



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:44 pm GMT

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/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

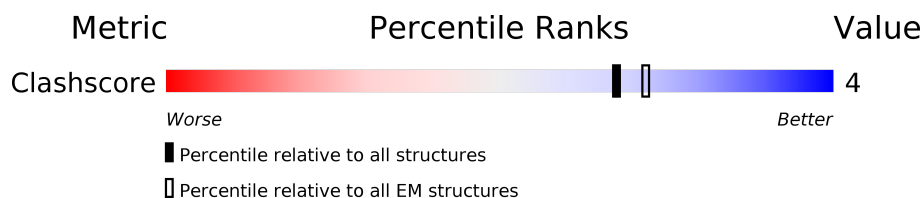
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY













The reported resolution of this entry is 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.




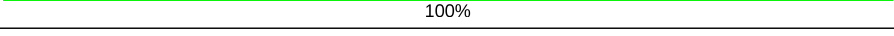
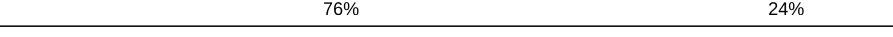
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336

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	 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%

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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 1374 1374	0	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

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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

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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

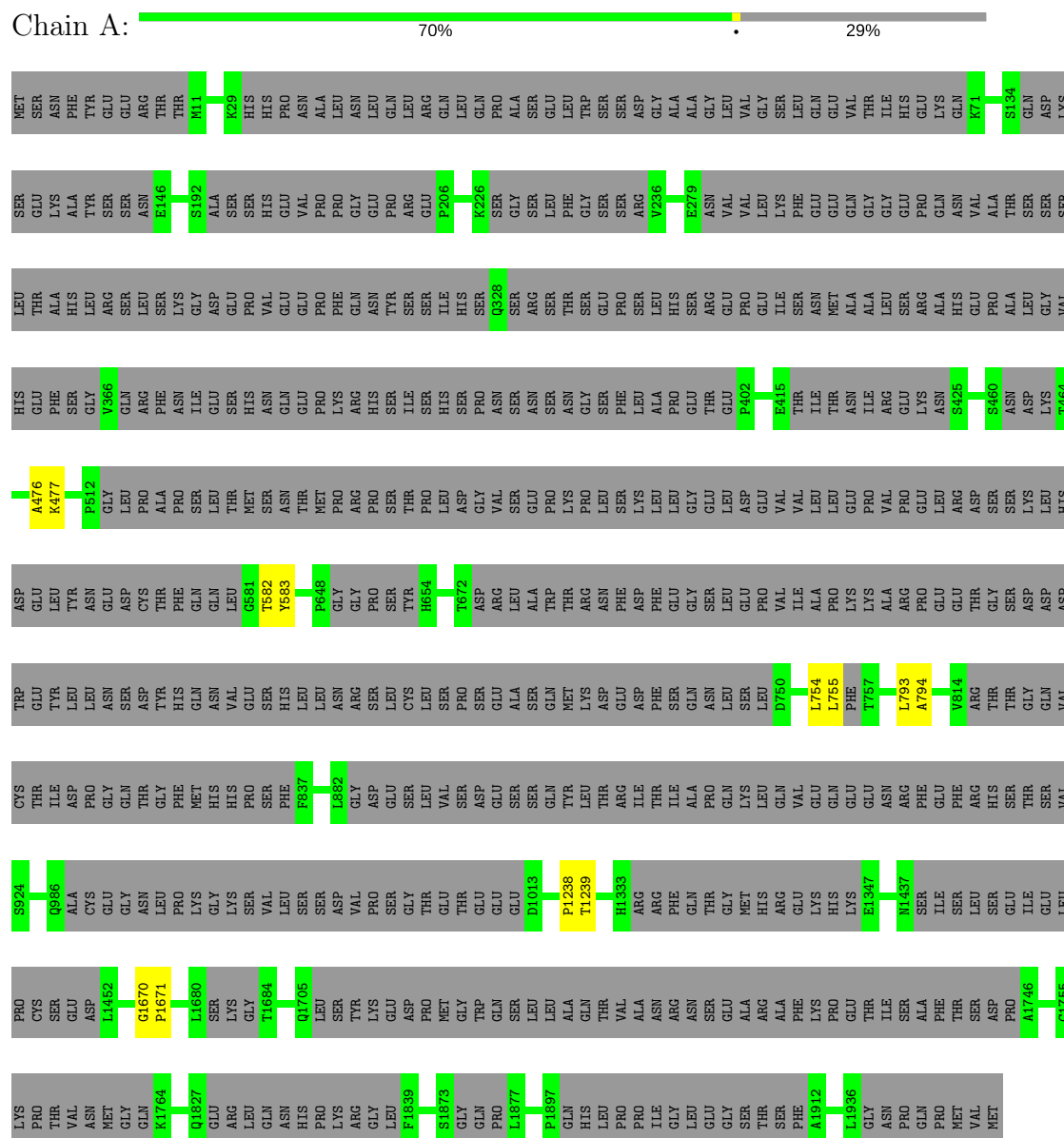
There are 10 discrepancies between the modelled and reference sequences:

