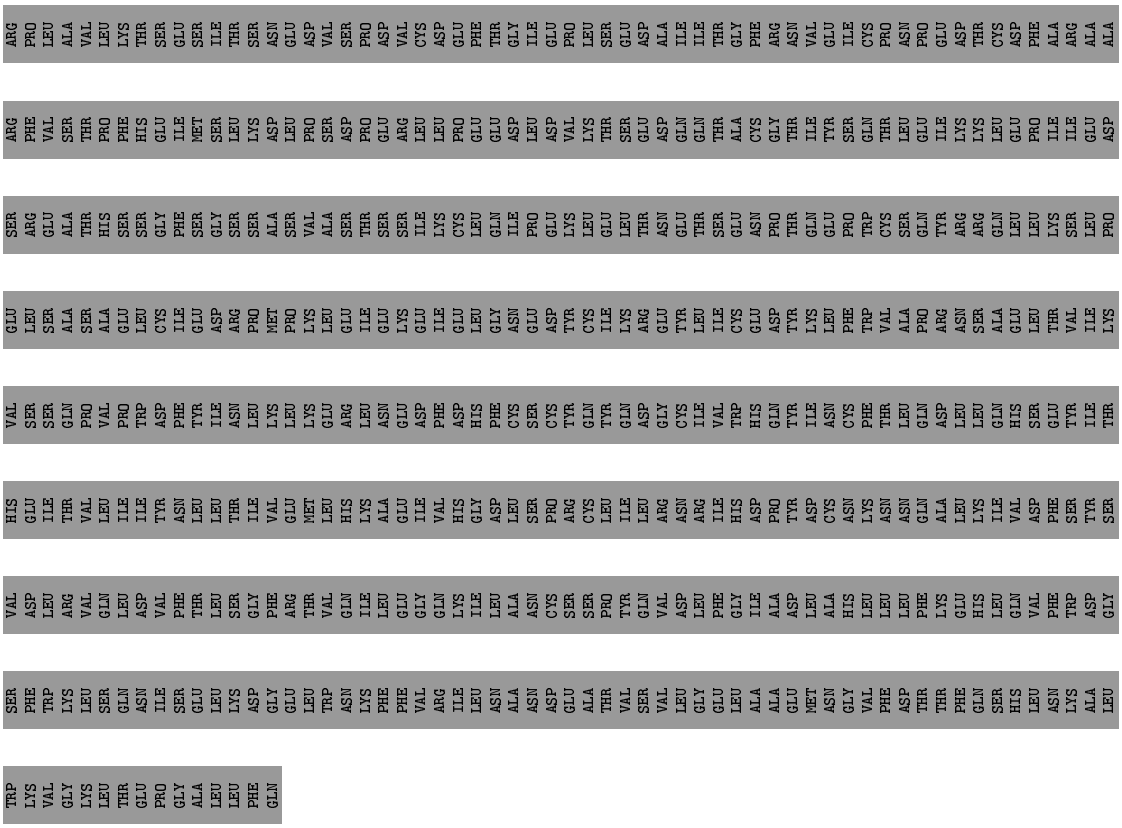
Chain O:



• Molecule 13: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta

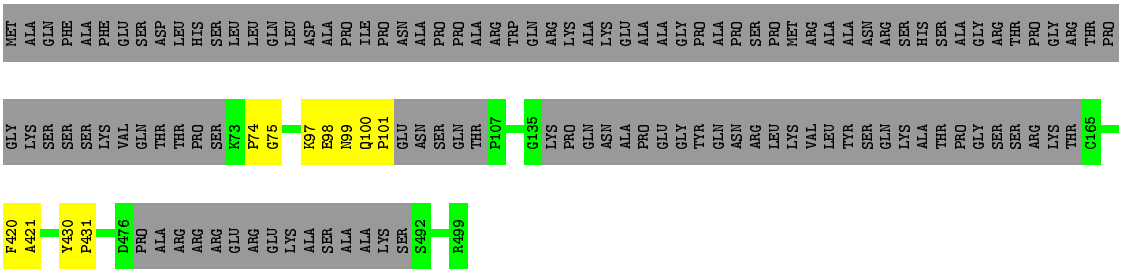
Chain Q:





