



Full wwPDB/EMDatabank EM Map/Model Validation 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 Full wwPDB/EMDatabank EM Map/Model Validation 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

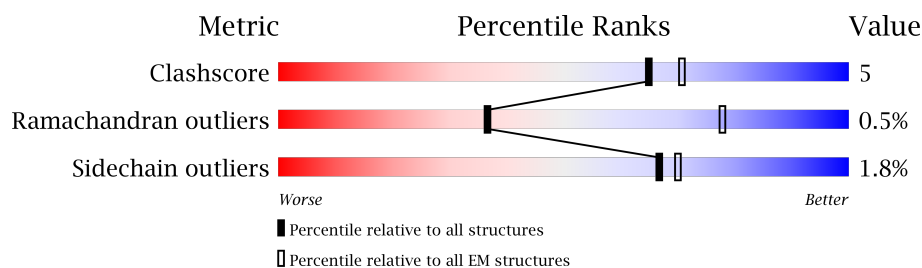
1 Overall quality at a glance

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.






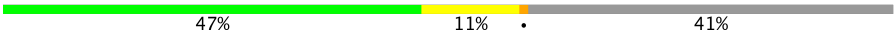




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	 86%10% . .
11	K	142	 61%10%29%
12	L	70	 54%10%36%
13	M	282	 47%11%.41%
14	N	422	 20%5%75%
15	O	654	 69%12%18%
16	P	317	 32%5%.61%
17	Q	251	 15%.84%

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	

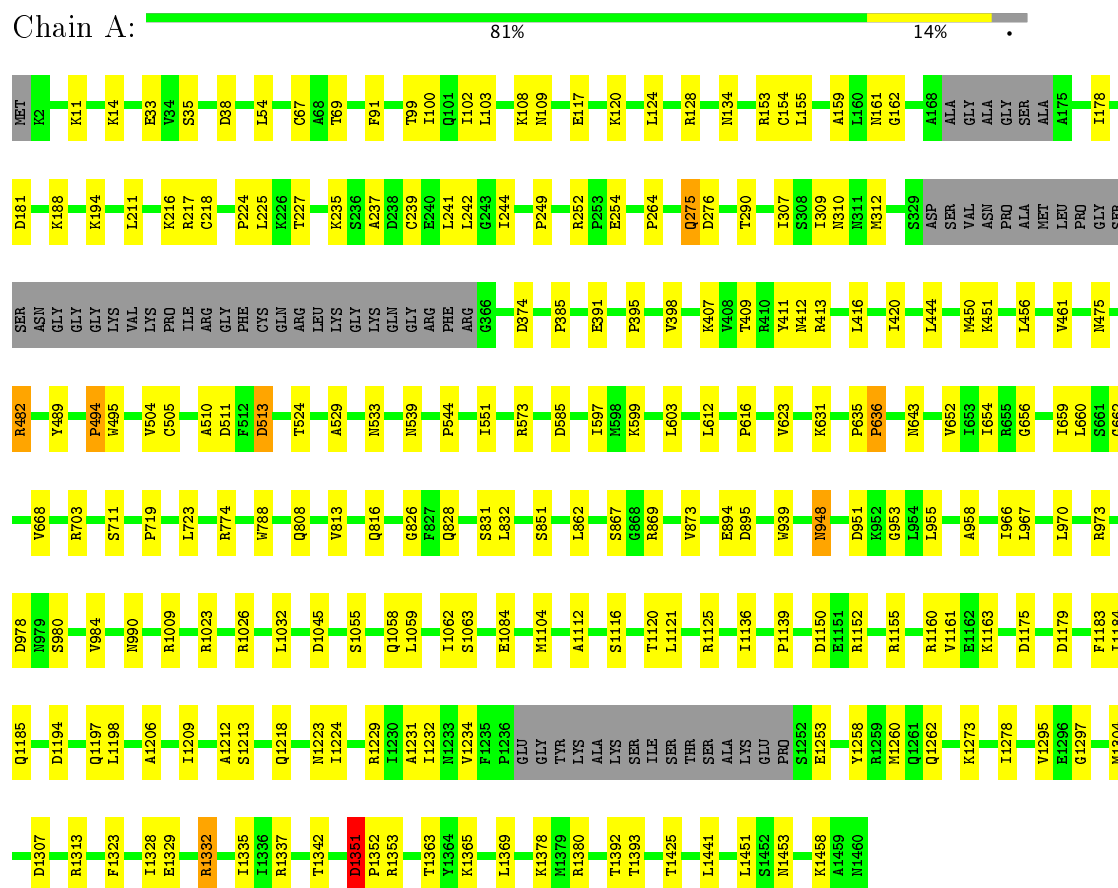
- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

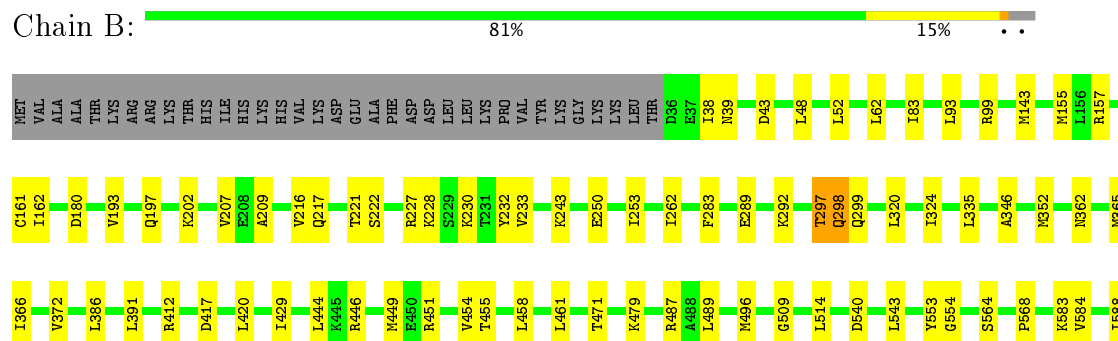
3 Residue-property plots

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: DNA-directed RNA polymerase III subunit RPC1

