



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 13, 2018 – 01:37 PM EDT

PDB ID : 6EXV  
EMDB ID: : EMD-3981  
Title : Structure of mammalian RNA polymerase II elongation complex inhibited by Alpha-amanitin  
Authors : Liu, X.; Farnung, L.; Wigge, C.; Cramer, P.  
Deposited on : 2017-11-09  
Resolution : 3.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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) : rb-20030736

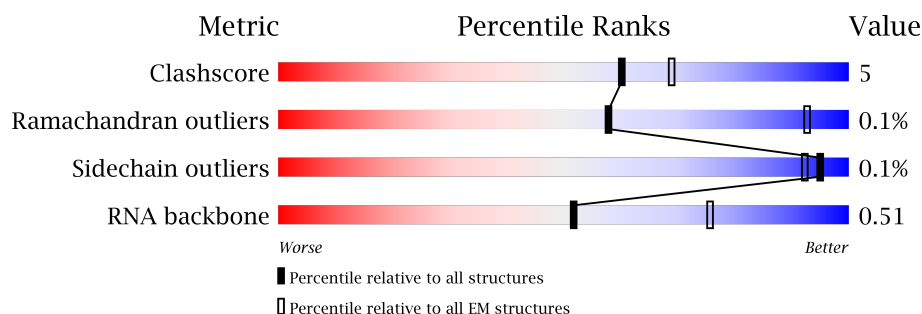
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	1970	61% 11% 28%
2	B	1167	83% 14% .
3	C	275	84% 9% 7%
4	D	142	65% 25% 10%
5	E	210	90% 9%
6	F	127	57% 8% 35%
7	G	172	79% 20% .
8	H	150	87% 11% ..

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Mol	Chain	Length	Quality of chain
9	I	125	 78%14%9%
10	J	67	 84%16%
11	K	117	 84%15%.
12	L	58	 55%21%24%
13	M	8	 50%50%
14	N	43	 53%5%42%
15	P	20	 50%10%10%30%
16	T	43	 81%.16%

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32717 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 DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1428	Total	C	N	O	S	0	0
			11317	7120	2025	2100	72		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	VAL	-	insertion	UNP I3LJR4
A	527	THR	-	insertion	UNP I3LJR4
A	528	PRO	-	insertion	UNP I3LJR4
A	529	GLN	-	insertion	UNP I3LJR4
A	1299	GLN	-	insertion	UNP I3LJR4
A	1300	GLY	-	insertion	UNP I3LJR4
A	1301	ILE	-	insertion	UNP I3LJR4
A	1302	GLU	-	insertion	UNP I3LJR4
A	1303	GLN	-	insertion	UNP I3LJR4
A	1304	ILE	-	insertion	UNP I3LJR4
A	1305	SER	-	insertion	UNP I3LJR4
A	1308	TYR	SER	conflict	UNP I3LJR4
A	1309	MET	ARG	conflict	UNP I3LJR4
A	1310	HIS	SER	conflict	UNP I3LJR4
A	1313	GLN	ALA	conflict	UNP I3LJR4

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a protein called AMATOXIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	8	Total	C	N	O	S	0	0
			64	39	10	14	1		

- Molecule 14 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	25	Total	C	N	O	P	0	0
			516	247	95	149	25		

- Molecule 15 is a RNA chain called RNA (5'-R(P\*CP\*AP\*UP\*AP\*AP\*AP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	14	Total	C	N	O	P	0	0
			301	135	59	93	14		

- Molecule 16 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	36	Total	C	N	O	P	0	0
			735	352	131	216	36		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	J	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
17	B	1	Total 1	Zn 1	0
17	I	2	Total 2	Zn 2	0
17	C	1	Total 1	Zn 1	0
17	A	2	Total 2	Zn 2	0
17	L	1	Total 1	Zn 1	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total 1	Mg 1	0


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.