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

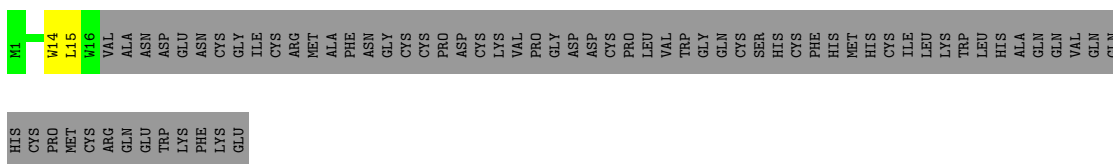
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

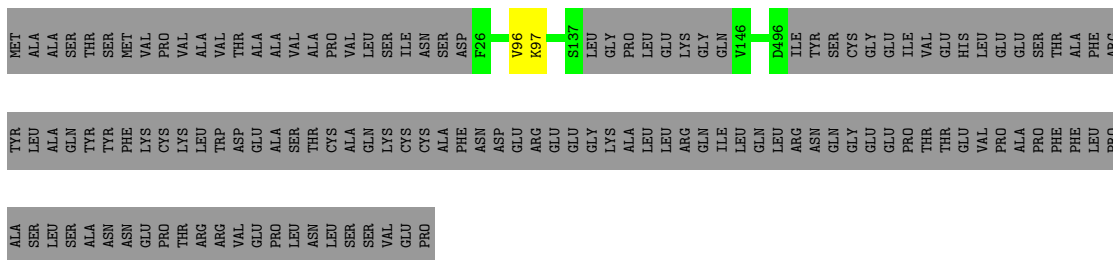
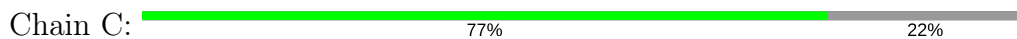