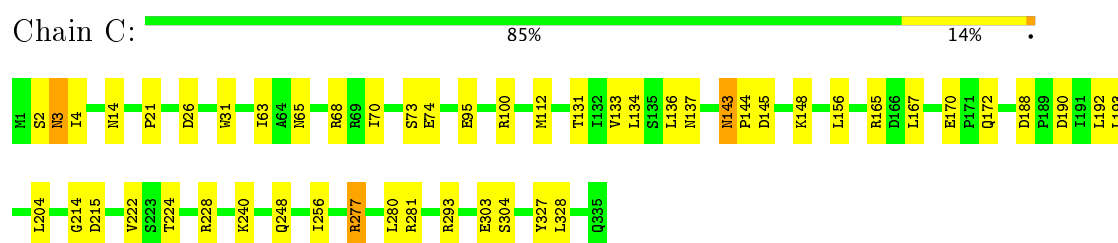


- Molecule 2: DNA-directed RNA polymerase III subunit RPC2

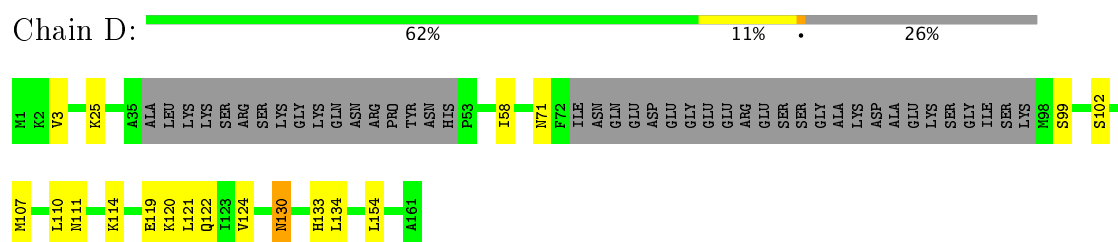




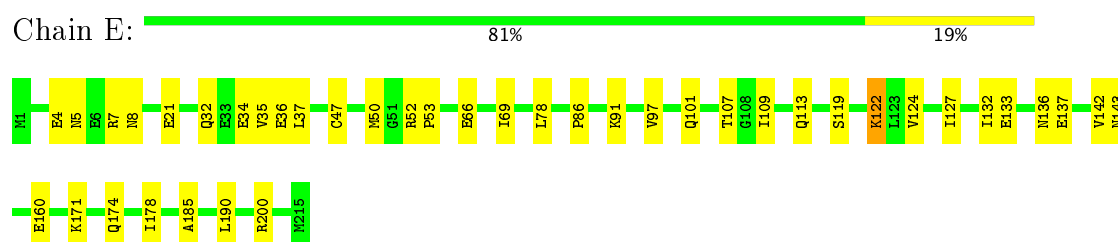
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



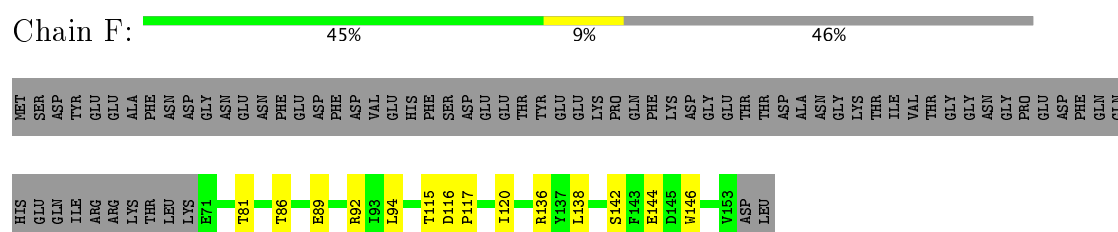
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9



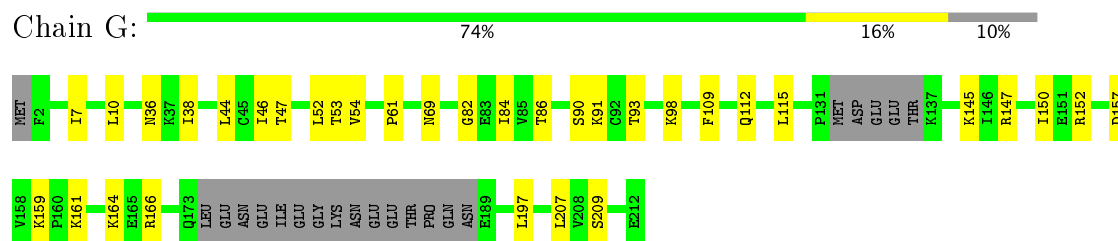
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



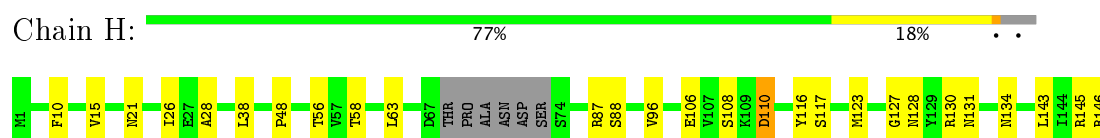
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



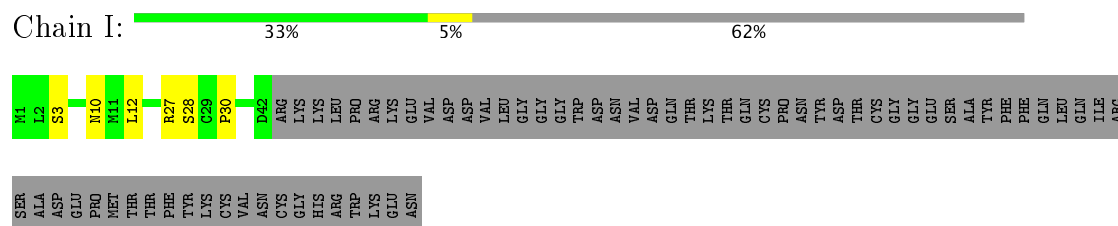
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



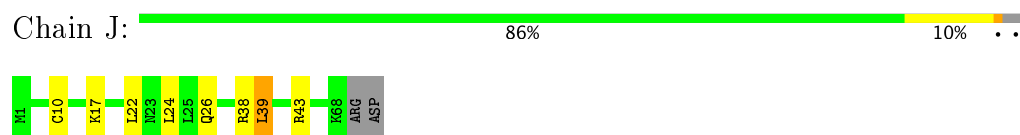
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