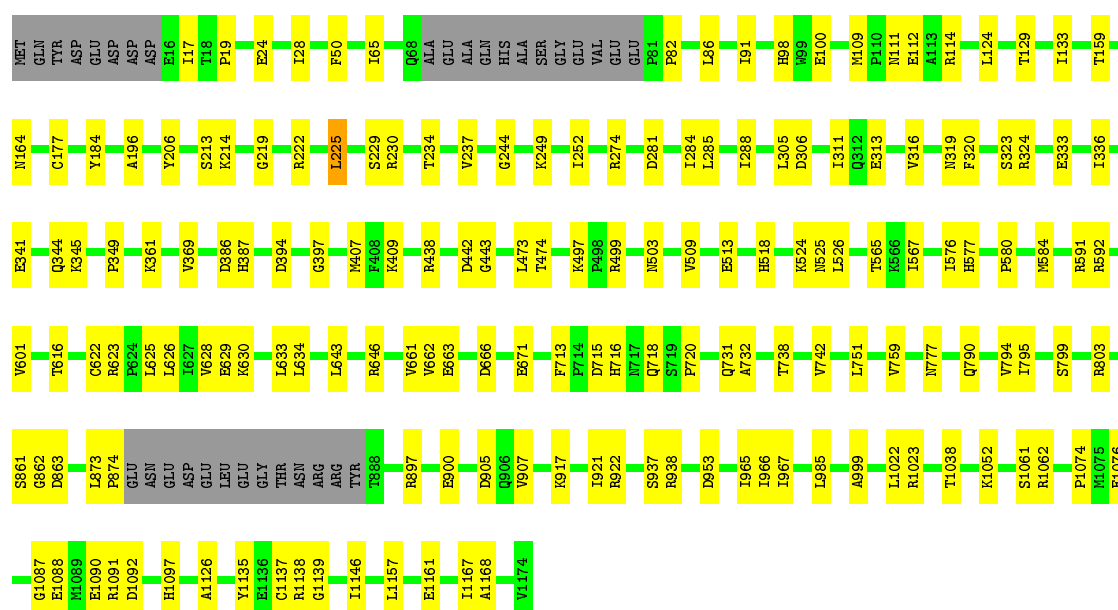
Chain A: 61%11%28%

Position	Most Conserved AA	Information Content (bits)
1	ASP	0.15
2	GLN	0.10
3	GLY	0.10
4	GLY	0.10
5	GLY	0.10
6	GLY	0.10
7	GLY	0.10
8	GLY	0.10
9	GLY	0.10
10	GLY	0.10
11	GLY	0.10
12	GLY	0.10
13	GLY	0.10
14	GLY	0.10
15	GLY	0.10
16	GLY	0.10
17	GLY	0.10
18	GLY	0.10
19	GLY	0.10
20	GLY	0.10
21	GLY	0.10
22	GLY	0.10
23	GLY	0.10
24	GLY	0.10
25	GLY	0.10
26	GLY	0.10
27	GLY	0.10
28	GLY	0.10
29	GLY	0.10
30	GLY	0.10
31	GLY	0.10
32	GLY	0.10
33	GLY	0.10
34	GLY	0.10
35	GLY	0.10
36	GLY	0.10
37	GLY	0.10
38	GLY	0.10
39	GLY	0.10
40	GLY	0.10
41	GLY	0.10
42	GLY	0.10
43	GLY	0.10
44	GLY	0.10
45	GLY	0.10
46	GLY	0.10
47	GLY	0.10
48	GLY	0.10
49	GLY	0.10
50	GLY	0.10
51	GLY	0.10
52	GLY	0.10
53	GLY	0.10
54	GLY	0.10
55	GLY	0.10
56	GLY	0.10
57	GLY	0.10
58	GLY	0.10
59	GLY	0.10
60	GLY	0.10
61	GLY	0.10
62	GLY	0.10
63	GLY	0.10
64	GLY	0.10
65	GLY	0.10
66	GLY	0.10
67	GLY	0.10
68	GLY	0.10
69	GLY	0.10
70	GLY	0.10
71	GLY	0.10
72	GLY	0.10
73	GLY	0.10
74	GLY	0.10
75	GLY	0.10
76	GLY	0.10
77	GLY	0.10
78	GLY	0.10
79	GLY	0.10
80	GLY	0.10
81	GLY	0.10
82	GLY	0.10
83	GLY	0.10
84	GLY	0.10
85	GLY	0.10
86	GLY	0.10
87	GLY	0.10
88	GLY	0.10
89	GLY	0.10
90	GLY	0.10
91	GLY	0.10
92	GLY	0.10
93	GLY	0.10
94	GLY	0.10
95	GLY	0.10
96	GLY	0.10
97	GLY	0.10
98	GLY	0.10
99	GLY	0.10
100	GLY	0.10
101	GLY	0.10
102	GLY	0.10
103	GLY	0.10
104	GLY	0.10
105	GLY	0.10
106	GLY	0.10
107	GLY	0.10
108	GLY	0.10
109	GLY	0.10
110	GLY	0.10
111	GLY	0.10
112	GLY	0.10
113	GLY	0.10
114	GLY	0.10
115	GLY	0.10
116	GLY	0.10
117	GLY	0.10
118	GLY	0.10
119	GLY	0.10
120	GLY	0.10
121	GLY	0.10
122	GLY	0.10
123	GLY	0.10
124	GLY	0.10
125	GLY	0.10
126	GLY	0.10
127	GLY	0.10
128	GLY	0.10
129	GLY	0.10
130	GLY	0.10
131	GLY	0.10
132	GLY	0.10
133	GLY	0.10
134	GLY	0.10
135	GLY	0.10
136	GLY	0.10
137	GLY	0.10
138		

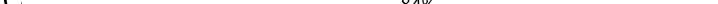
[illegible]

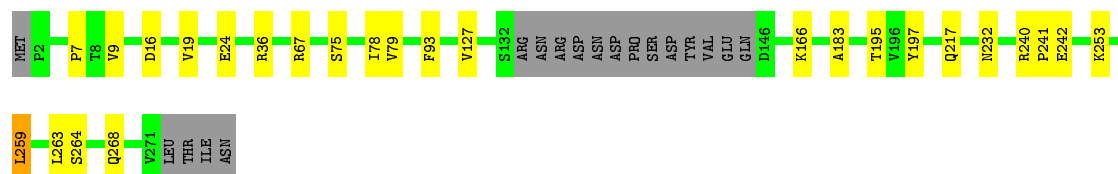
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B:  83% 14% 3%



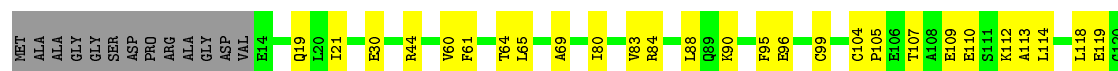
- Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

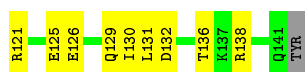
Chain C:  84% 9% 7%



- Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain D:  65% 25% 10%





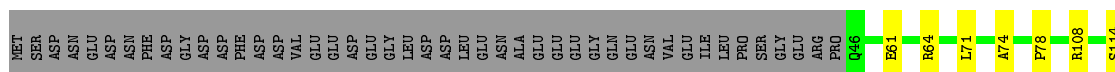
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E: 90% 9%



- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain F: 57% 8% 35%



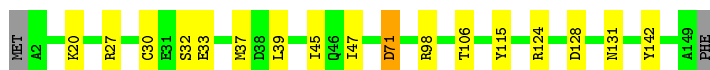
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 79% 20%



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

Chain H: 87% 11%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 78% 14% 9%




- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 84% 16%



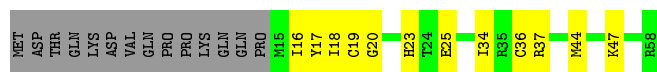
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

Chain K:  84% 15% .



