



wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 03:08 PM EDT

PDB ID : 5KHR
EMDB ID: : EMD-4025
Title : Model of human Anaphase-promoting complex/Cyclosome complex (APC15 deletion mutant) in complex with the E2 UBE2C/UBCH10 poised for ubiquitin ligation to substrate (APC/C-CDC20-substrate-UBE2C)
Authors : VanderLinden, R.; Yamaguchi, M.; Dube, P.; Haselbach, D.; Stark, H.; Schulman, B.A.
Deposited on : 2016-06-15
Resolution : 6.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

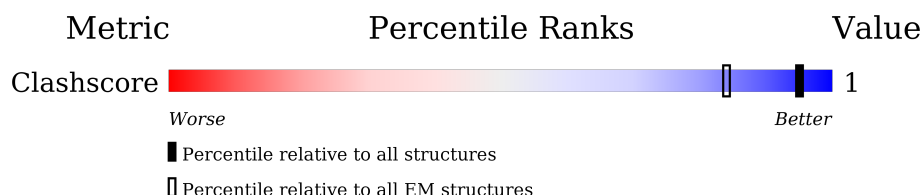
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY







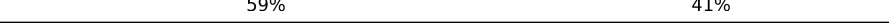
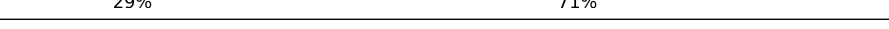
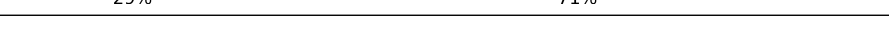

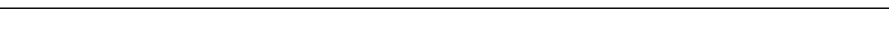

The reported resolution of this entry is 6.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



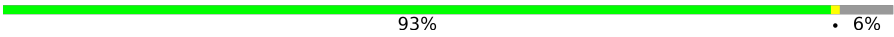







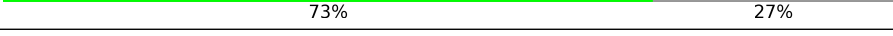
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924

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	1944		71% 28%
2	B	84		82% 18%
3	C	597		78% 22%
3	P	597		74% 26%
4	E	110		51% 49%
5	F	824		58% 42%
5	H	824		59% 41%
6	G	85		29% 71%
6	W	85		29% 71%
7	I	818		84% 15%
8	J	620		81% 19%
8	K	620		80% 20%

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Mol	Chain	Length	Quality of chain
9	L	185	 93% 6%
10	M	74	 64% 36%
11	N	822	 77% 22%
12	O	755	 80% 20%
13	Q	190	 76% 24%
14	R	499	 73% 26%
15	S	33	 30% 70%
16	X	565	 70% 30%
16	Y	565	 73% 27%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7936 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	1391	Total	C	0	1391
			1391	1391		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	69	Total	C	1	69
			70	70		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	468	Total	C	0	468
			468	468		
3	P	441	Total	C	0	441
			441	441		

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

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

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

Mol	Chain	Residues	Atoms		AltConf	Trace
5	F	481	Total	C	0	481
			481	481		
5	H	483	Total	C	0	483
			483	483		

- 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

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

Mol	Chain	Residues	Atoms	AltConf	Trace
7	I	693	Total C 693 693	0	693

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	809	GLY	-	expression tag	UNP Q9UJX5
I	810	GLY	-	expression tag	UNP Q9UJX5
I	811	SER	-	expression tag	UNP Q9UJX5
I	812	LEU	-	expression tag	UNP Q9UJX5
I	813	GLU	-	expression tag	UNP Q9UJX5
I	814	VAL	-	expression tag	UNP Q9UJX5
I	815	LEU	-	expression tag	UNP Q9UJX5
I	816	PHE	-	expression tag	UNP Q9UJX5
I	817	GLN	-	expression tag	UNP Q9UJX5
I	818	GLY	-	expression tag	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

