



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 22, 2018 – 09:20 PM EST

PDB ID : 6EU3
EMDB ID: : EMD-3958
Title : Apo RNA Polymerase III - closed conformation (cPOL3)
Authors : Abascal-Palacios, G.; Ramsay, E.P.; Beuron, F.; Morris, E.; Vannini, A.
Deposited on : 2017-10-27
Resolution : 3.30 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) : rb-20030736

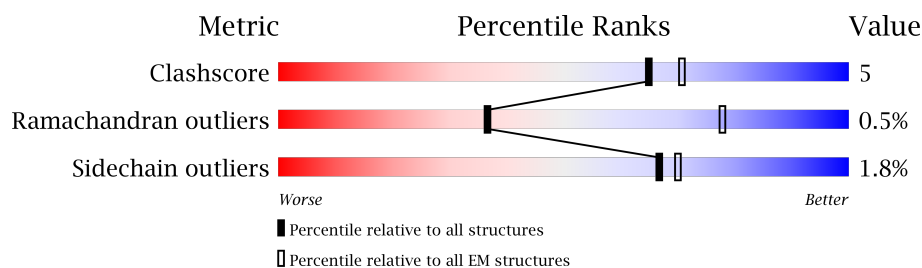
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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

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	1460	
2	B	1149	
3	C	335	
4	D	161	
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	

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Mol	Chain	Length	Quality of chain
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 38330 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1402	Total	C	N	O	S	0	0
			10980	6924	1930	2068	58		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	68	Total	C	N	O	S	0	0
			558	356	97	99	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	165	Total	C	N	O	S	0	0
			1347	862	229	255	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	105	Total	C	N	O	S	0	0
			802	508	144	147	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	537	Total	C	N	O	S	0	0
			4316	2748	739	810	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	123	Total	C	N	O	S	0	0
			1024	667	161	192	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	40	Total	C	N	O	0	0
			311	204	50	57		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Zn	0
			1	1	
18	A	2	Total	Zn	0
			2	2	
18	L	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

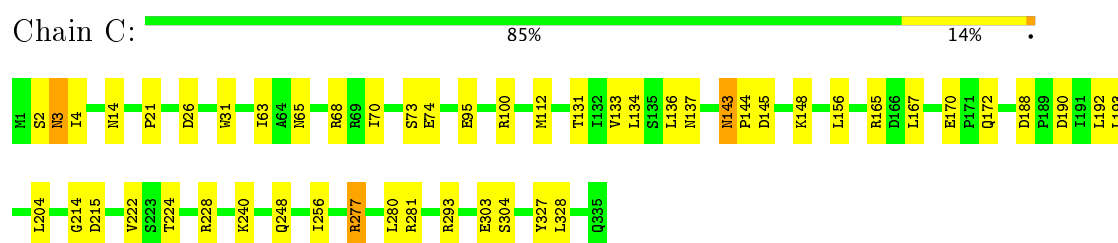
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1

- Molecule 2: DNA-directed RNA polymerase III subunit RPC2

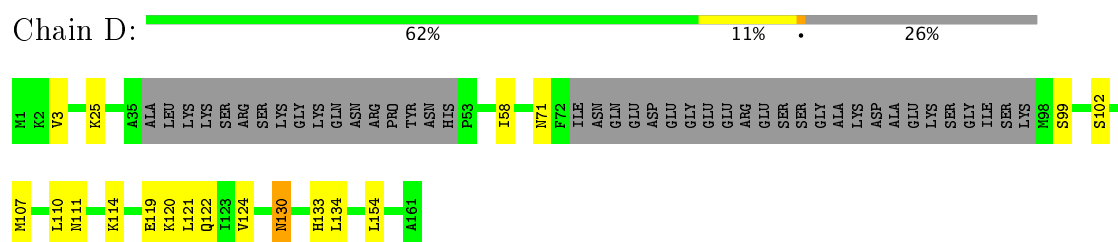
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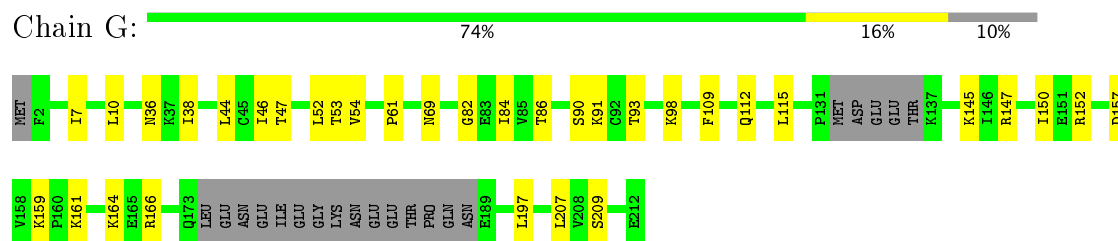
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