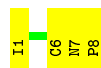
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

Chain L:  55% 21% 24%



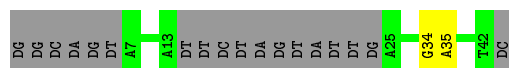
- Molecule 13: AMATOXIN

Chain M:  50% 50%



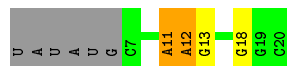
- Molecule 14: DNA (25-MER)

Chain N:  53% 5% 42%




- Molecule 15: RNA (5'-R(P\*CP\*AP\*UP\*AP\*AP\*AP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*C)-3')

Chain P:  50% 10% 10% 30%



- Molecule 16: DNA (36-MER)

Chain T:  81% . 16%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134512	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, HYP, TRX, CSX, ILX

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	0.40	0/11525	0.65	6/15559 (0.0%)
10	J	0.53	0/542	0.70	0/730
11	K	0.41	0/939	0.67	1/1271 (0.1%)
12	L	0.36	0/377	0.58	0/500
13	M	0.44	0/22	1.00	0/26
14	N	0.59	0/578	1.01	0/888
15	P	0.58	0/337	0.92	1/523 (0.2%)
16	T	0.70	0/823	0.98	1/1267 (0.1%)
2	B	0.41	0/9243	0.63	6/12475 (0.0%)
3	C	0.44	0/2102	0.62	1/2857 (0.0%)
4	D	0.26	0/1019	0.52	0/1374
5	E	0.36	0/1751	0.59	0/2366
6	F	0.39	0/667	0.61	0/901
7	G	0.28	0/1365	0.61	0/1853
8	H	0.42	0/1207	0.65	0/1628
9	I	0.33	0/948	0.56	0/1284
All	All	0.41	0/33445	0.66	16/45502 (0.0%)

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
1	A	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	80	ASP	CB-CG-OD1	8.88	126.29	118.30
1	A	503	LEU	CA-CB-CG	7.51	132.57	115.30
16	T	23	DC	O4'-C4'-C3'	-7.33	101.57	104.50
1	A	813	ASP	CB-CG-OD1	6.23	123.91	118.30
2	B	225	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	1049	LEU	CA-CB-CG	5.62	128.22	115.30
3	C	259	LEU	CB-CG-CD1	-5.54	101.58	111.00
2	B	751	LEU	CA-CB-CG	5.47	127.87	115.30
1	A	1029	LEU	CA-CB-CG	5.43	127.79	115.30
2	B	1157	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	1158	LEU	CA-CB-CG	5.26	127.40	115.30
2	B	1087	GLY	N-CA-C	5.25	126.24	113.10
1	A	1486	ILE	C-N-CD	5.25	139.43	128.40
2	B	526	LEU	CA-CB-CG	5.25	127.38	115.30
2	B	863	ASP	CB-CG-OD1	5.21	122.99	118.30
15	P	12	A	P-O3'-C3'	5.21	125.95	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
5	E	54	ARG	Peptide

## 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	11317	0	11439	144	0
2	B	9062	0	9109	108	0
3	C	2059	0	2009	22	0
4	D	1005	0	964	24	0
5	E	1720	0	1737	12	0
6	F	657	0	684	7	0
7	G	1334	0	1333	23	0
8	H	1186	0	1147	14	0
9	I	927	0	862	13	0
10	J	533	0	555	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	920	0	942	12	0
12	L	372	0	378	7	0
13	M	64	0	51	3	0
14	N	516	0	285	2	0
15	P	301	0	153	1	0
16	T	735	0	408	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32717	0	32056	346	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 5.

