



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:08 PM BST

PDB ID : 4V1A
EMDB ID: : EMD-2787
Title : Structure of the large subunit of the mammalian mitoribosome, part 2 of 2
Authors : Greber, B.J.; Boehringer, D.; Leibundgut, M.; Bieri, P.; Leitner, A.; Schmitz, N.; Aebersold, R.; Ban, N.
Deposited on : 2014-09-25
Resolution : 3.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

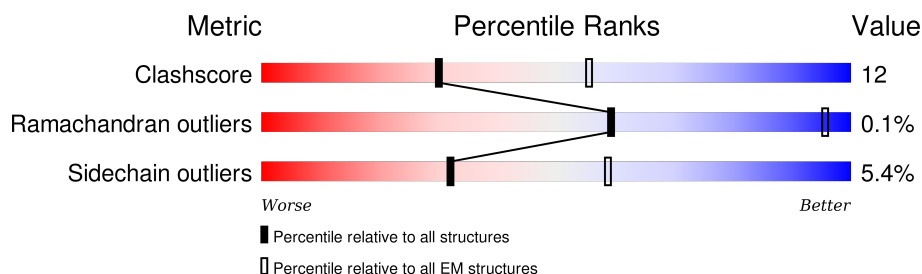
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	423	89% 7%
2	b	380	89% 7%
3	c	334	85% 12%
4	d	206	45% 52%
5	e	135	85% 10%
6	f	142	70% 6% 24%
7	g	159	84% 9% 7%
8	h	332	82% 5% 13%
9	i	312	75% 22%

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Mol	Chain	Length	Quality of chain
10	j	279	
11	k	212	
12	l	166	
13	m	159	
14	n	128	
15	o	124	
16	p	112	
17	q	138	
18	t	102	
19	u	205	
20	v	222	
21	w	433	
22	x	196	
23	z	47	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 31917 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 MITORIBOSOMAL PROTEIN ML37, MRPL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	121	Total	C	N	O	S	0	0
			968	626	167	172	3		

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	108	Total	C	N	O	S	0	0
			852	544	154	150	4		

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	242	Total	C	N	O	S	0	0
			1979	1266	352	351	10		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	131	Total	C	N	O	S	0	0
			1050	671	178	196	5		

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	94	Total	C	N	O	S	0	0
			747	466	143	136	2		

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	q	37	Total	C	N	O	0	0
			336	214	69	53		

- Molecule 18 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	t	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	151	Total	C	N	O	S	0	0
			1208	748	233	222	5		

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	131	Total	C	N	O	S	0	0
			1068	662	206	195	5		

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	w	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	x	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 23 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	z	47	Total	C	N	O	0	0
			282	188	47	47		

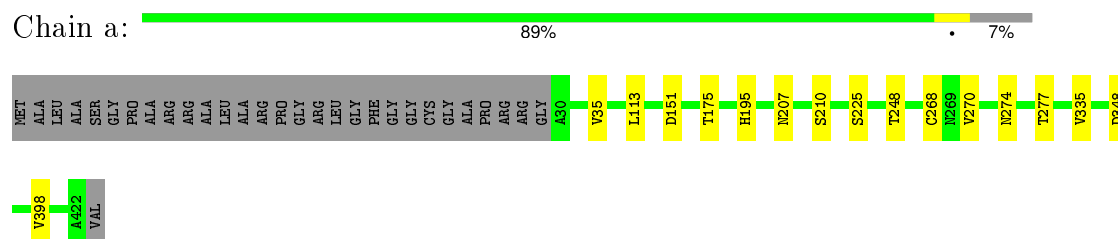
- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	x	1	Total	Zn	0
			1	1	

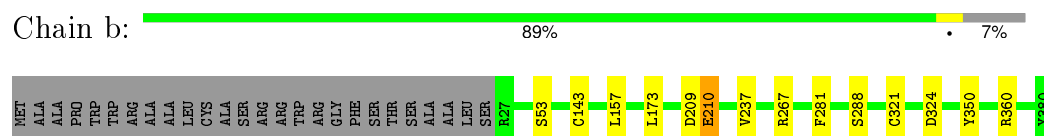
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

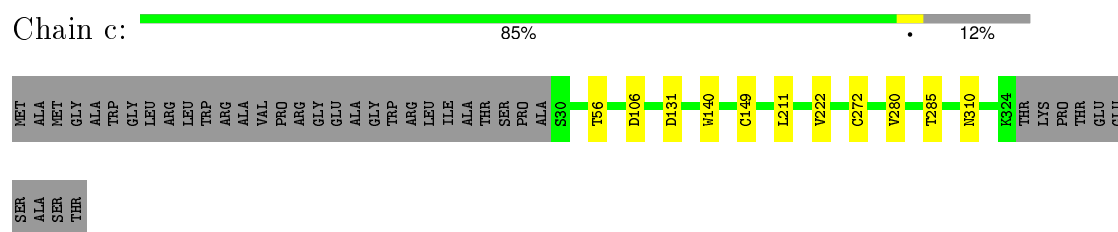
- Molecule 1: MITORIBOSOMAL PROTEIN ML37, MRPL37