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

Mol	Chain	Residues	Atoms	AltConf	Trace
9	L	174	Total C 174 174	0	174

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

Mol	Chain	Residues	Atoms	AltConf	Trace
10	M	47	Total C 47 47	0	47

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

Mol	Chain	Residues	Atoms	AltConf	Trace
11	N	645	Total C 645 645	0	645

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	603	Total C 603 603	0	603

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 13 is a protein called Ubiquitin-conjugating enzyme E2 C.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	Q	145	Total C 146 146	1	145

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	180	GLY	-	expression tag	UNP O00762
Q	181	GLY	-	expression tag	UNP O00762
Q	182	SER	-	expression tag	UNP O00762
Q	183	GLY	-	expression tag	UNP O00762
Q	184	SER	-	expression tag	UNP O00762
Q	185	LEU	-	expression tag	UNP O00762

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	186	GLU	-	expression tag	UNP O00762
Q	187	VAL	-	expression tag	UNP O00762
Q	188	LEU	-	expression tag	UNP O00762
Q	189	PHE	-	expression tag	UNP O00762
Q	190	GLN	-	expression tag	UNP O00762

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

Mol	Chain	Residues	Atoms	AltConf	Trace
14	R	368	Total C 370 370	2	368

- Molecule 15 is a protein called HSL1 peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	S	10	Total C 10 10	0	10

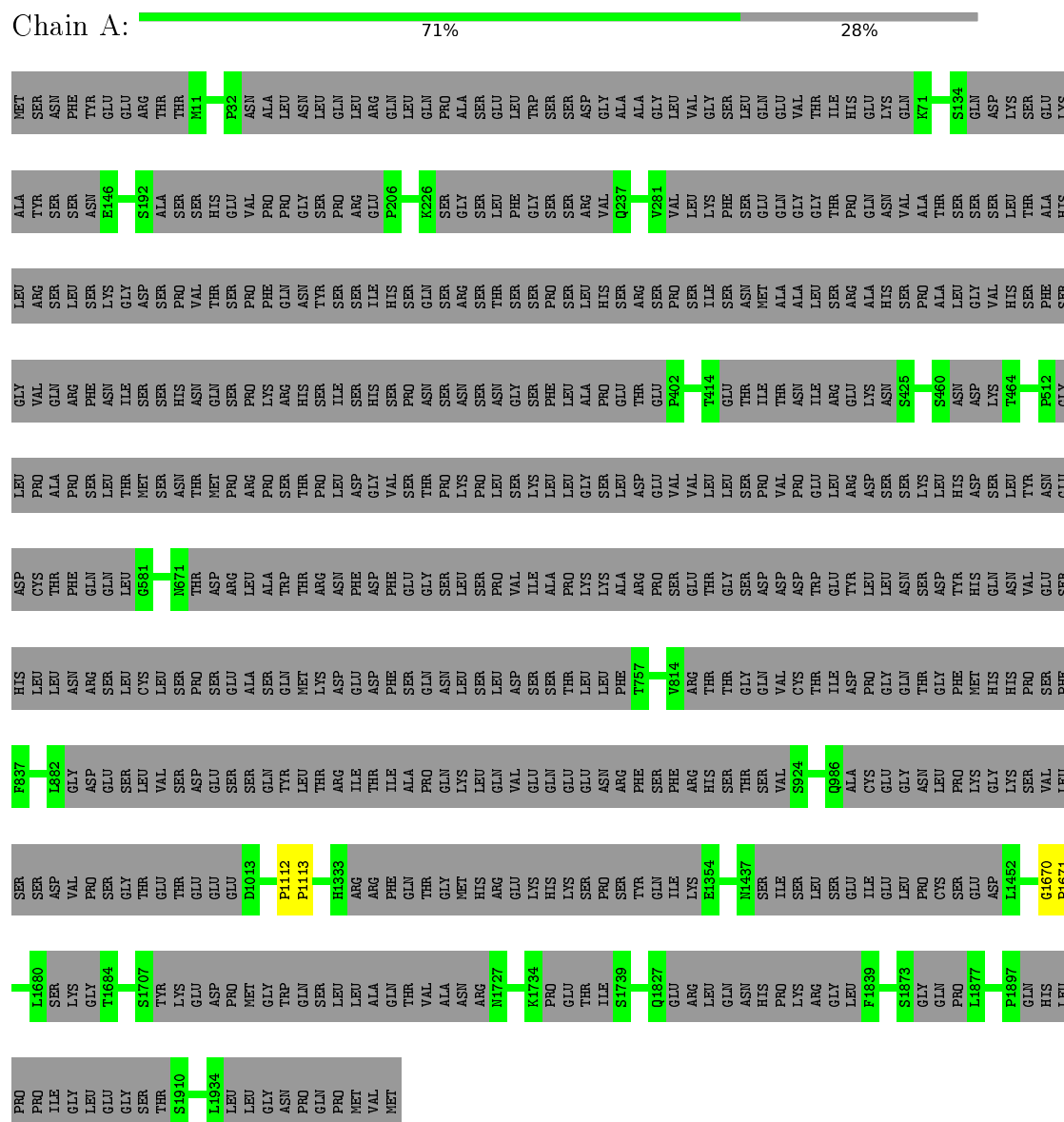
- Molecule 16 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	X	396	Total C 396 396	0	396
16	Y	415	Total C 415 415	0	415