All (346) 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:A:792:ASN:HD22	1:A:792:ASN:N	1.62	0.96
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.02	0.92
4:D:84:ARG:O	4:D:88:LEU:HB2	1.74	0.87
7:G:99:THR:O	7:G:106:CYS:HB3	1.74	0.86
4:D:104:CYS:SG	4:D:138:ARG:NH1	2.47	0.86
7:G:97:LEU:HB2	7:G:108:ILE:O	1.80	0.81
1:A:11:SER:N	2:B:1135:TYR:HH	1.79	0.81
2:B:344:GLN:OE1	2:B:345:LYS:NZ	2.14	0.80
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.52	0.75
1:A:321:GLU:OE2	1:A:340:LYS:NZ	2.20	0.75
3:C:36:ARG:HH12	11:K:40:HIS:HB2	1.50	0.75
3:C:253:LYS:NZ	11:K:102:GLU:OE1	2.20	0.74
1:A:358:ARG:HH12	2:B:1076:GLU:HG2	1.53	0.72
1:A:792:ASN:N	1:A:792:ASN:ND2	2.33	0.71
1:A:792:ASN:HD22	1:A:792:ASN:H	1.37	0.69
4:D:95:PHE:O	4:D:99:CYS:HB2	1.92	0.69
4:D:65:LEU:O	4:D:69:ALA:HB3	1.93	0.68
1:A:1190:GLN:O	1:A:1194:ASN:HB2	1.93	0.68
1:A:532:ARG:NH1	1:A:647:THR:OG1	2.27	0.68
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:71:ASP:OD1	8:H:71:ASP:N	2.24	0.68
1:A:546:ARG:HH12	1:A:550:LYS:NZ	1.93	0.67
2:B:1088:GLU:HB2	2:B:1091:ARG:NH1	2.10	0.67
7:G:6:SER:HB3	7:G:71:LYS:NZ	2.10	0.66
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.78	0.66
1:A:1416:ARG:NH1	1:A:1433:GLU:OE2	2.29	0.65
2:B:592:ARG:NE	2:B:663:GLU:OE1	2.30	0.65
8:H:71:ASP:OD2	8:H:142:TYR:OH	2.07	0.65
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.29	0.65
1:A:1211:LEU:HD11	1:A:1258:ARG:HE	1.63	0.64
4:D:105:PRO:HG2	4:D:131:LEU:HD21	1.80	0.64
8:H:30:CYS:HB2	8:H:39:LEU:HB3	1.78	0.64
1:A:125:LYS:O	1:A:129:ILE:HB	1.98	0.64
1:A:546:ARG:HH12	1:A:550:LYS:HZ1	1.46	0.63
7:G:6:SER:HB3	7:G:71:LYS:HZ3	1.63	0.63
7:G:44:PHE:HB2	7:G:77:PHE:HB3	1.78	0.63
1:A:395:THR:HG23	1:A:397:PHE:H	1.62	0.62
2:B:803:ARG:NH1	10:J:8:PHE:O	2.31	0.62
1:A:358:ARG:NH1	2:B:1076:GLU:HG2	2.15	0.61
1:A:1399:ALA:O	1:A:1403:ASP:HB2	2.00	0.61
1:A:1487:PRO:HG2	6:F:78:PRO:HA	1.82	0.61
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.33	0.60
1:A:379:GLY:HA2	1:A:475:ARG:O	2.00	0.60
1:A:864:LEU:HD23	1:A:1414:ILE:HG21	1.84	0.60
1:A:487:SER:OG	1:A:673:GLN:NE2	2.35	0.60
11:K:7:PHE:HB2	11:K:11:LEU:HD13	1.83	0.60
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.74	0.60
1:A:620:HIS:CE1	8:H:98:ARG:HH12	2.20	0.60
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.33	0.60
7:G:106:CYS:SG	7:G:107:PHE:N	2.76	0.59
2:B:237:VAL:HG11	2:B:369:VAL:HG22	1.84	0.58
7:G:11:ILE:HD11	7:G:30:LEU:HD23	1.84	0.58
5:E:13:ILE:HD11	5:E:132:GLN:HG3	1.85	0.58
1:A:904:GLN:NE2	1:A:980:PRO:O	2.37	0.58
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.83	0.58
2:B:17:ILE:HG23	2:B:19:PRO:HD3	1.86	0.58
2:B:1038:THR:HA	3:C:195:THR:HA	1.84	0.58
1:A:1430:CYS:HB2	1:A:1435:THR:HG23	1.85	0.58
1:A:1244:ASN:O	1:A:1259:ILE:HA	2.03	0.57
2:B:313:GLU:HB3	2:B:316:VAL:HG12	1.87	0.57
1:A:526:VAL:HA	1:A:533:PRO:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.38	0.57
1:A:421:ARG:NH2	1:A:437:ASP:OD2	2.38	0.56
1:A:791:GLN:HG3	13:M:1:ILX:HA	1.86	0.56
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.87	0.56
1:A:1130:ILE:HG12	1:A:1413:ALA:HB2	1.87	0.56
7:G:101:ILE:HG23	7:G:104:MET:HB3	1.87	0.56
2:B:320:PHE:O	2:B:324:ARG:NH1	2.38	0.56
2:B:65:ILE:HD11	2:B:86:LEU:HG	1.87	0.56
1:A:1130:ILE:HG21	1:A:1411:LEU:HB3	1.87	0.56
1:A:265:VAL:HG22	1:A:271:ARG:HG2	1.88	0.56
7:G:127:CYS:SG	7:G:128:TYR:N	2.77	0.56
2:B:713:PHE:HB3	2:B:716:HIS:HD2	1.71	0.56
12:L:36:CYS:SG	12:L:37:ARG:N	2.78	0.56
1:A:376:ASP:HB2	1:A:666:ARG:HD2	1.87	0.56
4:D:96:GLU:OE2	4:D:121:ARG:NH1	2.39	0.56
11:K:35:ILE:HB	11:K:71:ILE:HG22	1.89	0.55
1:A:1428:MET:HB2	1:A:1456:GLU:OE2	2.05	0.55
9:I:68:ILE:HG13	9:I:122:ARG:HD2	1.87	0.55
3:C:36:ARG:NH1	11:K:40:HIS:HB2	2.20	0.55
1:A:116:LYS:HZ1	1:A:183:GLY:H	1.55	0.55
7:G:89:VAL:HA	7:G:99:THR:HA	1.87	0.55
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.40	0.55
4:D:95:PHE:O	4:D:99:CYS:CB	2.55	0.54
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.41	0.54
1:A:1475:LEU:HB2	7:G:59:ILE:HD11	1.89	0.54
2:B:623:ARG:NH1	2:B:625:LEU:HD21	2.22	0.54
4:D:125:GLU:O	4:D:129:GLN:HB2	2.08	0.54
1:A:1173:THR:HG22	1:A:1214:VAL:HG22	1.90	0.54