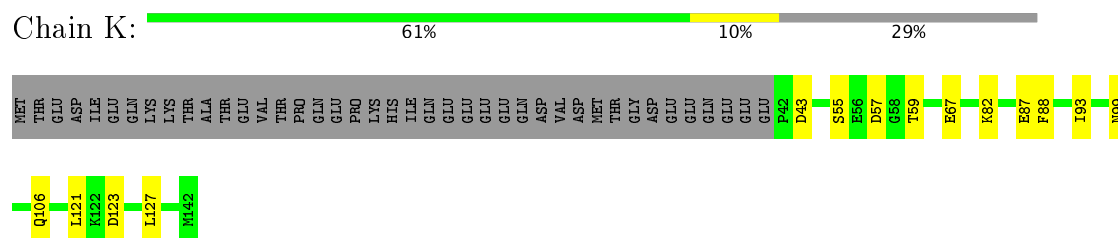
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



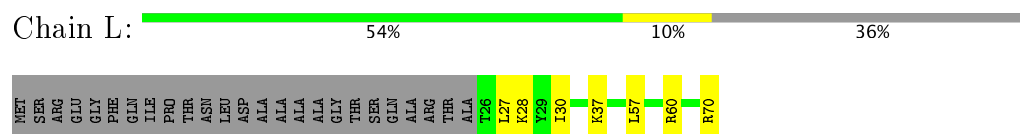
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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

Response	Percentage
Yes	47%
No	11%
Don't know	41%

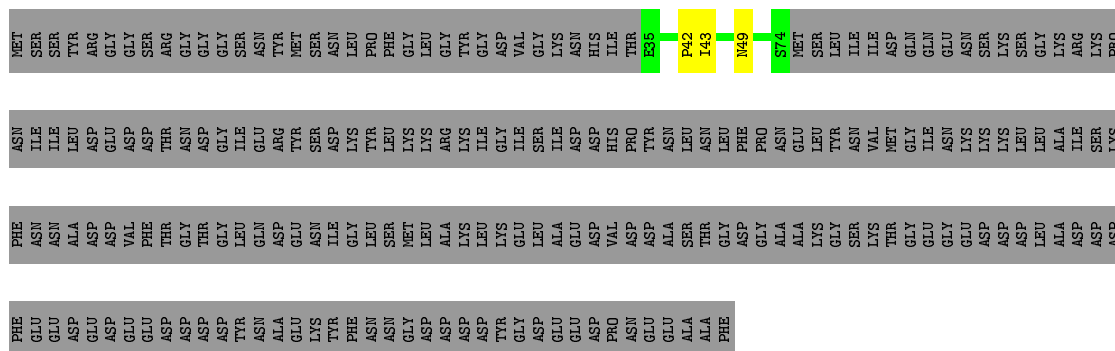


Frequency	Percentage
Daily	20%
Weekly	5%
Not at all	75%



Response	Percentage
U.S. is responsible	69%
U.S. is not responsible	12%
Unsure	18%





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.

All (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
2	B	335	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	1351	ASP	CB-CG-OD1	5.75	123.47	118.30
8	H	110	ASP	CB-CG-OD1	5.74	123.46	118.30
11	K	57	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	513	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	275	GLN	C-N-CA	5.19	134.69	121.70
1	A	585	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	839	GLY	N-CA-C	5.01	125.64	113.10