• Molecule 2: Anaphase-promoting complex subunit 11

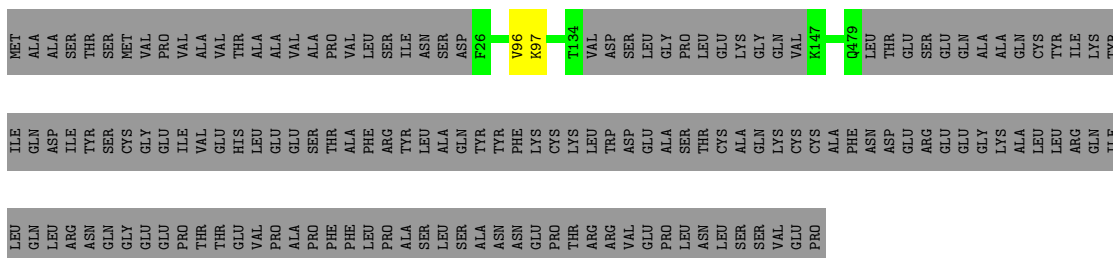




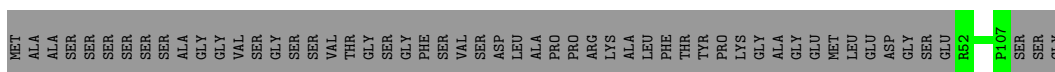
- Molecule 3: Cell division cycle protein 23 homolog



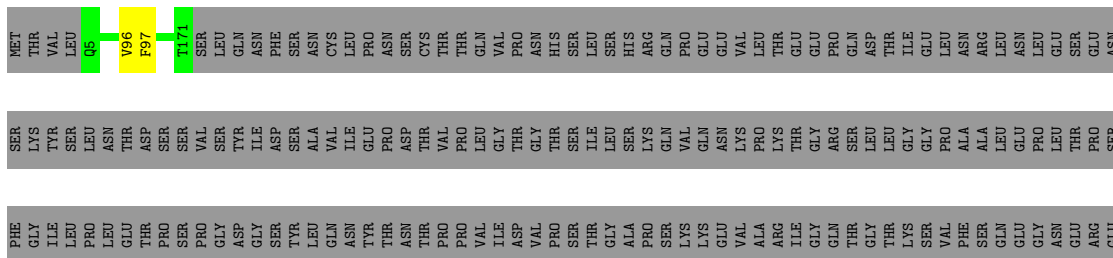
- Molecule 3: Cell division cycle protein 23 homolog

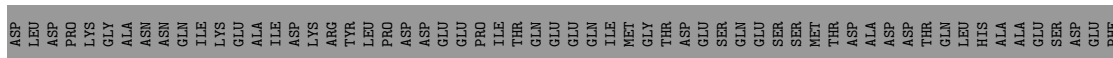
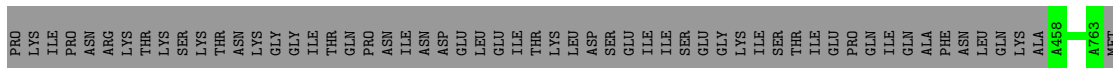
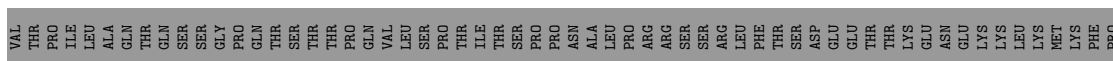


- Molecule 4: Anaphase-promoting complex subunit 16



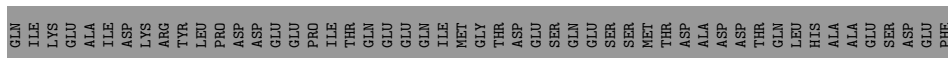
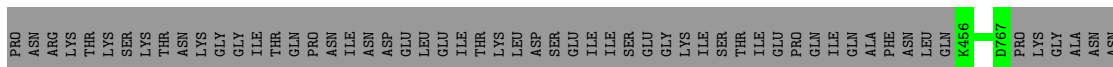
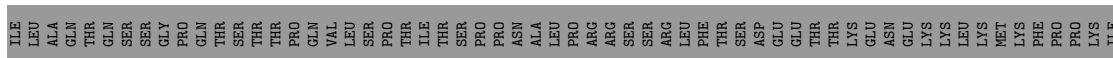
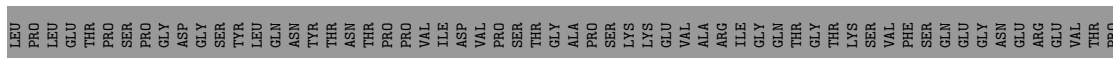
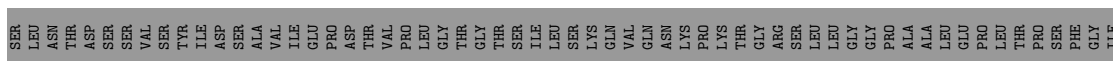
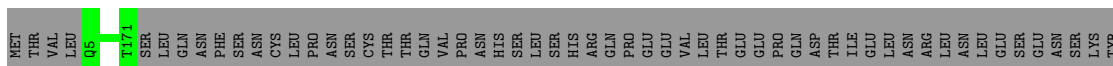
- Molecule 5: Cell division cycle protein 27 homolog