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.90	0.53
1:A:358:ARG:NH1	2:B:1076:GLU:HA	2.22	0.53
8:H:32:SER:HB3	8:H:37:MET:H	1.73	0.53
1:A:689:ILE:HD11	2:B:985:LEU:HD22	1.91	0.53
5:E:195:ARG:HH12	5:E:205:THR:HG21	1.72	0.53
2:B:1022:LEU:HD12	2:B:1023:ARG:HG2	1.91	0.53
2:B:285:LEU:HA	2:B:288:ILE:HG22	1.90	0.53
1:A:1408:ARG:O	5:E:172:ARG:NH1	2.41	0.53
2:B:1062:ARG:HH12	2:B:1074:PRO:HB3	1.73	0.53
2:B:795:ILE:HB	2:B:966:ILE:HB	1.90	0.53
4:D:65:LEU:O	4:D:69:ALA:CB	2.57	0.53
5:E:24:ARG:HH12	5:E:184:GLY:HA3	1.74	0.53
9:I:15:ARG:HB3	9:I:24:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:128:ASP:OD1	8:H:131:ASN:ND2	2.42	0.53
8:H:32:SER:OG	8:H:33:GLU:N	2.41	0.53
7:G:12:LEU:HD23	7:G:67:LEU:HB3	1.90	0.52
12:L:19:CYS:SG	12:L:20:GLY:N	2.81	0.52
2:B:111:ASN:HD21	2:B:742:VAL:HG11	1.74	0.52
1:A:342:ARG:NE	2:B:1161:GLU:OE2	2.42	0.52
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.90	0.52
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.92	0.52
2:B:230:ARG:HH11	2:B:409:LYS:HD2	1.75	0.52
4:D:90:LYS:HE2	4:D:130:ILE:HD11	1.90	0.52
1:A:955:GLU:OE2	1:A:1010:VAL:HG22	2.09	0.52
1:A:32:LYS:HE3	1:A:89:GLU:OE2	2.10	0.52
2:B:319:ASN:O	2:B:323:SER:HB2	2.10	0.52
4:D:61:PHE:O	4:D:65:LEU:HB2	2.10	0.52
4:D:107:THR:HG23	4:D:110:GLU:H	1.75	0.51
6:F:61:GLU:OE2	6:F:108:ARG:NH1	2.44	0.51
1:A:1016:LEU:HD11	1:A:1072:ILE:HB	1.92	0.51
1:A:1281:ASP:HA	1:A:1284:PHE:HB3	1.93	0.51
1:A:576:GLN:HE21	1:A:580:LEU:HD21	1.76	0.51
1:A:721:HIS:HD2	9:I:110:LEU:HD13	1.74	0.51
3:C:78:ILE:HD11	3:C:127:VAL:HG23	1.91	0.51
10:J:14:VAL:HG13	10:J:49:LEU:HD12	1.92	0.51
1:A:606:HIS:HB3	1:A:626:THR:HG23	1.92	0.51
2:B:114:ARG:NH2	2:B:184:TYR:OH	2.43	0.51
1:A:137:PRO:HA	1:A:140:ARG:HE	1.75	0.51
1:A:1472:ASP:N	1:A:1472:ASP:OD1	2.43	0.51
1:A:1374:VAL:O	1:A:1378:LEU:HB2	2.10	0.51
1:A:619:LYS:NZ	1:A:627:LYS:HE3	2.26	0.50
1:A:129:ILE:HD11	1:A:143:HIS:HB3	1.93	0.50
1:A:511:THR:HA	1:A:514:GLU:HG2	1.94	0.50
1:A:546:ARG:NH1	1:A:550:LYS:NZ	2.59	0.50
1:A:864:LEU:HD21	1:A:1128:ILE:HD12	1.94	0.50
9:I:81:THR:HG22	9:I:83:ASP:H	1.76	0.50
1:A:322:LEU:HD22	1:A:325:LEU:HD12	1.93	0.50
2:B:1062:ARG:NH1	2:B:1074:PRO:HB3	2.27	0.50
7:G:90:THR:HA	7:G:139:GLN:HE22	1.77	0.50
2:B:438:ARG:O	2:B:442:ASP:HB2	2.11	0.50
3:C:264:SER:O	3:C:268:GLN:HB2	2.11	0.49
4:D:132:ASP:O	4:D:136:THR:CB	2.60	0.49
2:B:196:ALA:HA	2:B:394:ASP:O	2.12	0.49
4:D:84:ARG:O	4:D:88:LEU:CB	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:114:LEU:HD22	7:G:84:VAL:HG21	1.94	0.49
1:A:394:VAL:HG22	1:A:402:LEU:HD13	1.94	0.49
1:A:65:ILE:CG2	1:A:271:ARG:HH12	2.26	0.49
1:A:832:THR:OG1	1:A:835:GLU:OE1	2.30	0.49
2:B:580:PRO:O	2:B:584:MET:HB2	2.12	0.49
2:B:341:GLU:O	2:B:345:LYS:HB2	2.12	0.49
9:I:80:ARG:HB3	9:I:93:GLU:OE2	2.13	0.49
7:G:1:MET:N	7:G:78:ARG:O	2.44	0.49
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	1.94	0.49
3:C:259:LEU:HD11	11:K:42:LEU:HD21	1.95	0.49
1:A:1122:PRO:HA	1:A:1125:LYS:HG2	1.95	0.48
1:A:554:PHE:HB3	1:A:585:LEU:HD23	1.95	0.48
3:C:259:LEU:O	3:C:263:LEU:HB3	2.13	0.48
3:C:93:PHE:HE1	3:C:166:LYS:HZ3	1.61	0.48
2:B:917:LYS:NZ	12:L:34:ILE:HD11	2.28	0.48
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.95	0.48
1:A:604:ARG:HH21	1:A:643:LYS:HE2	1.77	0.48
3:C:197:TYR:HD2	3:C:217:GLN:HE21	1.60	0.48
1:A:1365:ILE:HG23	1:A:1369:LEU:HD12	1.95	0.48
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.12	0.48
1:A:860:ILE:HD11	1:A:1125:LYS:HB3	1.96	0.48
1:A:137:PRO:HB3	1:A:140:ARG:HH21	1.79	0.48
1:A:555:LEU:HD12	1:A:591:ILE:HG13	1.95	0.48
3:C:7:PRO:HA	3:C:24:GLU:O	2.13	0.48
2:B:306:ASP:OD1	9:I:25:TYR:OH	2.29	0.48
2:B:623:ARG:HH12	2:B:625:LEU:HD21	1.79	0.48
2:B:794:VAL:HG22	2:B:967:ILE:HG22	1.96	0.48
4:D:132:ASP:O	4:D:136:THR:HB	2.14	0.48
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.96	0.48
2:B:159:THR:HA	2:B:164:ASN:HD22	1.78	0.47
12:L:18:ILE:HD11	12:L:47:LYS:NZ	2.30	0.47
2:B:225:LEU:HB3	2:B:349:PRO:HB2	1.96	0.47
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.78	0.47
1:A:823:VAL:HG22	1:A:835:GLU:HG3	1.96	0.47
4:D:19:GLN:HG3	4:D:21:ILE:HG12	1.96	0.47
1:A:648:SER:OG	1:A:651:SER:OG	2.32	0.47