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1351	ASP	Peptide
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
2	B	297	THR	Peptide
2	B	298	GLN	Peptide
2	B	583	LYS	Peptide
2	B	838	SER	Peptide
2	B	856	ASN	Peptide
2	B	889	SER	Peptide
2	B	932	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	934	ASN	Peptide
3	C	3	ASN	Peptide
8	H	108	SER	Peptide
12	L	28	LYS	Peptide
13	M	107	ILE	Peptide
13	M	117	HIS	Peptide
13	M	166	MET	Peptide
13	M	96	LEU	Peptide
14	N	377	ASN	Peptide
14	N	379	VAL	Peptide
14	N	410	GLY	Peptide
15	O	238	ARG	Peptide
15	O	248	ASP	Peptide
15	O	326	ILE	Peptide
16	P	205	ASN	Peptide
16	P	209	ALA	Peptide
16	P	236	THR	Peptide
16	P	306	ASP	Peptide
16	P	307	LYS	Peptide
16	P	308	GLU	Peptide
16	P	312	PHE	Peptide
16	P	313	ASP	Peptide
17	Q	43	ILE	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
7:G:90:SER:HB2	7:G:98:LYS:HG3	1.80	0.64
2:B:589:SER:HB3	2:B:653:GLU:HG3	1.81	0.63
2:B:607:ARG:HH11	2:B:651:VAL:HB	1.64	0.63
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.81	0.63
4:D:58:ILE:HD12	7:G:36:ASN:HD21	1.64	0.63
2:B:887:SER:HB2	2:B:895:LEU:HB3	1.81	0.62
1:A:869:ARG:HH21	2:B:509:GLY:HA2	1.62	0.62
15:O:552:PRO:HG3	15:O:557:ARG:HA	1.80	0.62
1:A:1328:ILE:HD13	5:E:178:ILE:HG13	1.83	0.61
1:A:235:LYS:HG3	1:A:237:ALA:H	1.64	0.61
1:A:216:LYS:HD3	1:A:217:ARG:HG3	1.83	0.61
3:C:277:ARG:HB2	3:C:280:LEU:HD12	1.83	0.60
15:O:40:ARG:NH2	16:P:313:ASP:OD1	2.34	0.60
1:A:482:ARG:HH11	1:A:544:PRO:HG3	1.66	0.60
2:B:694:ASN:HD21	2:B:916:HIS:HD2	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.84	0.59
2:B:52:LEU:HD22	2:B:743:LEU:HD23	1.84	0.59
1:A:38:ASP:HB2	1:A:290:THR:HG23	1.83	0.59
1:A:1369:LEU:HD11	1:A:1378:LYS:HB3	1.85	0.59
1:A:1152:ARG:NH1	1:A:1197:GLN:OE1	2.36	0.59
1:A:573:ARG:HH22	11:K:87:GLU:HB3	1.67	0.58
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.36	0.58
3:C:63:ILE:HD13	11:K:127:LEU:HD21	1.85	0.58
2:B:675:ILE:HG22	2:B:676:GLU:HG3	1.83	0.58
2:B:776:SER:O	2:B:780:ARG:NH1	2.37	0.58
3:C:2:SER:O	3:C:14:ASN:ND2	2.37	0.58
1:A:252:ARG:NH2	1:A:254:GLU:OE2	2.36	0.58
1:A:652:VAL:HG22	1:A:662:GLY:HA3	1.87	0.57
1:A:1184:ILE:HD12	1:A:1232:ILE:HB	1.86	0.57
1:A:154:CYS:SG	1:A:155:LEU:N	2.77	0.57
10:J:24:LEU:HD12	10:J:39:LEU:HD12	1.86	0.57
1:A:103:LEU:O	1:A:108:LYS:NZ	2.37	0.57
2:B:612:LEU:HD12	2:B:649:LEU:HD12	1.84	0.57
10:J:22:LEU:O	10:J:26:GLN:NE2	2.38	0.57
2:B:788:ARG:NH1	2:B:882:ASP:OD2	2.38	0.56
2:B:588:ILE:HA	2:B:602:ALA:O	2.05	0.56
1:A:1206:ALA:HB2	1:A:1224:ILE:HD11	1.87	0.56
2:B:496:MET:HB3	2:B:608:ILE:HD12	1.87	0.56
15:O:620:LEU:HD22	15:O:623:GLU:HG2	1.87	0.56
1:A:869:ARG:HD3	2:B:489:LEU:HB2	1.88	0.56
6:F:92:ARG:HH21	7:G:61:PRO:HG3	1.69	0.56
1:A:505:CYS:HB2	1:A:510:ALA:HB3	1.88	0.56
8:H:58:THR:HB	8:H:143:LEU:HB2	1.88	0.56
1:A:1185:GLN:OE1	1:A:1229:ARG:NH1	2.39	0.56
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.86	0.56
16:P:203:LYS:HB2	16:P:206:VAL:HG22	1.87	0.55
2:B:299:GLN:HG3	13:M:190:ASN:HD22	1.71	0.55
1:A:533:ASN:O	1:A:539:ASN:ND2	2.40	0.55
2:B:622:VAL:HG22	2:B:645:LEU:HD23	1.88	0.55
15:O:137:ILE:HA	15:O:140:ILE:HG22	1.89	0.55
4:D:110:LEU:HD21	4:D:120:LYS:HB2	1.87	0.55
9:I:28:SER:O	13:M:185:TYR:OH	2.25	0.55
2:B:202:LYS:HB3	2:B:222:SER:HB2	1.89	0.55
2:B:882:ASP:HB3	2:B:901:ARG:HE	1.72	0.54
14:N:304:PHE:CE1	14:N:409:LEU:HB3	2.41	0.54
7:G:84:ILE:HD11	7:G:147:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:THR:HG22	7:G:145:LYS:HD2	1.89	0.54
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.90	0.54
1:A:654:ILE:HG12	1:A:659:ILE:HG13	1.90	0.54
1:A:1441:LEU:HD21	7:G:54:VAL:HG22	1.89	0.54
1:A:1059:LEU:HD11	8:H:106:GLU:HB2	1.89	0.54
2:B:838:SER:O	2:B:840:GLN:N	2.39	0.54
14:N:409:LEU:HD12	14:N:409:LEU:N	2.23	0.54
6:F:89:GLU:OE2	6:F:136:ARG:NH2	2.41	0.53
1:A:1055:SER:HB2	8:H:131:ASN:HD22	1.73	0.53
1:A:1023:ARG:NH2	1:A:1045:ASP:OD1	2.41	0.53
15:O:43:ASN:HB2	15:O:47:PHE:HB2	1.90	0.53
15:O:312:TYR:HB2	15:O:460:LEU:HD21	1.89	0.53
3:C:143:ASN:HD22	3:C:144:PRO:HD2	1.73	0.53
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.40	0.53
1:A:391:GLU:HG2	1:A:489:TYR:HB2	1.91	0.53
2:B:62:LEU:HA	2:B:155:MET:HE1	1.90	0.53
2:B:207:VAL:HG22	2:B:217:GLN:HG3	1.90	0.53
1:A:504:VAL:HG12	1:A:551:ILE:HD11	1.91	0.53
2:B:774:ASN:ND2	2:B:775:LYS:O	2.42	0.53
1:A:1278:ILE:HG13	1:A:1297:GLY:HA3	1.89	0.53
5:E:4:GLU:O	5:E:8:ASN:ND2	2.38	0.53
6:F:117:PRO:HA	6:F:120:ILE:HG12	1.91	0.52
2:B:209:ALA:HB2	2:B:366:ILE:HG21	1.90	0.52