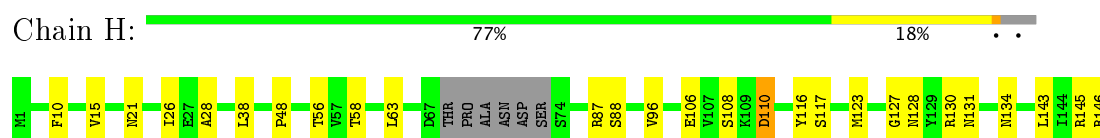
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9



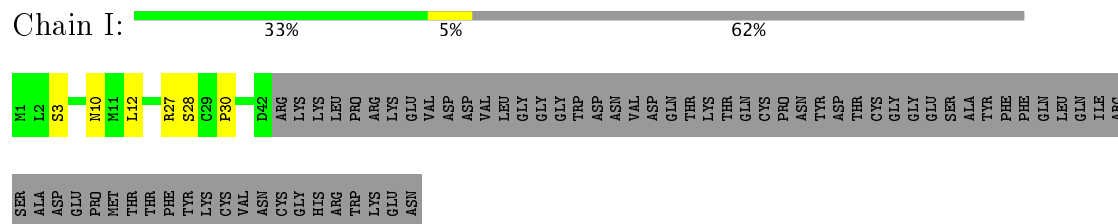
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



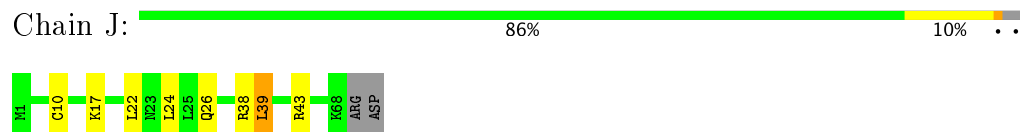
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



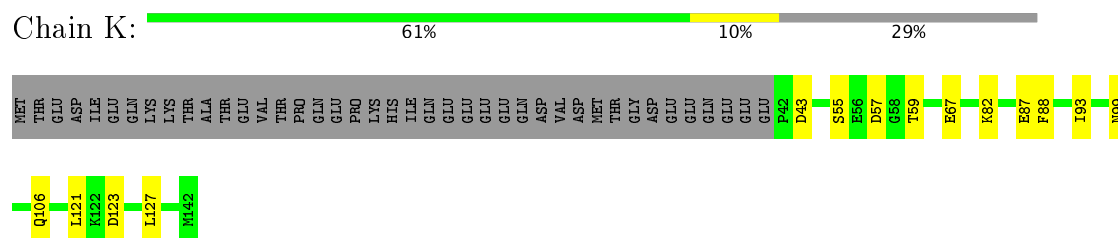
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



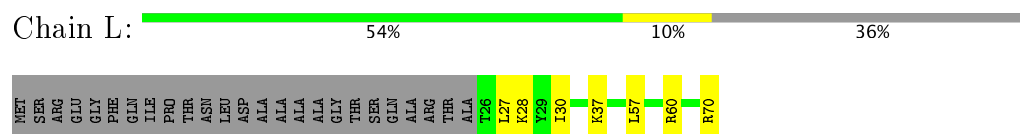
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