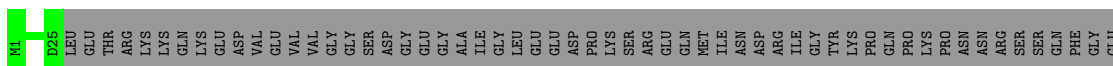
- Molecule 5: Cell division cycle protein 27 homolog

Chain H: 58% 42%



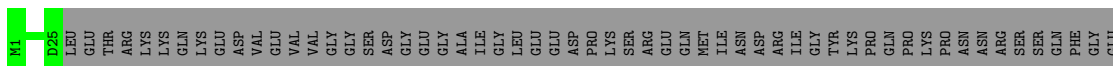
- Molecule 6: Anaphase-promoting complex subunit CDC26

Chain G:  29% 71%



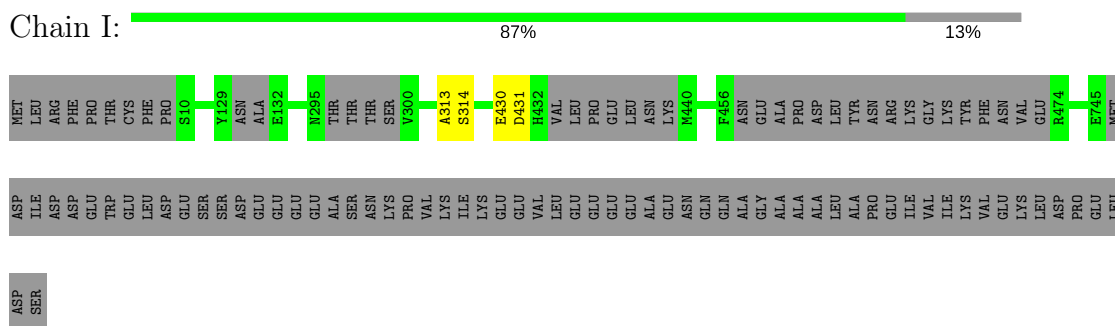
- Molecule 6: Anaphase-promoting complex subunit CDC26

Chain W: 29% 71%



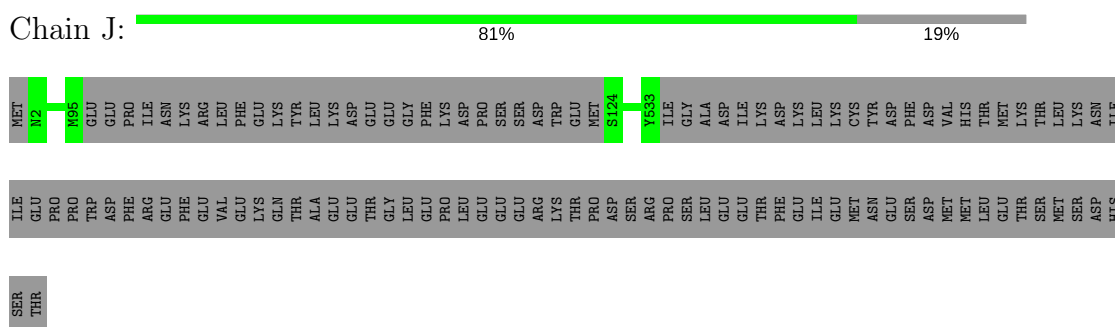
- Molecule 7: Anaphase-promoting complex subunit 4