7:G:98:LYS:HB3	7:G:109:PHE:HD1	1.74	0.52
7:G:91:LYS:NZ	7:G:93:THR:OG1	2.42	0.52
14:N:303:ARG:HG3	14:N:411:ARG:HB2	1.91	0.52
15:O:194:LEU:HD22	15:O:200:LEU:HG	1.91	0.52
1:A:1332:ARG:HB3	1:A:1363:THR:HG21	1.92	0.52
2:B:543:LEU:HG	13:M:176:VAL:HG11	1.91	0.52
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.92	0.52
8:H:48:PRO:O	8:H:146:ARG:NH2	2.42	0.52
14:N:409:LEU:N	14:N:409:LEU:CD1	2.73	0.52
2:B:927:LYS:NZ	3:C:214:GLY:O	2.43	0.52
1:A:1304:MET:HG2	5:E:142:VAL:HG11	1.90	0.52
13:M:230:SER:O	13:M:234:HIS:ND1	2.41	0.52
2:B:612:LEU:HD22	2:B:674:GLU:HA	1.90	0.51
15:O:150:GLU:HG2	15:O:151:GLU:HG3	1.92	0.51
1:A:652:VAL:HG21	1:A:668:VAL:HG21	1.91	0.51
1:A:1425:THR:HG22	6:F:92:ARG:HD2	1.91	0.51
1:A:224:PRO:HA	1:A:227:THR:HG22	1.91	0.51
1:A:1253:GLU:OE2	9:I:27:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:736:VAL:HG12	2:B:974:GLU:HB2	1.92	0.51
14:N:380:MET:SD	14:N:421:GLN:NE2	2.83	0.51
1:A:873:VAL:HG21	2:B:487:ARG:HB3	1.92	0.51
1:A:1329:GLU:OE2	5:E:200:ARG:NE	2.44	0.51
7:G:161:LYS:HZ2	7:G:166:ARG:HA	1.76	0.51
2:B:553:TYR:HD2	2:B:568:PRO:HG2	1.76	0.51
14:N:372:SER:HB2	14:N:382:ILE:HG22	1.91	0.51
15:O:102:ARG:O	15:O:123:ASN:ND2	2.43	0.51
1:A:1351:ASP:O	1:A:1353:ARG:N	2.44	0.51
1:A:894:GLU:OE2	2:B:1067:ARG:NH1	2.44	0.51
2:B:623:LYS:H	2:B:626:HIS:HD2	1.58	0.51
1:A:307:ILE:HD11	1:A:312:MET:HG2	1.91	0.50
1:A:808:GLN:HE21	1:A:813:VAL:HG13	1.77	0.50
7:G:52:LEU:HD12	7:G:53:THR:HG22	1.93	0.50
2:B:197:GLN:HE22	2:B:454:VAL:HG22	1.75	0.50
1:A:813:VAL:HG23	1:A:851:SER:HA	1.92	0.50
2:B:616:SER:HG	2:B:621:ARG:HH21	1.57	0.50
1:A:413:ARG:NH1	1:A:456:LEU:O	2.41	0.50
2:B:554:GLY:HA2	2:B:564:SER:HA	1.93	0.50
2:B:372:VAL:HB	2:B:651:VAL:HG11	1.93	0.50
3:C:100:ARG:NH1	3:C:193:LEU:O	2.45	0.50
1:A:1323:PHE:HE1	1:A:1328:ILE:HG13	1.77	0.50
3:C:143:ASN:ND2	3:C:145:ASP:OD1	2.44	0.50
15:O:308:THR:HG23	15:O:456:HIS:HB3	1.94	0.50
11:K:67:GLU:HA	11:K:99:ASN:HB3	1.93	0.50
15:O:163:VAL:HA	15:O:169:LEU:HD13	1.93	0.50
1:A:124:LEU:HD23	1:A:128:ARG:HH12	1.77	0.50
8:H:127:GLY:HA3	8:H:130:ARG:HH21	1.77	0.49
1:A:1160:ARG:NH1	1:A:1307:ASP:O	2.45	0.49
2:B:738:THR:HG23	2:B:977:THR:HA	1.95	0.49
1:A:124:LEU:HD12	1:A:241:LEU:HD21	1.94	0.49
2:B:543:LEU:O	13:M:89:GLN:NE2	2.43	0.49
1:A:788:TRP:NE1	8:H:21:ASN:OD1	2.45	0.49
14:N:304:PHE:CE1	14:N:409:LEU:CB	2.96	0.49
9:I:3:SER:HB2	9:I:12:LEU:HD11	1.95	0.49
1:A:1258:TYR:O	1:A:1262:GLN:NE2	2.45	0.49
5:E:50:MET:SD	5:E:52:ARG:NH1	2.79	0.49
13:M:113:LYS:HE3	13:M:118:LEU:HB3	1.93	0.49
1:A:1223:ASN:HD21	1:A:1231:ALA:HB3	1.78	0.48
1:A:1365:LYS:NZ	1:A:1378:LYS:O	2.46	0.48
1:A:623:VAL:HG13	1:A:656:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:VAL:HG22	2:B:233:VAL:HG23	1.94	0.48
1:A:1121:LEU:O	1:A:1342:THR:OG1	2.32	0.48
2:B:800:ASN:HD22	2:B:855:PRO:HG2	1.78	0.48
2:B:1005:TYR:OH	3:C:293:ARG:NH1	2.47	0.48
5:E:109:ILE:HG22	5:E:133:GLU:HB2	1.94	0.48
12:L:27:LEU:HD11	12:L:37:LYS:HD2	1.95	0.48
1:A:1120:THR:HG22	1:A:1125:ARG:HB2	1.96	0.48
1:A:1194:ASP:O	1:A:1197:GLN:NE2	2.46	0.48
1:A:14:LYS:HD3	2:B:1144:GLU:HB3	1.96	0.48
2:B:901:ARG:NH1	3:C:95:GLU:OE1	2.38	0.48
5:E:47:CYS:HA	5:E:53:PRO:HA	1.94	0.48
5:E:171:LYS:H	5:E:174:GLN:HE21	1.61	0.48
5:E:32:GLN:HE21	5:E:36:GLU:HG3	1.79	0.48
1:A:109:ASN:HD22	1:A:159:ALA:HB2	1.79	0.48
1:A:249:PRO:HB2	15:O:42:LEU:HD22	1.94	0.48
2:B:243:LYS:HA	2:B:250:GLU:HG2	1.96	0.48
3:C:224:THR:OG1	3:C:303:GLU:OE1	2.30	0.48
3:C:327:TYR:OH	11:K:43:ASP:OD2	2.32	0.48
1:A:1136:ILE:HD11	1:A:1139:PRO:HB3	1.96	0.48
1:A:409:THR:HG23	1:A:411:TYR:H	1.78	0.48
1:A:1451:LEU:HD13	4:D:107:MET:HG3	1.95	0.48
2:B:711:GLY:HA2	2:B:728:MET:HB2	1.96	0.48
2:B:940:PRO:HG3	2:B:1019:PHE:HE1	1.78	0.47
2:B:929:GLU:OE2	3:C:73:SER:OG	2.25	0.47
7:G:152:ARG:HB3	7:G:197:LEU:HD12	1.96	0.47
1:A:211:LEU:O	15:O:553:ARG:NH2	2.48	0.47
16:P:222:LEU:HB2	16:P:241:ARG:NH1	2.28	0.47
2:B:38:ILE:HG13	2:B:628:ARG:HG2	1.96	0.47
4:D:130:ASN:H	4:D:133:HIS:CE1	2.33	0.47
2:B:161:CYS:SG	2:B:162:ILE:N	2.87	0.47
1:A:117:GLU:HG3	15:O:212:GLU:HG3	1.96	0.47
5:E:119:SER:O	5:E:122:LYS:NZ	2.47	0.47
13:M:134:ASP:O	13:M:138:SER:CB	2.63	0.47
1:A:832:LEU:HD21	1:A:862:LEU:HD23	1.97	0.47
2:B:43:ASP:HB3	2:B:627:LEU:HD13	1.97	0.47
5:E:91:LYS:HE3	15:O:231:PRO:HG2	1.96	0.47
15:O:499:THR:HG23	17:Q:42:PRO:HA	1.97	0.47
2:B:217:GLN:HB3	2:B:232:TYR:HB3	1.96	0.47
3:C:188:ASP:N	3:C:188:ASP:OD1	2.46	0.47
15:O:581:LEU:HD11	15:O:647:LEU:HD12	1.97	0.47