2:B:344:GLN:O	2:B:361:LYS:NZ	2.47	0.47
1:A:1220:HIS:HB3	1:A:1224:ARG:HH12	1.79	0.47
7:G:59:ILE:HG12	7:G:66:VAL:HG22	1.96	0.47
1:A:11:SER:N	2:B:1135:TYR:OH	2.43	0.47
1:A:466:LYS:HE3	2:B:1097:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.95	0.47
4:D:109:GLU:O	4:D:113:ALA:HB2	2.14	0.47
4:D:60:VAL:O	4:D:64:THR:CB	2.63	0.47
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.97	0.47
1:A:865:ILE:HG12	2:B:1092:ASP:OD2	2.14	0.47
4:D:44:ARG:NH2	7:G:35:GLU:OE2	2.48	0.47
1:A:1032:GLN:OE1	1:A:1036:ASN:ND2	2.48	0.47
5:E:24:ARG:NH1	5:E:184:GLY:HA3	2.30	0.47
14:N:35:DA:OP2	14:N:35:DA:H8	1.98	0.47
1:A:1205:ALA:HB1	1:A:1267:ASN:HB2	1.97	0.47
1:A:1440:MET:HG2	2:B:1167:ILE:HD11	1.98	0.46
1:A:201:GLU:HG3	1:A:213:LYS:HG2	1.97	0.46
1:A:130:LEU:HD21	1:A:235:VAL:HG12	1.96	0.46
2:B:177:CYS:HG	2:B:738:THR:HG1	1.53	0.46
1:A:364:ARG:NH1	1:A:502:ASN:OD1	2.45	0.46
7:G:151:ARG:HH11	7:G:158:PHE:HE1	1.63	0.46
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	1.98	0.46
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.97	0.46
7:G:11:ILE:O	7:G:67:LEU:HA	2.14	0.46
7:G:112:SER:HB3	7:G:163:LEU:H	1.81	0.46
1:A:477:LEU:HB2	1:A:483:ARG:HH21	1.81	0.46
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.98	0.46
1:A:387:ASN:ND2	2:B:1061:SER:OG	2.47	0.46
2:B:474:THR:OG1	2:B:732:ALA:O	2.33	0.46
10:J:1:MET:HA	10:J:55:LEU:HB2	1.97	0.46
11:K:38:GLU:OE2	11:K:42:LEU:HD13	2.16	0.46
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.98	0.46
1:A:545:VAL:HG23	1:A:676:ILE:HG21	1.98	0.46
1:A:1281:ASP:O	1:A:1285:LEU:HB2	2.15	0.45
1:A:1218:ARG:HA	1:A:1221:MET:HB2	1.98	0.45
1:A:1218:ARG:NH2	1:A:1253:GLU:OE1	2.41	0.45
9:I:25:TYR:O	9:I:37:TYR:HA	2.16	0.45
2:B:473:LEU:HD13	2:B:731:GLN:HA	1.98	0.45
1:A:621:ILE:HD11	8:H:124:ARG:HB2	1.97	0.45
2:B:206:TYR:O	2:B:219:GLY:HA2	2.16	0.45
1:A:393:ILE:HD11	6:F:74:ALA:HB1	1.98	0.45
2:B:509:VAL:HG11	2:B:524:LYS:HD2	1.96	0.45
2:B:567:ILE:HD11	2:B:577:HIS:HB2	1.98	0.45
1:A:510:GLU:OE2	6:F:71:LEU:HD13	2.17	0.45
1:A:620:HIS:HB2	8:H:115:TYR:HE2	1.82	0.45
1:A:33:ARG:HE	2:B:1139:GLY:HA2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:LEU:HD23	4:D:121:ARG:HG3	1.99	0.45
15:P:11:A:H8	15:P:11:A:OP2	2.00	0.45
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.99	0.45
1:A:542:LEU:HD21	1:A:642:LYS:HB3	1.98	0.45
2:B:643:LEU:O	2:B:646:ARG:NH1	2.50	0.45
9:I:69:ILE:HG22	9:I:71:ASP:H	1.81	0.45
2:B:499:ARG:NH2	2:B:518:HIS:O	2.50	0.44
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.98	0.44
6:F:114:SER:OG	6:F:115:TYR:N	2.50	0.44
11:K:106:ARG:HA	11:K:109:ILE:HG22	1.99	0.44
1:A:585:LEU:HD22	8:H:47:ILE:HD11	1.98	0.44
2:B:473:LEU:HD11	2:B:1052:LYS:HD3	1.98	0.44
11:K:13:PHE:N	11:K:16:GLU:OE2	2.49	0.44
2:B:109:MET:HB2	2:B:112:GLU:HG2	1.99	0.44
9:I:96:PHE:HD2	9:I:110:LEU:HD11	1.83	0.44
1:A:1196:TYR:OH	1:A:1201:ASP:O	2.35	0.44
1:A:1160:ARG:NH2	1:A:1350:LYS:O	2.50	0.44
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.99	0.44
5:E:104:ILE:HD11	5:E:127:LEU:HD23	1.99	0.44
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	2.00	0.44
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.98	0.44
10:J:46:ARG:O	10:J:50:LEU:CB	2.66	0.44
11:K:61:TYR:HA	11:K:72:ILE:O	2.17	0.44
1:A:70:ARG:HD2	1:A:75:ALA:HB1	2.00	0.44
3:C:264:SER:O	3:C:268:GLN:CB	2.66	0.44
1:A:45:GLU:HB3	1:A:53:LYS:HE2	1.99	0.44
2:B:897:ARG:HB2	2:B:900:GLU:OE2	2.17	0.44
1:A:1179:PRO:HA	1:A:1209:PRO:HB3	2.00	0.43
1:A:119:VAL:HG22	1:A:151:LYS:NZ	2.33	0.43
2:B:861:SER:OG	2:B:862:GLY:N	2.51	0.43
3:C:16:ASP:OD1	3:C:240:ARG:NE	2.51	0.43
3:C:240:ARG:NH2	3:C:242:GLU:OE2	2.51	0.43
3:C:7:PRO:HG3	11:K:97:GLU:OE2	2.17	0.43
14:N:34:DG:OP2	14:N:34:DG:H2'	2.18	0.43
2:B:1092:ASP:OD1	2:B:1092:ASP:N	2.43	0.43
2:B:438:ARG:HD3	2:B:442:ASP:OD2	2.18	0.43
2:B:565:THR:O	2:B:576:ILE:HA	2.18	0.43
1:A:1374:VAL:O	1:A:1378:LEU:CB	2.65	0.43
2:B:222:ARG:HG2	2:B:234:THR:HG22	2.00	0.43
2:B:333:GLU:HA	2:B:336:ILE:HG22	1.99	0.43
2:B:98:HIS:NE2	2:B:100:GLU:OE1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:40:LEU:O	10:J:46:ARG:NH1	2.51	0.43
1:A:1416:ARG:HA	1:A:1432:PHE:HE2	1.83	0.43
1:A:42:LYS:O	1:A:288:ASN:ND2	2.46	0.43