Chain I:



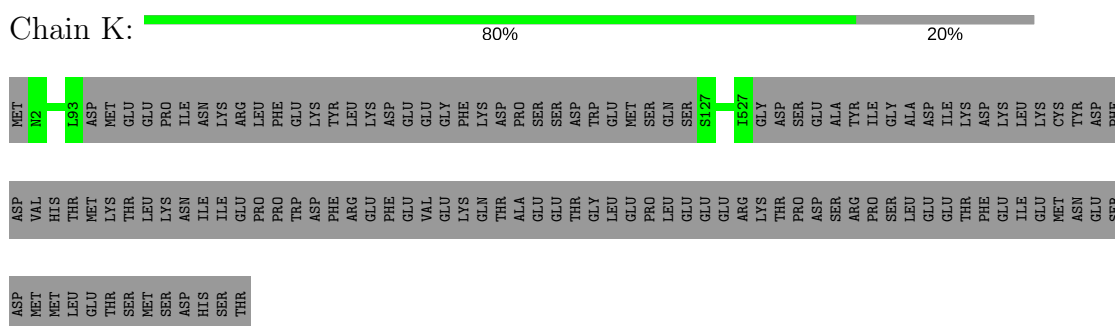
- Molecule 8: Cell division cycle protein 16 homolog

Chain J:



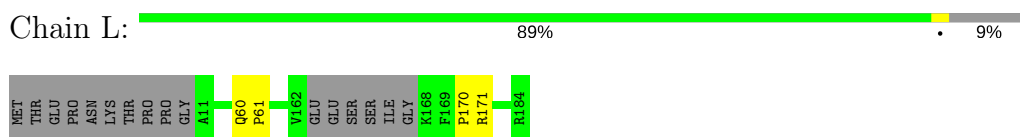
- Molecule 8: Cell division cycle protein 16 homolog

Chain K:



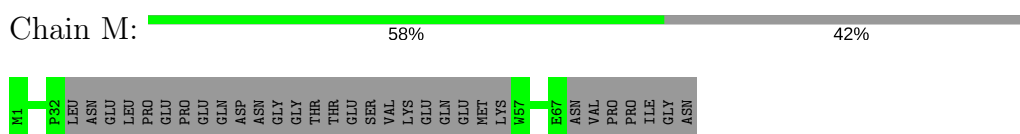
- Molecule 9: Anaphase-promoting complex subunit 10

Chain L:



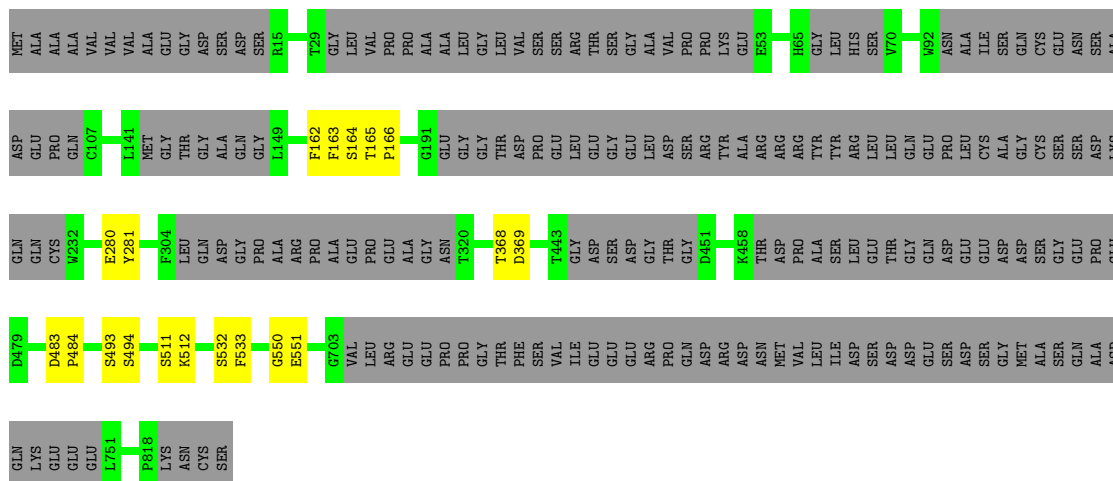
- Molecule 10: Anaphase-promoting complex subunit 13