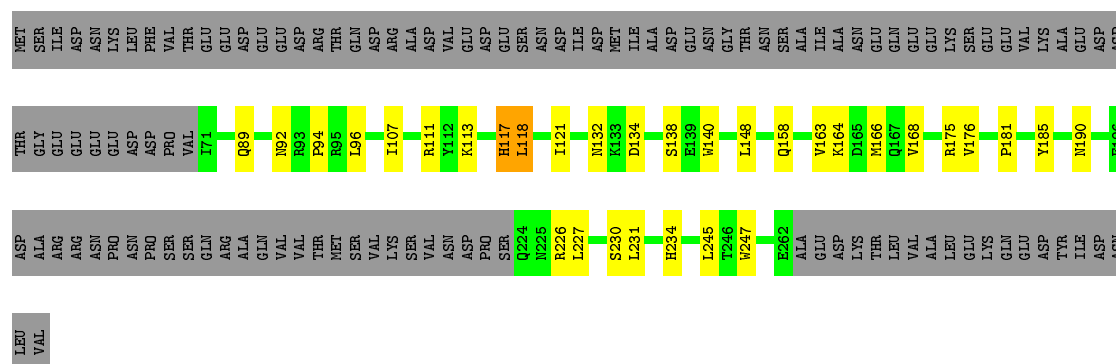


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



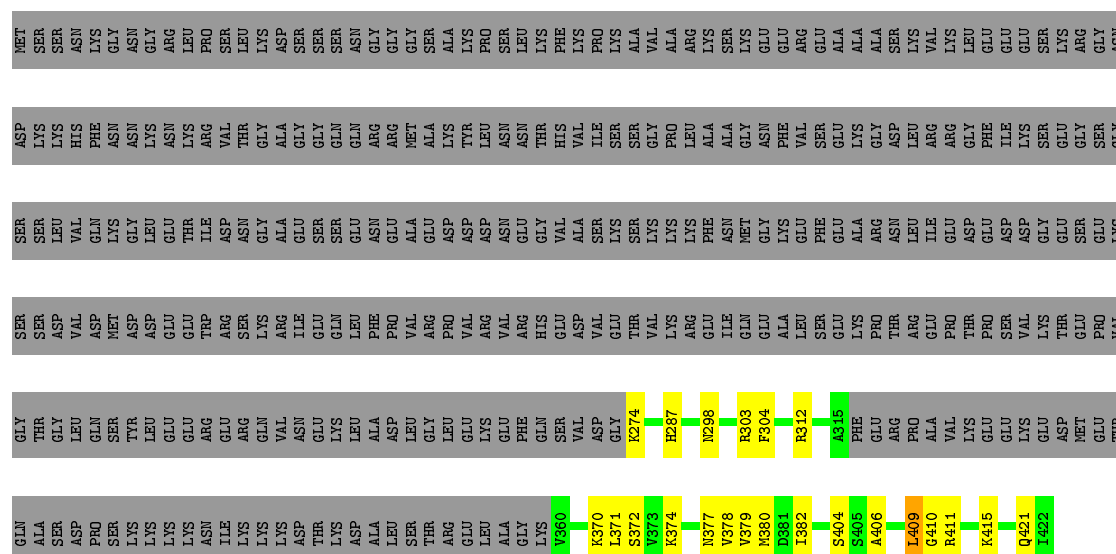
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

Chain M:



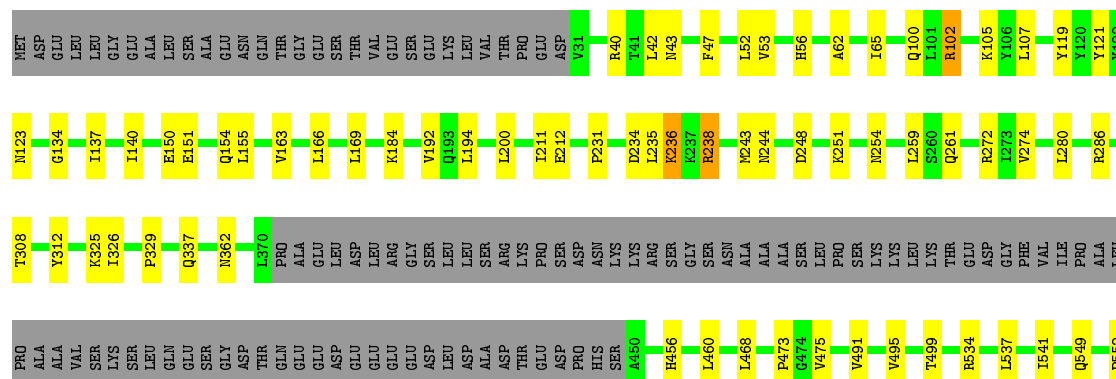
- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

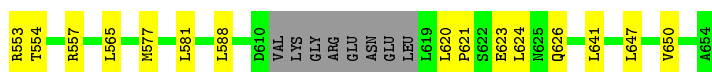
Chain N:



- Molecule 15: DNA-directed RNA polymerase III subunit RPC3

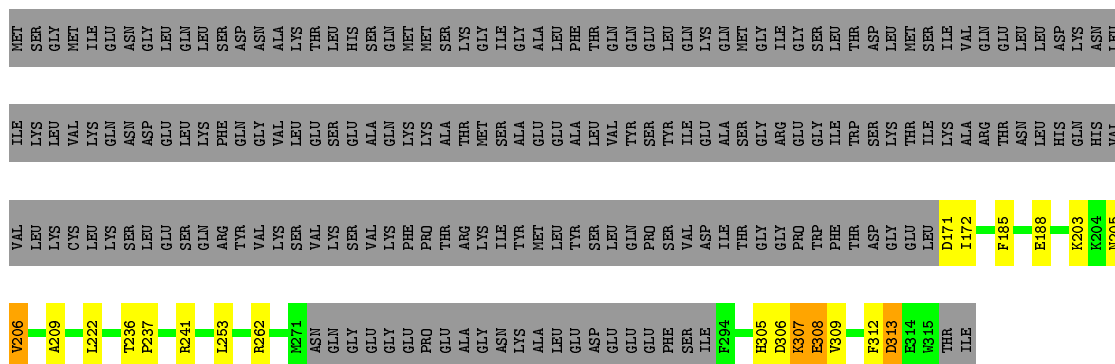
Chain O:





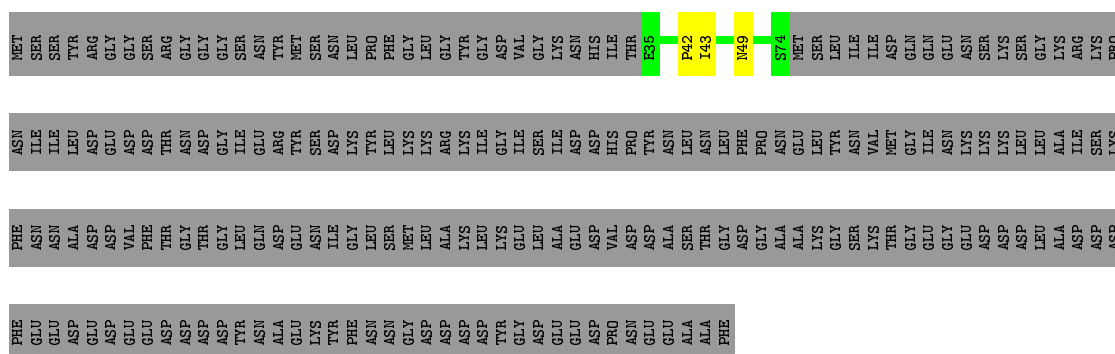
- Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P: 32% 5% 61%



- Molecule 17: DNA-directed RNA polymerase III subunit RPC7

Chain Q: 15% 84%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62306	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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

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	0.28	0/11176	0.61	6/15104 (0.0%)
10	J	0.30	0/567	0.66	1/761 (0.1%)
11	K	0.27	0/803	0.62	1/1083 (0.1%)
12	L	0.30	0/360	0.67	0/478
13	M	0.29	0/1378	0.64	0/1863
14	N	0.29	0/810	0.73	1/1088 (0.1%)
15	O	0.27	0/4380	0.61	0/5908
16	P	0.33	0/1050	0.74	0/1424
17	Q	0.42	0/320	0.73	0/434
2	B	0.28	0/8943	0.60	2/12068 (0.0%)
3	C	0.28	0/2711	0.57	1/3676 (0.0%)
4	D	0.27	0/991	0.58	0/1328
5	E	0.30	0/1795	0.52	0/2416
6	F	0.28	0/683	0.58	0/923
7	G	0.28	0/1583	0.57	0/2146
8	H	0.29	0/1138	0.61	1/1540 (0.1%)
9	I	0.29	0/328	0.62	0/445
All	All	0.29	0/39016	0.61	13/52685 (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	6
12	L	0	1
13	M	0	4
14	N	0	3
15	O	0	3
16	P	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	Q	0	1
2	B	0	8
3	C	0	1
8	H	0	1
All	All	0	36

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	409	LEU	N-CA-C	-6.86	92.49	111.00
1	A	54	LEU	CA-CB-CG	6.78	130.89	115.30
3	C	156	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	276	ASP	CB-CG-OD1	6.42	124.08	118.30
10	J	39	LEU	CA-CB-CG	6.10	129.33	115.30