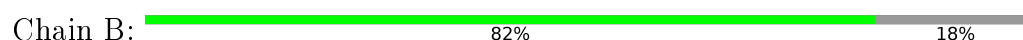
3 Residue-property plots

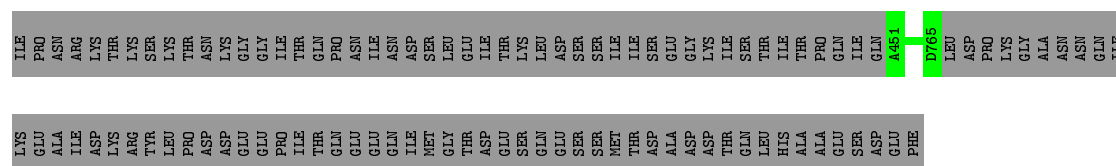
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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



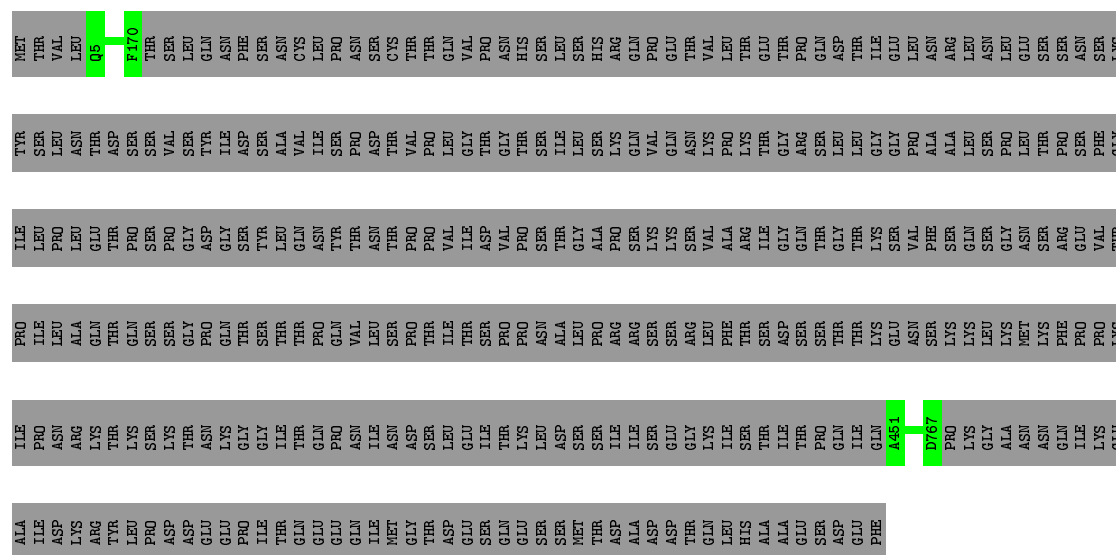
- Molecule 2: Anaphase-promoting complex subunit 11