2:B:227:ARG:NH2	2:B:449:MET:SD	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:287:HIS:HB3	14:N:371:LEU:HD13	1.96	0.47
15:O:140:ILE:HD11	15:O:194:LEU:HD21	1.96	0.47
1:A:1058:GLN:NE2	8:H:134:ASN:O	2.48	0.47
14:N:374:LYS:HA	14:N:380:MET:HG2	1.97	0.47
1:A:385:PRO:HD2	2:B:765:TYR:CD1	2.50	0.46
2:B:931:MET:HB3	2:B:940:PRO:HD2	1.97	0.46
2:B:702:GLN:HE22	2:B:1025:GLN:HE22	1.63	0.46
2:B:193:VAL:HG21	2:B:458:LEU:HD23	1.96	0.46
2:B:850:ASN:ND2	2:B:862:VAL:O	2.45	0.46
15:O:552:PRO:HB2	15:O:554:THR:HG22	1.96	0.46
1:A:33:GLU:HG2	1:A:35:SER:H	1.80	0.46
2:B:788:ARG:HB3	2:B:899:LEU:HD11	1.98	0.46
13:M:245:LEU:HD21	14:N:404:SER:HA	1.96	0.46
5:E:97:VAL:HG13	5:E:127:ILE:HD11	1.97	0.46
4:D:119:GLU:HA	4:D:122:GLN:HB2	1.97	0.46
13:M:117:HIS:CE1	13:M:175:ARG:HH12	2.34	0.46
15:O:549:GLN:O	15:O:565:LEU:HB2	2.15	0.46
2:B:776:SER:HB2	2:B:928:GLN:HB2	1.98	0.46
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.98	0.46
1:A:264:PRO:HG3	2:B:1134:SER:HB2	1.98	0.46
1:A:529:ALA:O	1:A:533:ASN:ND2	2.49	0.46
7:G:10:LEU:HA	7:G:69:ASN:HA	1.97	0.46
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.98	0.46
13:M:158:GLN:HE22	14:N:415:LYS:HE3	1.81	0.46
1:A:967:LEU:HD22	1:A:1009:ARG:HH21	1.81	0.46
2:B:262:ILE:HG12	2:B:346:ALA:HB1	1.98	0.46
2:B:540:ASP:HB3	2:B:543:LEU:HD13	1.96	0.46
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.84	0.46
15:O:52:LEU:O	15:O:56:HIS:ND1	2.47	0.46
7:G:112:GLN:HG2	7:G:115:LEU:HD22	1.98	0.45
7:G:157:ASP:HB3	7:G:159:LYS:HG3	1.97	0.45
2:B:832:VAL:HB	12:L:60:ARG:HA	1.98	0.45
15:O:621:PRO:HA	15:O:624:LEU:HD23	1.97	0.45
1:A:374:ASP:OD1	2:B:1038:ARG:NH1	2.36	0.45
2:B:934:ASN:O	2:B:936:GLN:N	2.48	0.45
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.99	0.45
1:A:1332:ARG:HA	1:A:1335:ILE:HG22	1.98	0.45
1:A:597:ILE:HB	1:A:603:LEU:HB2	1.98	0.45
2:B:1094:VAL:HG23	2:B:1143:LEU:HD11	1.97	0.45
13:M:121:ILE:HG22	13:M:148:LEU:HB2	1.98	0.45
1:A:1112:ALA:HB1	1:A:1116:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ASP:HB3	1:A:984:VAL:HG12	1.98	0.45
1:A:1458:LYS:NZ	4:D:111:ASN:O	2.45	0.45
5:E:124:VAL:HG23	5:E:132:ILE:HG13	1.99	0.45
14:N:304:PHE:N	14:N:304:PHE:CD1	2.85	0.45
14:N:382:ILE:HG12	14:N:421:GLN:HB3	1.99	0.45
15:O:100:GLN:NE2	15:O:166:LEU:O	2.48	0.45
15:O:588:LEU:HD23	15:O:641:LEU:HD23	1.97	0.45
3:C:215:ASP:OD1	12:L:70:ARG:NH2	2.50	0.45
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.99	0.45
1:A:895:ASP:OD2	1:A:1380:ARG:NH1	2.50	0.45
1:A:955:LEU:HB3	1:A:958:ALA:HB3	1.98	0.45
2:B:157:ARG:NH2	2:B:180:ASP:OD1	2.50	0.45
2:B:461:LEU:HD23	2:B:708:GLN:HA	1.99	0.45
4:D:99:SER:HA	4:D:102:SER:HB2	1.98	0.45
1:A:980:SER:HB3	5:E:160:GLU:HG2	1.98	0.45
1:A:225:LEU:HD23	15:O:541:ILE:HG22	1.99	0.45
5:E:101:GLN:HE21	5:E:127:ILE:HG13	1.82	0.45
1:A:239:CYS:HB3	1:A:244:ILE:HB	1.98	0.44
2:B:253:ILE:HD11	2:B:283:PHE:HE1	1.81	0.44
7:G:38:ILE:HG12	7:G:44:LEU:HD13	1.99	0.44
16:P:171:ASP:HA	16:P:172:ILE:HA	1.65	0.44
1:A:1209:ILE:HA	1:A:1212:ALA:HB2	2.00	0.44
1:A:420:ILE:HG23	1:A:444:LEU:HD21	1.99	0.44
15:O:235:LEU:HD13	15:O:238:ARG:HB2	1.99	0.44
1:A:1084:GLU:HB3	6:F:86:THR:HG23	1.98	0.44
1:A:703:ARG:NH2	11:K:93:ILE:O	2.50	0.44
12:L:30:ILE:N	12:L:57:LEU:O	2.51	0.44
15:O:200:LEU:HB3	15:O:280:LEU:HD12	1.99	0.44
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.44
1:A:1198:LEU:HD23	1:A:1273:LYS:HD3	1.99	0.44
2:B:765:TYR:HD2	2:B:924:ILE:HB	1.82	0.44
1:A:533:ASN:HD21	6:F:94:LEU:HD23	1.82	0.44
11:K:67:GLU:N	11:K:99:ASN:O	2.50	0.44
13:M:247:TRP:HD1	14:N:406:ALA:HB1	1.82	0.44
15:O:53:VAL:HG11	15:O:65:ILE:HG21	1.99	0.44
2:B:709:ALA:HA	2:B:1027:LEU:HA	1.98	0.44
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.00	0.44
2:B:935:ASP:HB2	3:C:228:ARG:HB3	1.99	0.44
3:C:100:ARG:NH2	3:C:192:LEU:O	2.50	0.44
14:N:304:PHE:N	14:N:304:PHE:HD1	2.15	0.44
15:O:192:VAL:HG23	15:O:274:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:ASN:HB3	1:A:951:ASP:HB2	1.99	0.44
2:B:1004:LEU:HB2	2:B:1013:LEU:HD12	1.98	0.44
2:B:289:GLU:HA	2:B:292:LYS:HD3	1.99	0.44
2:B:386:LEU:HB3	2:B:444:LEU:HD21	2.00	0.44
8:H:96:VAL:HG12	8:H:143:LEU:HD23	1.99	0.44
1:A:1175:ASP:HA	1:A:1183:PHE:O	2.18	0.44
1:A:1161:VAL:HG11	1:A:1295:VAL:HG11	1.98	0.44
4:D:121:LEU:HA	4:D:124:VAL:HG12	2.00	0.44
16:P:222:LEU:HD21	16:P:237:PRO:HG3	1.99	0.44
1:A:153:ARG:HB3	15:O:337:GLN:HB3	1.99	0.43
2:B:417:ASP:HA	2:B:420:LEU:HB2	2.00	0.43
3:C:136:LEU:HB3	3:C:204:LEU:HG	2.00	0.43
4:D:134:LEU:HD13	4:D:154:LEU:HD11	2.00	0.43
1:A:1026:ARG:HH22	8:H:110:ASP:H	1.66	0.43