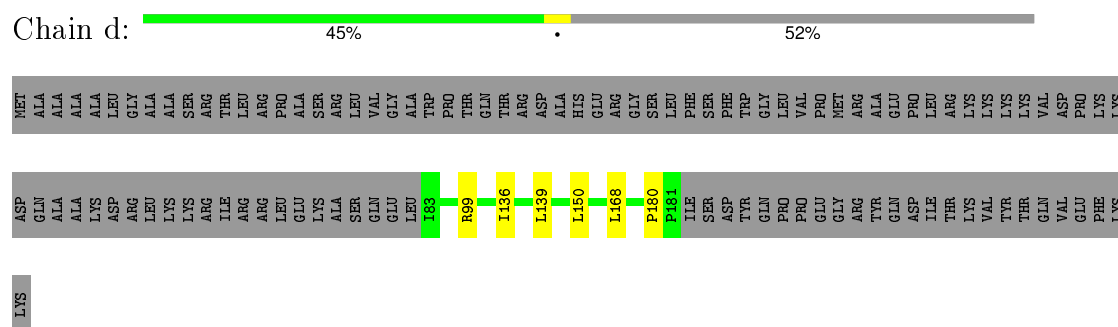
- Molecule 2: MITORIBOSOMAL PROTEIN ML38, MRPL38




- Molecule 3: MITORIBOSOMAL PROTEIN ML39, MRPL39

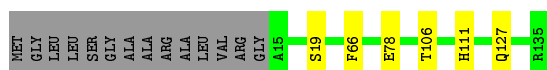


- Molecule 4: MITORIBOSOMAL PROTEIN ML40, MRPL40



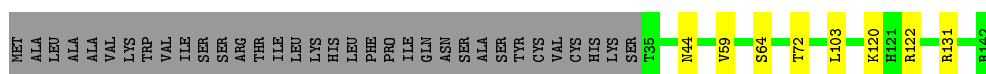
- Molecule 5: MITORIBOSOMAL PROTEIN ML41, MRPL41

Chain e:  85% 10%




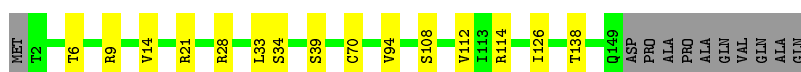
- Molecule 6: MITORIBOSOMAL PROTEIN ML42, MRPL42

Chain f:  70% 6% 24%




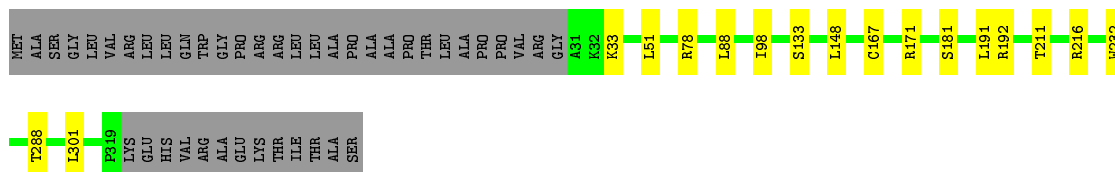
- Molecule 7: MITORIBOSOMAL PROTEIN ML43, MRPL43

Chain g:  84% 9% 7%



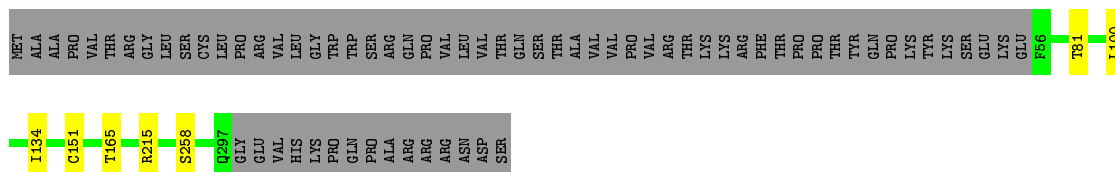
- Molecule 8: MITORIBOSOMAL PROTEIN ML44, MRPL44

Chain h:  82% 5% 13%



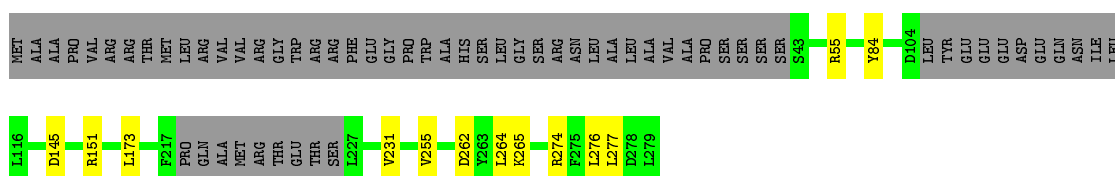
- Molecule 9: MITORIBOSOMAL PROTEIN ML45, MRPL45