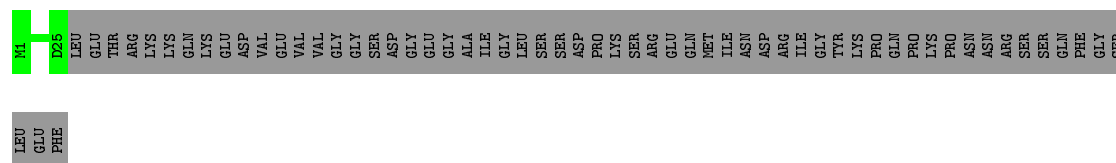
- Molecule 5: Cell division cycle protein 27 homolog

Chain H:  59% 41%



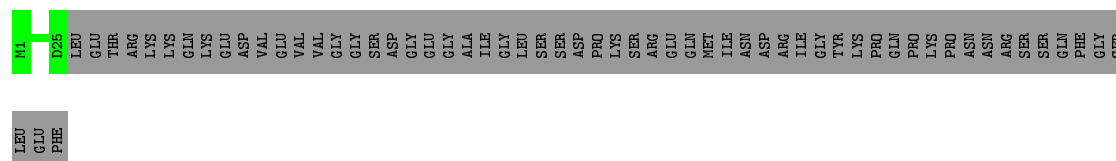
- Molecule 6: Anaphase-promoting complex subunit CDC26

Chain G: 29% 71%



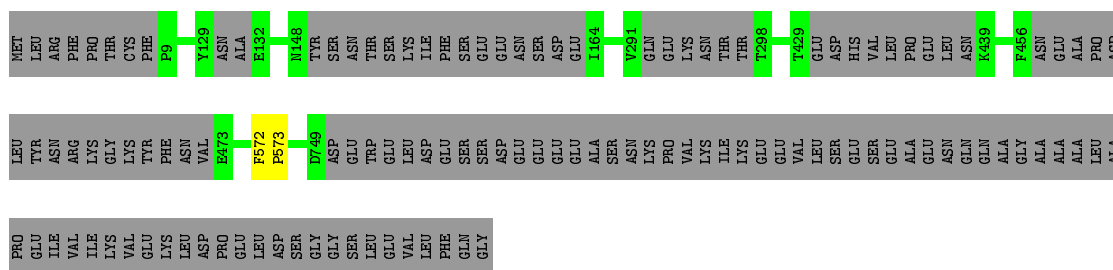
- Molecule 6: Anaphase-promoting complex subunit CDC26

Chain W:  29% 71%



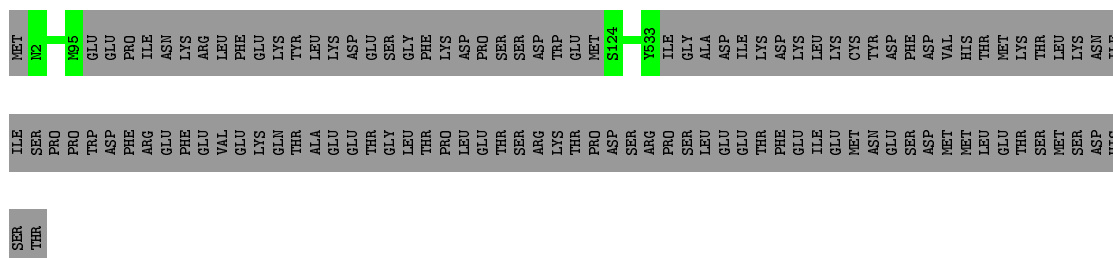
- Molecule 7: Anaphase-promoting complex subunit 4

Chain I: 84% 15%



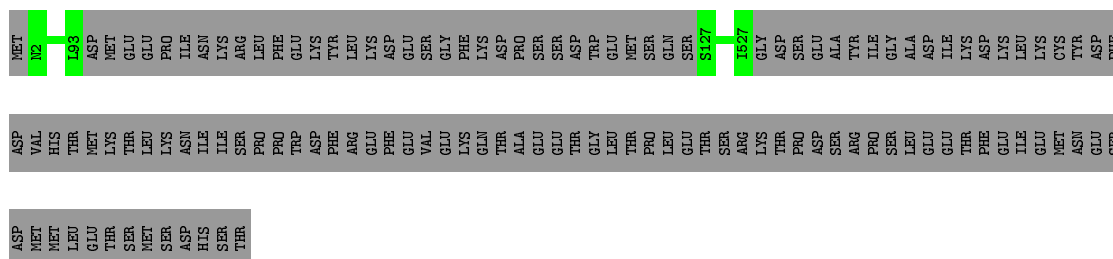
- Molecule 8: Cell division cycle protein 16 homolog