Chain M:



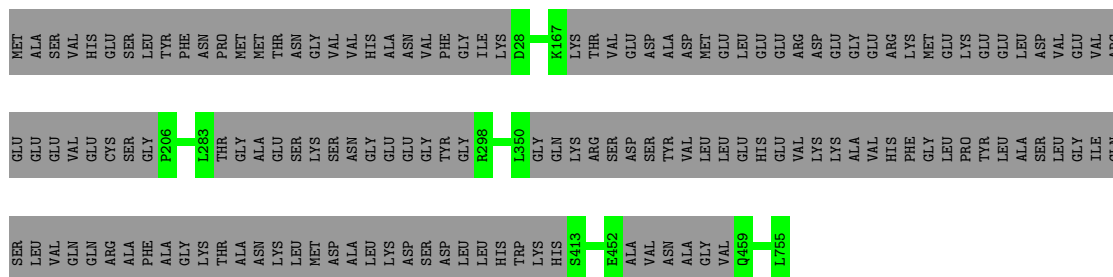
- Molecule 11: Anaphase-promoting complex subunit 2

Chain N:  74% . 24%



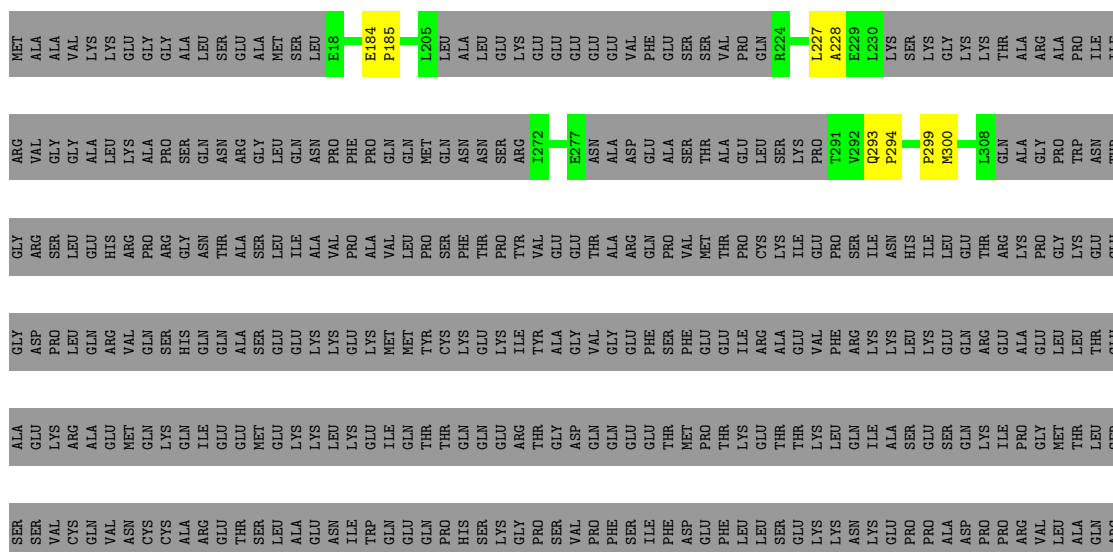
- Molecule 12: Anaphase-promoting complex subunit 5

Chain 0: 81% 19%



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

Chain Q: 20% 79%



[illegible]