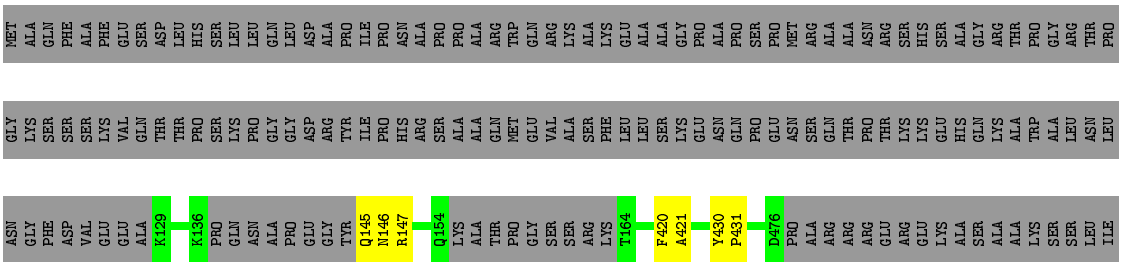
- Molecule 14: Cell division cycle protein 20 homolog

Chain R:



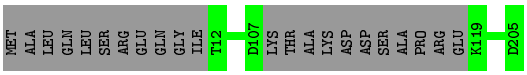
- Molecule 14: Cell division cycle protein 20 homolog

Chain S:



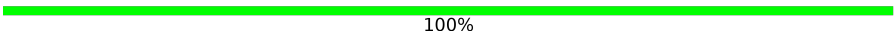
• Molecule 15: Mitotic spindle assembly checkpoint protein MAD2A

Chain T:



• Molecule 16: unknown

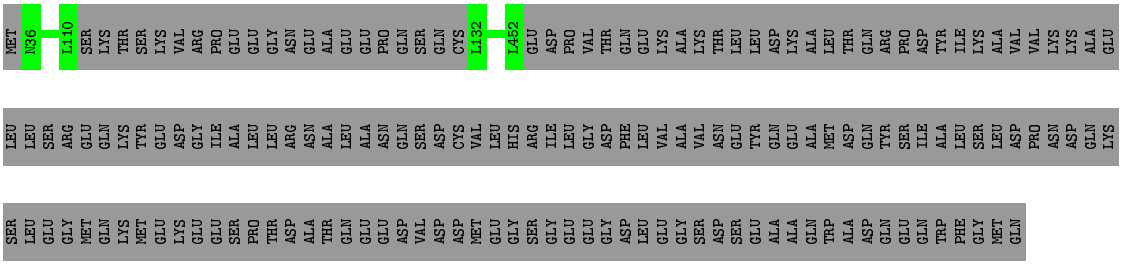
Chain U:



There are no outlier residues recorded for this chain.

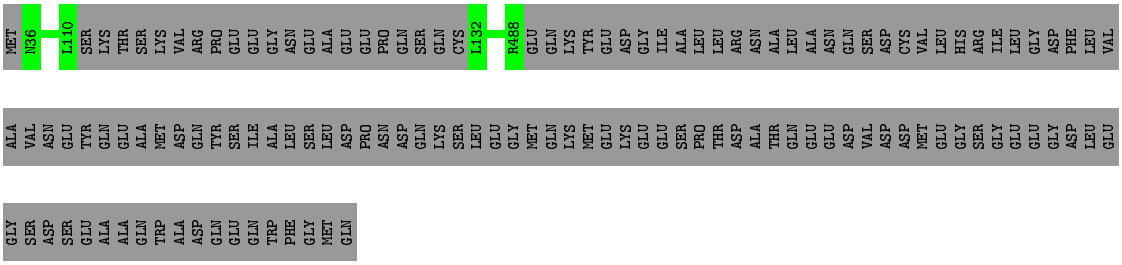
• Molecule 17: Anaphase-promoting complex subunit 7

Chain X:



• Molecule 17: Anaphase-promoting complex subunit 7

Chain Y:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	268851	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)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	1374	0	0	6	0
2	B	16	0	0	1	0
3	C	463	0	0	1	0
3	P	442	0	0	1	0
4	E	56	0	0	0	0
5	F	473	0	0	1	0
5	H	479	0	0	0	0
6	G	25	0	0	0	0
6	W	25	0	0	0	0
7	I	706	0	0	2	0
8	J	504	0	0	0	0
8	K	493	0	0	0	0
9	L	169	0	0	2	0
10	M	43	0	0	0	0
11	N	627	0	0	10	0
12	O	608	0	0	0	0
13	Q	219	0	0	4	0
14	R	378	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	S	333	0	0	4	0
15	T	183	0	0	0	0
16	U	9	0	0	0	0
17	X	396	0	0	0	0
17	Y	432	0	0	0	0
All	All	8453	0	0	38	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 4.

The worst 5 of 38 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)
14:R:97:LYS:CA	14:R:98:GLU:CA	2.65	0.74
14:R:420:PHE:CA	14:R:421:ALA:CA	2.75	0.65
14:R:99:ASN:CA	14:R:100:GLN:CA	2.77	0.62
11:N:164:SER:CA	11:N:165:THR:CA	2.78	0.60
11:N:280:GLU:CA	11:N:281:TYR:CA	2.82	0.57

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.