Chain J: 81% 19%



- Molecule 8: Cell division cycle protein 16 homolog

Chain K: 80% 20%



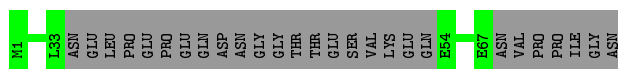
- Molecule 9: Anaphase-promoting complex subunit 10

Chain L: 93% 6%



- Molecule 10: Anaphase-promoting complex subunit 13

Chain M: 64% 36%



- Molecule 11: Anaphase-promoting complex subunit 2

Chain N: 77% 22%

- | | | |
|-----|-----|------|
| GLU | ALA | MET |
| GLU | ASN | N36 |
| ASP | GLN | L110 |
| VAL | SER | SER |
| ASP | ASP | LYS |
| ASP | CYS | THR |
| MET | VAL | THR |
| GLU | LEU | SER |
| GLY | HTS | LYS |
| SER | ARG | VAL |
| GLY | ILE | ARG |
| GLU | LEU | PRO |
| GLU | GLY | SER |
| GLY | ASP | THR |
| ASP | PHE | GLY |
| LEU | LEU | ASN |
| GLU | VAL | SER |
| GLY | ALA | ALA |
| SER | VAL | SER |
| SER | ASN | THR |
| ASP | GLU | PRO |
| SER | TYR | GLN |
| GLU | GLN | SER |
| ALA | GLU | GLN |
| ALA | GLU | CYS |
| GLN | ALA | L132 |
| TRP | MET | L132 |
| ALA | ASP | Q471 |
| ASP | GLN | ARG |
| GLN | TYR | PRO |
| GLU | SER | ASP |
| GLN | ILE | THR |
| TRP | ALA | ILE |
| PHE | LEU | LYS |
| GLY | SER | LYS |
| MET | LEU | ALA |
| GLN | ASP | VAL |
| | PRO | VAL |
| | ASN | LYS |
| | ASP | LYS |
| | GLN | ALA |
| | LYS | GLU |
| | SER | LEU |
| | LEU | LEU |
| | GLY | SER |
| | GLY | ARG |
| | GLN | GLN |
| | LYS | LYS |
| | MET | TYR |
| | GLU | GLU |
| | LYS | ASP |
| | GLY | GLY |
| | GLU | ILE |
| | SER | ALA |
| | PRO | LEU |
| | THR | LEU |
| | ASP | ARG |
| | ALA | ASN |
| | THR | ALA |
| | GLN | LEU |

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	222697	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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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 [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	1391	0	0	2	0
2	B	70	0	0	0	0
3	C	468	0	0	0	0
3	P	441	0	0	0	0
4	E	56	0	0	0	0
5	F	481	0	0	0	0
5	H	483	0	0	0	0
6	G	25	0	0	0	0
6	W	25	0	0	0	0
7	I	693	0	0	1	0
8	J	504	0	0	0	0
8	K	493	0	0	0	0
9	L	174	0	0	1	0
10	M	47	0	0	0	0
11	N	645	0	0	4	0
12	O	603	0	0	0	0
13	Q	146	0	0	0	0
14	R	370	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	S	10	0	0	0	0
16	X	396	0	0	0	0
16	Y	415	0	0	0	0
All	All	7936	0	0	11	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 1.

The worst 5 of 11 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)
11:N:532:SER:CA	11:N:533:PHE:CA	2.83	0.56
1:A:1670:GLY:CA	1:A:1671:PRO:CA	2.84	0.55
11:N:550:GLY:CA	11:N:551:GLU:CA	2.85	0.55
11:N:368:THR:CA	11:N:369:ASP:CA	2.90	0.49
14:R:420:PHE:CA	14:R:421:ALA:CA	2.92	0.48

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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

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](#)

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.