1:A:620:HIS:CE1	8:H:98:ARG:NH1	2.86	0.43
2:B:777:ASN:O	10:J:47:ARG:NH1	2.52	0.43
1:A:589:LYS:NZ	1:A:625:ASP:OD2	2.40	0.43
2:B:284:ILE:HD13	2:B:284:ILE:HG21	1.84	0.43
2:B:873:LEU:HD12	2:B:874:PRO:HD2	2.00	0.43
1:A:26:LEU:HG	2:B:1168:ALA:HB2	2.01	0.43
3:C:19:VAL:HG23	3:C:241:PRO:HB2	2.00	0.43
3:C:75:SER:HB3	3:C:79:VAL:HG11	2.01	0.43
10:J:67:LYS:NZ	12:L:23:HIS:CE1	2.87	0.43
2:B:715:ASP:OD1	2:B:715:ASP:N	2.48	0.42
4:D:112:LYS:HD2	4:D:119:GLU:HG2	2.00	0.42
9:I:110:LEU:HD12	9:I:110:LEU:HA	1.88	0.42
1:A:1163:HIS:CE1	1:A:1302:GLU:HG3	2.54	0.42
2:B:513:GLU:HG2	2:B:525:ASN:HD22	1.85	0.42
1:A:831:LEU:H	2:B:715:ASP:HB2	1.85	0.42
12:L:17:TYR:HB3	12:L:44:MET:HB3	2.00	0.42
13:M:6:CSX:HB2	13:M:7:ASN:H	1.43	0.42
2:B:601:VAL:HG12	2:B:616:THR:HG23	2.01	0.42
2:B:626:LEU:HD23	2:B:662:VAL:HG12	2.01	0.42
1:A:1227:THR:HG23	1:A:1229:GLU:H	1.84	0.42
1:A:963:ARG:NH2	1:A:967:ARG:HH21	2.18	0.42
1:A:466:LYS:HE3	2:B:1097:HIS:HD2	1.83	0.42
2:B:249:LYS:HA	2:B:252:ILE:HB	2.00	0.42
2:B:24:GLU:O	2:B:28:ILE:HB	2.19	0.42
5:E:116:GLN:HA	5:E:119:VAL:HG22	2.02	0.42
5:E:139:ILE:H	5:E:139:ILE:HG13	1.67	0.42
1:A:358:ARG:HH12	2:B:1076:GLU:HA	1.83	0.42
2:B:629:GLU:HB3	2:B:630:LYS:H	1.64	0.42
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	2.00	0.42
1:A:546:ARG:NH1	1:A:550:LYS:HZ3	2.17	0.42
2:B:285:LEU:HD11	2:B:305:LEU:HD11	2.00	0.42
4:D:30:GLU:O	7:G:4:HIS:N	2.47	0.42
1:A:734:ARG:NH1	9:I:108:MET:HG3	2.35	0.42
1:A:823:VAL:HG13	1:A:835:GLU:OE2	2.20	0.42
1:A:721:HIS:CD2	9:I:110:LEU:HD13	2.55	0.42
1:A:551:ARG:HH12	8:H:27:ARG:HH21	1.67	0.42
2:B:622:CYS:HB3	2:B:666:ASP:HB3	2.02	0.42
1:A:1005:HIS:HA	1:A:1006:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:125:ILE:HG22	6:F:127:ASP:H	1.85	0.41
7:G:137:ILE:HG23	7:G:141:ASP:OD2	2.20	0.41
1:A:184:CYS:SG	1:A:185:GLY:N	2.93	0.41
2:B:86:LEU:HA	2:B:129:THR:O	2.20	0.41
9:I:86:CYS:SG	9:I:87:GLN:N	2.93	0.41
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.54	0.41
2:B:177:CYS:SG	2:B:738:THR:OG1	2.64	0.41
1:A:928:ARG:HE	8:H:106:THR:HB	1.86	0.41
2:B:937:SER:OG	2:B:938:ARG:N	2.53	0.41
3:C:259:LEU:O	3:C:263:LEU:CB	2.69	0.41
1:A:365:THR:OG1	1:A:366:VAL:N	2.53	0.41
2:B:1088:GLU:HB2	2:B:1091:ARG:HH12	1.84	0.41
2:B:213:SER:OG	2:B:214:LYS:N	2.53	0.41
2:B:82:PRO:HA	2:B:133:ILE:O	2.21	0.41
1:A:792:ASN:HD21	13:M:8:HYP:HA	1.85	0.41
1:A:892:GLY:HA3	1:A:1396:ARG:HH11	1.85	0.41
2:B:1126:ALA:HB3	2:B:1146:ILE:HD11	2.03	0.41
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.25	0.41
1:A:139:LYS:HA	1:A:142:THR:HG22	2.03	0.41
5:E:177:ASP:OD1	5:E:177:ASP:N	2.54	0.41
5:E:194:ILE:HG12	5:E:204:ILE:HG12	2.02	0.41
8:H:20:LYS:NZ	8:H:45:ILE:HD12	2.35	0.41
1:A:1052:ARG:NE	1:A:1056:GLU:OE1	2.49	0.41
5:E:102:ALA:HB3	5:E:127:LEU:HG	2.03	0.41
1:A:408:ARG:HH21	1:A:412:GLN:HB3	1.86	0.41
7:G:60:GLN:HE22	7:G:65:PHE:HB2	1.86	0.41
1:A:41:ILE:HB	1:A:88:ILE:HG12	2.03	0.41
2:B:244:GLY:H	2:B:249:LYS:NZ	2.19	0.41
3:C:67:ARG:NH1	10:J:2:ILE:HG23	2.35	0.41
2:B:799:SER:O	2:B:803:ARG:NH1	2.54	0.40
1:A:52:PRO:HB2	1:A:60:PRO:HD3	2.04	0.40
2:B:225:LEU:HD23	2:B:229:SER:HB3	2.03	0.40
1:A:290:LEU:HD11	1:A:307:VAL:HG22	2.04	0.40
4:D:80:ILE:HA	4:D:83:VAL:HG12	2.04	0.40
2:B:1137:CYS:SG	2:B:1138:ARG:N	2.94	0.40
2:B:386:ASP:OD2	2:B:497:LYS:HG3	2.21	0.40
1:A:806:THR:O	2:B:503:ASN:ND2	2.54	0.40
2:B:634:LEU:HB3	2:B:661:VAL:HG12	2.03	0.40
2:B:407:MET:SD	2:B:443:GLY:HA3	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1418/1970 (72%)	1287 (91%)	129 (9%)	2 (0%)	55	88
2	B	1128/1167 (97%)	1027 (91%)	101 (9%)	0	100	100
3	C	253/275 (92%)	227 (90%)	26 (10%)	0	100	100
4	D	126/142 (89%)	114 (90%)	12 (10%)	0	100	100
5	E	207/210 (99%)	194 (94%)	13 (6%)	0	100	100
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
8	H	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
9	I	112/125 (90%)	93 (83%)	19 (17%)	0	100	100
10	J	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
13	M	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
All	All	3863/4588 (84%)	3518 (91%)	343 (9%)	2 (0%)	58	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	539	GLN
1	A	540	ASP