8:H:10:PHE:HD2	8:H:38:LEU:HD22	1.83	0.43
2:B:197:GLN:OE1	2:B:451:ARG:NH1	2.51	0.43
2:B:391:LEU:HD23	2:B:429:ILE:HA	1.99	0.43
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.99	0.43
1:A:719:PRO:HB3	1:A:723:LEU:HD23	2.00	0.43
1:A:966:ILE:HA	1:A:970:LEU:HD12	2.01	0.43
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.99	0.43
1:A:309:ILE:HG13	1:A:310:ASN:H	1.83	0.43
1:A:91:PHE:HE1	1:A:99:THR:HG21	1.83	0.43
3:C:131:THR:O	3:C:172:GLN:NE2	2.51	0.43
3:C:70:ILE:HB	3:C:74:GLU:HB2	2.01	0.43
5:E:113:GLN:NE2	5:E:137:GLU:OE2	2.51	0.43
6:F:115:THR:HG22	6:F:116:ASP:H	1.84	0.43
6:F:81:THR:HG1	6:F:146:TRP:HE1	1.66	0.43
13:M:134:ASP:O	13:M:138:SER:HB3	2.18	0.43
15:O:259:LEU:HG	15:O:261:GLN:H	1.83	0.43
1:A:612:LEU:HD23	1:A:616:PRO:HA	2.00	0.43
1:A:67:CYS:SG	1:A:69:THR:OG1	2.72	0.43
2:B:961:LEU:HD11	2:B:1022:ILE:HD11	2.00	0.43
3:C:133:VAL:HG23	3:C:170:GLU:HB2	2.01	0.43
5:E:34:GLU:HA	5:E:37:LEU:HD23	2.01	0.43
1:A:1213:SER:OG	1:A:1218:GLN:NE2	2.52	0.43
2:B:843:ILE:HB	2:B:871:VAL:HG12	2.01	0.43
15:O:134:GLY:HA2	15:O:137:ILE:HG12	2.01	0.43
2:B:935:ASP:HB3	2:B:1005:TYR:HE2	1.84	0.43
11:K:55:SER:OG	11:K:59:THR:O	2.36	0.43
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:723:THR:HA	2:B:790:LYS:HB3	2.01	0.42
7:G:46:ILE:HG22	7:G:47:THR:HG23	2.00	0.42
1:A:524:THR:HG22	2:B:1081:GLU:HG3	2.01	0.42
15:O:495:VAL:HG21	15:O:577:MET:HE1	2.00	0.42
2:B:730:TYR:O	2:B:753:GLN:NE2	2.40	0.42
15:O:211:ILE:HG23	15:O:329:PRO:HB3	2.01	0.42
2:B:885:MET:SD	2:B:887:SER:OG	2.76	0.42
15:O:154:GLN:HG2	15:O:155:LEU:HD22	2.02	0.42
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.52	0.42
3:C:328:LEU:HB3	11:K:121:LEU:HD21	2.01	0.42
15:O:623:GLU:HA	15:O:626:GLN:HB3	2.01	0.42
5:E:35:VAL:HG13	5:E:36:GLU:HG2	2.01	0.42
4:D:3:VAL:HA	7:G:7:ILE:HG22	2.01	0.42
8:H:28:ALA:HB3	8:H:38:LEU:HB3	2.02	0.42
2:B:320:LEU:HA	2:B:324:ILE:HB	2.02	0.42
2:B:471:THR:HG22	2:B:514:LEU:HB2	2.02	0.42
2:B:615:VAL:HG12	2:B:620:SER:HA	2.01	0.42
9:I:30:PRO:HG3	13:M:140:TRP:HZ2	1.84	0.42
16:P:185:PHE:HA	16:P:188:GLU:HG2	2.02	0.42
1:A:102:ILE:HG13	1:A:242:LEU:HD22	2.01	0.41
1:A:828:GLN:HB3	2:B:655:ASN:HD21	1.84	0.41
2:B:983:LYS:HG3	2:B:985:GLU:H	1.84	0.41
8:H:15:VAL:HG22	8:H:26:ILE:HG22	2.02	0.41
2:B:774:ASN:HB3	2:B:777:SER:HB3	2.02	0.41
1:A:1392:THR:HG22	1:A:1393:THR:H	1.85	0.41
2:B:913:SER:HB2	2:B:1027:LEU:HD11	2.01	0.41
3:C:26:ASP:N	3:C:26:ASP:OD1	2.52	0.41
5:E:78:LEU:HB3	5:E:107:THR:HG23	2.03	0.41
5:E:86:PRO:HA	5:E:113:GLN:HG2	2.02	0.41
1:A:953:GLY:HA2	1:A:1063:SER:HA	2.02	0.41
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	2.01	0.41
13:M:227:LEU:HB3	13:M:231:LEU:HB2	2.03	0.41
15:O:62:ALA:HA	15:O:65:ILE:HG22	2.03	0.41
2:B:932:PRO:HB2	2:B:1004:LEU:HD13	2.01	0.41
1:A:100:ILE:HD11	1:A:178:ILE:HD12	2.01	0.41
1:A:1234:VAL:HG11	1:A:1260:MET:HE1	2.02	0.41
3:C:248:GLN:HA	3:C:256:ILE:HD11	2.01	0.41
7:G:207:LEU:HD23	7:G:209:SER:H	1.85	0.41
3:C:222:VAL:HA	3:C:304:SER:HA	2.03	0.41
1:A:11:LYS:HA	2:B:1145:ASP:HA	2.02	0.41
2:B:590:ILE:HA	2:B:600:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:LEU:HD12	3:C:167:LEU:HB3	2.02	0.41
6:F:144:GLU:HG2	6:F:146:TRP:CD1	2.56	0.41
13:M:92:ASN:HD21	13:M:181:PRO:HD3	1.86	0.41
2:B:193:VAL:O	2:B:455:THR:HA	2.21	0.41
2:B:230:LYS:NZ	2:B:352:MET:SD	2.89	0.41
3:C:31:TRP:CE2	11:K:123:ASP:HB3	2.56	0.41
15:O:491:VAL:HG11	15:O:650:VAL:HG11	2.03	0.41
1:A:1150:ASP:O	1:A:1155:ARG:NH1	2.54	0.40
14:N:303:ARG:C	14:N:304:PHE:HD1	2.25	0.40
15:O:235:LEU:HD12	15:O:236:LYS:H	1.86	0.40
1:A:939:TRP:HZ2	1:A:1062:ILE:HD12	1.85	0.40
2:B:83:ILE:HD11	2:B:93:LEU:HD13	2.02	0.40
1:A:412:ASN:HB2	1:A:416:LEU:HD13	2.03	0.40
1:A:816:GLN:NE2	1:A:867:SER:OG	2.51	0.40
2:B:935:ASP:HB3	2:B:1005:TYR:CE2	2.57	0.40
7:G:82:GLY:H	7:G:150:ILE:HB	1.86	0.40
1:A:660:LEU:HD12	8:H:117:SER:HB3	2.03	0.40
15:O:473:PRO:HG2	15:O:475:VAL:HG12	2.02	0.40
15:O:534:ARG:HD3	15:O:537:LEU:HD12	2.03	0.40
1:A:826:GLY:H	1:A:831:SER:HA	1.86	0.40
1:A:711:SER:OG	2:B:1016:TYR:O	2.39	0.40
2:B:221:THR:HB	2:B:228:LYS:HB2	2.03	0.40
2:B:932:PRO:HG3	2:B:1006:SER:HA	2.04	0.40
8:H:56:THR:HB	8:H:145:ARG:HB3	2.04	0.40
15:O:231:PRO:HB3	15:O:234:ASP:HA	2.04	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	1394/1460 (96%)	1213 (87%)	174 (12%)	7 (0%)	32 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	A	513	ASP
2	B	298	GLN
3	C	4	ILE
13	M	118	LEU
16	P	206	VAL
1	A	494	PRO
1	A	1179	ASP
15	O	236	LYS
16	P	307	LYS
1	A	1352	PRO