- Molecule 14: Cell division cycle protein 20 homolog

Chain R:  74% . 24%

F420	F431	F436	F439	F440	F441	F442	F443	F444	F445	F446	F447	F448	F449	F450	F451	F452	F453	F454	F455	F456	F457	F458	F459	F460	F461	F462	F463	F464	F465	F466	F467	F468	F469	F470	F471	F472	F473	F474	F475	F476	F477	F478	F479	F480	F481	F482	F483	F484	F485	F486	F487	F488	F489	F490	F491	F492	F493	F494	F495	F496	F497	F498	F499	F500	F501	F502	F503	F504	F505	F506	F507	F508	F509	F510	F511	F512	F513	F514	F515	F516	F517	F518	F519	F520	F521	F522	F523	F524	F525	F526	F527	F528	F529	F530	F531	F532	F533	F534	F535	F536	F537	F538	F539	F540	F541	F542	F543	F544	F545	F546	F547	F548	F549	F550	F551	F552	F553	F554	F555	F556	F557	F558	F559	F560	F561	F562	F563	F564	F565	F566	F567	F568	F569	F570	F571	F572	F573	F574	F575	F576	F577	F578	F579	F580	F581	F582	F583	F584	F585	F586	F587	F588	F589	F590	F591	F592	F593	F594	F595	F596	F597	F598	F599	F600	F601	F602	F603	F604	F605	F606	F607	F608	F609	F610	F611	F612	F613	F614	F615	F616	F617	F618	F619	F620	F621	F622	F623	F624	F625	F626	F627	F628	F629	F630	F631	F632	F633	F634	F635	F636	F637	F638	F639	F640	F641	F642	F643	F644	F645	F646	F647	F648	F649	F650	F651	F652	F653	F654	F655	F656	F657	F658	F659	F660	F661	F662	F663	F664	F665	F666	F667	F668	F669	F670	F671	F672	F673	F674	F675	F676	F677	F678	F679	F680	F681	F682	F683	F684	F685	F686	F687	F688	F689	F690	F691	F692	F693	F694	F695	F696	F697	F698	F699	F700	F701	F702	F703	F704	F705	F706	F707	F708	F709	F710	F711	F712	F713	F714	F715	F716	F717	F718	F719	F720	F721	F722	F723	F724	F725	F726	F727	F728	F729	F730	F731	F732	F733	F734	F735	F736	F737	F738	F739	F740	F741	F742	F743	F744	F745	F746	F747	F748	F749	F750	F751	F752	F753	F754	F755	F756	F757	F758	F759	F760	F761	F762	F763	F764	F765	F766	F767	F768	F769	F770	F771	F772	F773	F774	F775	F776	F777	F778	F779	F780	F781	F782	F783	F784	F785	F786	F787	F788	F789	F790	F791	F792	F793	F794	F795	F796	F797	F798	F799	F800	F801	F802	F803	F804	F805	F806	F807	F808	F809	F810	F811	F812	F813	F814	F815	F816	F817	F818	F819	F820	F821	F822	F823	F824	F825	F826	F827	F828	F829	F830	F831	F832	F833	F834	F835	F836	F837	F838	F839	F840	F841	F842	F843	F844	F845	F846	F847	F848	F849	F850	F851	F852	F853	F854	F855	F856	F857	F858	F859	F860	F861	F862	F863	F864	F865	F866	F867	F868	F869	F870	F871	F872	F873	F874	F875	F876	F877	F878	F879	F880	F881	F882	F883	F884	F885	F886	F887	F888	F889	F890	F891	F892	F893	F894	F895	F896	F897	F898	F899	F900	F901	F902	F903	F904	F905	F906	F907	F908	F909	F910	F911	F912	F913	F914	F915	F916	F917	F918	F919	F920	F921	F922	F923	F924	F925	F926	F927	F928	F929	F930	F931	F932	F933	F934	F935	F936	F937	F938	F939	F940	F941	F942	F943	F944	F945	F946	F947	F948	F949	F950	F951	F952	F953	F954	F955	F956	F957	F958	F959	F960	F961	F962	F963	F964	F965	F966	F967	F968	F969	F970	F971	F972	F973	F974	F975	F976	F977	F978	F979	F980	F981	F982	F983	F984	F985	F986	F987	F988	F989	F990	F991	F992	F993	F994	F995	F996	F997	F998	F999	F1000
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- Molecule 14: Cell division cycle protein 20 homolog