### 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	1258/1749 (72%)	1257 (100%)	1 (0%)	94	99
2	B	993/1021 (97%)	993 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	106/126 (84%)	105 (99%)	1 (1%)	82	92
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/153 (96%)	147 (100%)	0	100	100
8	H	129/131 (98%)	128 (99%)	1 (1%)	85	94
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3435/4066 (84%)	3432 (100%)	3 (0%)	95	99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	792	ASN
4	D	126	GLU
8	H	71	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	576	GLN
1	A	673	GLN
1	A	739	ASN
1	A	792	ASN
1	A	1230	GLN
1	A	1420	ASN
2	B	111	ASN
2	B	639	HIS
2	B	790	GLN
2	B	941	GLN
2	B	970	HIS
3	C	66	HIS

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Mol	Chain	Res	Type
7	G	139	GLN
9	I	22	ASN
9	I	45	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	13/20 (65%)	3 (23%)	1 (7%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	11	A
15	P	13	G
15	P	18	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	12	A

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
13	ILX	M	1	13	9,9,10	0.80	0	9,11,13	1.37	2 (22%)
13	TRX	M	2	13	15,16,17	1.08	1 (6%)	15,22,24	1.52	3 (20%)
13	CSX	M	6	13	4,6,7	1.37	1 (25%)	2,6,8	1.52	1 (50%)
13	HYP	M	8	13	7,8,9	0.69	0	5,10,12	2.29	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ILX	M	1	13	-	0/11/12/14	0/0/0/0
13	TRX	M	2	13	-	0/3/6/8	0/2/2/2
13	CSX	M	6	13	-	0/1/5/7	0/0/0/0
13	HYP	M	8	13	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	2	TRX	CA-C	2.03	1.52	1.50
13	M	6	CSX	CA-C	2.24	1.53	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	8	HYP	O-C-CA	-3.85	116.16	125.15
13	M	2	TRX	CH2-CZ2-CE2	-3.74	116.69	119.17
13	M	2	TRX	CB-CG-CD1	-2.98	124.28	127.97
13	M	1	ILX	OD1-CD1-CG1	-2.88	104.75	111.11
13	M	1	ILX	CB-CA-C	-2.02	110.19	112.96
13	M	6	CSX	CA-CB-SG	2.13	118.24	113.47
13	M	2	TRX	CB-CG-CD2	2.27	129.77	126.25
13	M	8	HYP	CB-CG-CD	2.84	107.08	103.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	ILX	1	0
13	M	6	CSX	1	0
13	M	8	HYP	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.