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Mol	Chain	Res	Type
13	M	94	PRO
16	P	253	LEU
16	P	305	HIS
16	P	308	GLU
1	A	599	LYS
1	A	636	PRO
3	C	3	ASN
2	B	584	VAL
14	N	378	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4266/5405 (79%)	4191 (98%)	75 (2%)	67 83

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	161	ASN
1	A	188	LYS
1	A	194	LYS
1	A	450	MET
1	A	451	LYS
1	A	482	ARG
1	A	643	ASN
1	A	774	ARG
1	A	948	ASN
1	A	973	ARG
1	A	990	ASN
1	A	1032	LEU
1	A	1104	MET
1	A	1163	LYS
1	A	1313	ARG
1	A	1332	ARG
1	A	1337	ARG
1	A	1453	ASN
2	B	39	ASN
2	B	48	LEU
2	B	99	ARG
2	B	143	MET
2	B	362	ASN
2	B	365	MET
2	B	412	ARG
2	B	446	ARG
2	B	479	LYS
2	B	664	LYS
2	B	774	ASN
2	B	861	ASN
2	B	919	LYS
2	B	997	ASN
2	B	1048	ARG
3	C	112	MET
3	C	137	ASN
3	C	143	ASN

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Mol	Chain	Res	Type
3	C	148	LYS
3	C	240	LYS
3	C	277	ARG
3	C	281	ARG
4	D	25	LYS
4	D	71	ASN
4	D	114	LYS
4	D	130	ASN
5	E	5	ASN
5	E	7	ARG
5	E	122	LYS
5	E	136	ASN
7	G	164	LYS
8	H	87	ARG
8	H	128	ASN
9	I	10	ASN
10	J	38	ARG
13	M	111	ARG
13	M	132	ASN
13	M	164	LYS
13	M	226	ARG
14	N	274	LYS
14	N	298	ASN
14	N	312	ARG
14	N	370	LYS
15	O	102	ARG
15	O	184	LYS
15	O	243	MET
15	O	244	ASN
15	O	251	LYS
15	O	254	ASN
15	O	272	ARG
15	O	286	ARG
15	O	325	LYS
15	O	362	ASN
15	O	468	LEU
16	P	262	ARG
17	Q	49	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	109	ASN
1	A	161	ASN
1	A	229	ASN
1	A	386	ASN
1	A	533	ASN
1	A	566	HIS
1	A	643	ASN
1	A	808	GLN
1	A	816	GLN
1	A	899	GLN
1	A	948	ASN
1	A	990	ASN
1	A	1218	GLN
1	A	1233	ASN
1	A	1254	ASN
1	A	1262	GLN
1	A	1354	HIS
1	A	1419	GLN
1	A	1453	ASN
2	B	39	ASN
2	B	334	HIS
2	B	362	ASN
2	B	456	HIS
2	B	593	ASN
2	B	596	GLN
2	B	626	HIS
2	B	774	ASN
2	B	861	ASN
2	B	893	GLN
2	B	916	HIS
2	B	997	ASN
2	B	1025	GLN
3	C	137	ASN
3	C	143	ASN
3	C	207	HIS
4	D	71	ASN
4	D	130	ASN
5	E	5	ASN
5	E	32	GLN
5	E	54	GLN
5	E	101	GLN
5	E	113	GLN

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Mol	Chain	Res	Type
5	E	136	ASN
5	E	174	GLN
7	G	36	ASN
8	H	128	ASN
10	J	26	GLN
13	M	92	ASN
13	M	117	HIS
13	M	132	ASN
13	M	155	ASN
13	M	158	GLN
13	M	190	ASN
14	N	298	ASN
14	N	421	GLN
15	O	244	ASN
15	O	254	ASN
15	O	362	ASN
15	O	464	ASN
15	O	544	ASN
15	O	579	GLN
15	O	584	ASN
15	O	631	ASN
17	Q	49	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.