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	CYS	Peptide
1	A	275	GLN	Peptide
1	A	494	PRO	Peptide
1	A	511	ASP	Peptide
1	A	631	LYS	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	10980	0	11096	118	0
2	B	8788	0	8903	104	0
3	C	2655	0	2628	29	0
4	D	977	0	983	10	0
5	E	1759	0	1788	23	0
6	F	671	0	692	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1544	0	1540	19	0
8	H	1120	0	1089	16	0
9	I	321	0	306	4	0
10	J	558	0	573	4	0
11	K	792	0	790	11	0
12	L	358	0	382	4	0
13	M	1347	0	1315	17	0
14	N	802	0	851	16	0
15	O	4316	0	4485	44	0
16	P	1024	0	992	6	0
17	Q	311	0	315	1	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
All	All	38330	0	38728	373	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.

The worst 5 of 373 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:162:GLY:HA3	1:A:181:ASP:O	1.86	0.75
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.73	0.70
15:O:107:LEU:O	15:O:119:TYR:HB2	1.92	0.69
1:A:475:ASN:HD21	2:B:1066:GLU:HG2	1.60	0.65
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.79	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1394/1460 (96%)	1213 (87%)	174 (12%)	7 (0%)	32	66
2	B	1112/1149 (97%)	979 (88%)	128 (12%)	5 (0%)	38	71
3	C	333/335 (99%)	299 (90%)	32 (10%)	2 (1%)	28	63
4	D	113/161 (70%)	96 (85%)	17 (15%)	0	100	100
5	E	213/215 (99%)	195 (92%)	18 (8%)	0	100	100
6	F	81/155 (52%)	68 (84%)	13 (16%)	0	100	100
7	G	185/212 (87%)	162 (88%)	23 (12%)	0	100	100
8	H	136/146 (93%)	115 (85%)	21 (15%)	0	100	100
9	I	40/110 (36%)	35 (88%)	5 (12%)	0	100	100
10	J	66/70 (94%)	56 (85%)	10 (15%)	0	100	100
11	K	99/142 (70%)	88 (89%)	11 (11%)	0	100	100
12	L	43/70 (61%)	36 (84%)	7 (16%)	0	100	100
13	M	161/282 (57%)	123 (76%)	36 (22%)	2 (1%)	15	50
14	N	101/422 (24%)	82 (81%)	18 (18%)	1 (1%)	18	53
15	O	531/654 (81%)	470 (88%)	60 (11%)	1 (0%)	51	81
16	P	119/317 (38%)	82 (69%)	31 (26%)	6 (5%)	2	17
17	Q	38/251 (15%)	28 (74%)	10 (26%)	0	100	100
All	All	4765/6151 (78%)	4127 (87%)	614 (13%)	24 (0%)	37	66

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	839	GLY
2	B	935	ASP
1	A	495	TRP
2	B	297	THR
16	P	309	VAL

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	1215/1257 (97%)	1196 (98%)	19 (2%)	68	84
2	B	975/1006 (97%)	960 (98%)	15 (2%)	70	85
3	C	296/296 (100%)	289 (98%)	7 (2%)	54	79
4	D	110/145 (76%)	106 (96%)	4 (4%)	40	72
5	E	197/197 (100%)	193 (98%)	4 (2%)	60	81
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	170/190 (90%)	169 (99%)	1 (1%)	89	93
8	H	123/128 (96%)	121 (98%)	2 (2%)	68	84
9	I	38/98 (39%)	37 (97%)	1 (3%)	51	77
10	J	63/65 (97%)	62 (98%)	1 (2%)	68	84
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	143/249 (57%)	139 (97%)	4 (3%)	49	76
14	N	88/360 (24%)	84 (96%)	4 (4%)	32	67
15	O	493/593 (83%)	482 (98%)	11 (2%)	57	80
16	P	116/285 (41%)	115 (99%)	1 (1%)	82	90
17	Q	35/212 (16%)	34 (97%)	1 (3%)	48	75
All	All	4266/5405 (79%)	4191 (98%)	75 (2%)	67	83

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1048	ARG
4	D	25	LYS
15	O	286	ARG
3	C	112	MET
3	C	240	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	893	GLN
4	D	71	ASN
15	O	544	ASN

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Mol	Chain	Res	Type
2	B	916	HIS
3	C	137	ASN

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 ⓘ

Of 7 ligands modelled in this entry, 7 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.