Chain S: 65% . 33%

[illegible]

HIS
GLN
GLY
T1498
R499

- Molecule 15: Mitotic spindle assembly checkpoint protein MAD2A

Chain T:  89% 11%

MET	ALA	LEU	GLN	LEU	SER	ARG	GLU	GLY	ILE	T112	D107	LYS	THR	ALA	LYS	ASP	SER	ALA	PRO	ARG	GLU	K119	D205
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- Molecule 16: unknown

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: Anaphase-promoting complex subunit 7

Chain X:  70% 30%

MET	R36	L110	LYS	THR	SER	VAL	GLY	PRO	GLU	GLY	L132	L452	GLU	ASP	PRO	VAL	THR	GLN	LEU	LEU	ASP	LYS	ALA	LEU	THR	GLN	ASP	TYR	ILE	LYS	ALA	VAL	LYS	LYS	GLU
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LEU	LEU	SER	ARG	GLN	LYS	TYR	ASP	ILE	ALA	LEU	LEU	ASN	ALA	LEU	ASN	GLN	SER	VAL	ASP	CYS	VAL	LEU	HIS	ARG	ILE	LEU	GLY	ASP	PHE	LEU	VAL	ALA	VAL	ASN	GLU	TYR	GLN	ALA	GLU	ALA	MET	ASP	GLN	ASP	TYR	ILE	ALA	SER	LEU	LEU	ASP	PRO	ASN	ASP	LYS	LYS
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SER	LEU	GLU	GLY	MET	GLN	LYS	MET	GLU	LYS	ARG	GLU	GLU	PRO	THR	ASP	THR	ALA	THR	GLN	GLU	GLU	PRO	ASN	GLN	ASP	VAL	SER	ASP	ASP	MET	GLU	GLY	SER	GLN	GLY	GLU	GLU	GLY	ASP	LEU	GLU	ILE	GLY	SER	ASP	GLU	ALA	ALA	GLN	TRP	ALA	ASP	GLN	GLN	GLN	TRP	PHE	GLY	MET	GLN
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- Molecule 17: Anaphase-promoting complex subunit 7

Chain Y:  76% 24%

MET	R36	L110	SER	LYS	THR	SER	VAL	GLN	ARG	GLU	PRO	GLU	GLY	ASN	GLU	ALA	GLU	GLU	PRO	ASN	GLN	SER	LYS	CYS	L132	R498	GLU	GLN	LYS	TYR	GLU	ASP	GLY	LEU	ILE	ALA	LEU	LEU	ASN	GLN	SER	VAL	ASP	ASP	GLN	GLU	LEU	HIS	ARG	ILE	LEU	GLY	ASP	PHE	LEU	VAL
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ALA	VAL	ASN	SER	TYR	GLN	GLU	ALA	GLN	ASP	ALA	TYR	SER	ILE	ALA	LEU	SER	LEU	ASP	PRO	ASN	ASP	GLN	LYS	SER	LEU	GLU	GLY	MET	GLN	LYS	MET	GLU	LYS	LEU	GLU	PRO	THR	ALA	THR	GLN	GLU	GLU	ASP	VAL	ASP	ASP	MET	GLU	GLY	SER	GLY	GLY	GLU	GLY	ASP	GLY	LEU	GLU
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GLY	SER	ASP	SER	GLU	ALA	ALA	GLN	TRP	TRP	PHE	GLY	MET	GLN
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4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	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

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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 [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.