Chain i:  75% 22%



- Molecule 10: MITORIBOSOMAL PROTEIN ML46, MRPL46

Chain j:  73% 5% 22%




- Molecule 11: MITORIBOSOMAL PROTEIN ML48, MRPL48

Chain k:  60% 38%

MET ASN GLY ALA LEU LEU LYS ALA CYS LEU LEU LEU ASN ASP THR VAL LEU LYS GLN ALA LEU SER SER LYS LEU ARG ARG VAL ARG ALA SER SER GLY GLY SER PRO CYS SER ALA GLY GLY ILE LEU LEU SER THR SER ARG HIS Y48 Q66 GLU PRO LYS LYS LYS LYS GLY VAL GLU

Y77 Y98 Q138 Q138 LYS LYS M144 T154 L162 D193 PHE LYS GLY ARG PHE LYS LEU ARG ALA ARG PRO GLU LEU ALA ALA LYS LEU ASN

- Molecule 12: MITORIBOSOMAL PROTEIN ML49, MRPL49

Chain l:  76% 20%

MET ALA ALA THR VAL LEU CYS GLY VAL LEU LEU ARG ALA TRP ARG THR GLY VAL PRO LEU LYS CYS GLY LEU ARG ARG LEU SER GLN THR GLY THR PRO E34 S89 R90 N93 D99 I100 T101 M141 F166

- Molecule 13: MITORIBOSOMAL PROTEIN ML50, MRPL50

Chain m:  67% 31%

MET ALA ALA ARG TRP VAL SER GLY LEU LEU ARG ARG ALA TRP LEU THR CYS GLY VAL SER GLY CYS PRO ARG ARG ARG PHE TRP SER PRO PHE ARG LYS GLU GLN LYS PRO VAL VAL ALA GLU THR VAL VAL GLU VAL VAL LYS LYS GLU PRO ILE L51 I90 M121 Y159

- Molecule 14: MITORIBOSOMAL PROTEIN ML51, MRPL51

Chain n:  70% 6% 24%


MET ALA GLY SER LEU TRP VAL THR GLY ARG GLY TRP GLN LEU LEU THR CYS ALA ALA THR ARG SER PHE SER LEU GLY ILE PRO ARG LEU F32 R46 V56 N65 F66 I92 V98 R101 D105 R128

- Molecule 15: MITORIBOSOMAL PROTEIN ML52, MRPL52

Chain o:  71% 5% 24%

MET ALA TRP GLY ILE LEU LEU SER THR GLY VAL ARG ALA HIS CYS GLY THR ALA ALA ALA GLN A23 Y40 L43 T94 D48 R65 R76 L116 LEU GLN ASN PRO VAL PRO PRO SER GLN

- Molecule 16: MITORIBOSOMAL PROTEIN ML53, MRPL53

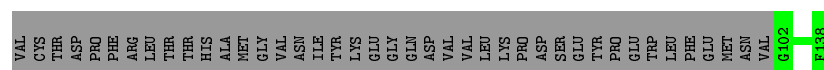
Chain p:  86% 13%

MET A2 S60 G98 ALA ALA GLY ALA SER GLY ASP LYS PRO ALA TRP ARG ALA THR GLY ARG

- Molecule 17: MITORIBOSOMAL PROTEIN ML54, MRPL54

Chain q:  27% 73%

MET ALA ALA ARG ARG LEU PHE GLY ALA ALA ARG ALA TRP TRP ARG ALA TRP GLU LEU SER ASP ALA VAL SER GLY ARG HIS VAL ARG ASN TYR ALA LYS ARG PRO VAL ILE LYS GLY LYS GLY GLY LYS GLY VAL VAL VAL GLY GLU GLU LEU LYS ASP PRO GLU



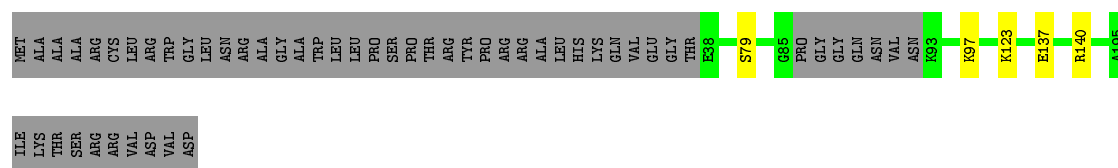
- Molecule 18: MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63

Chain t: 84% 8% 8%



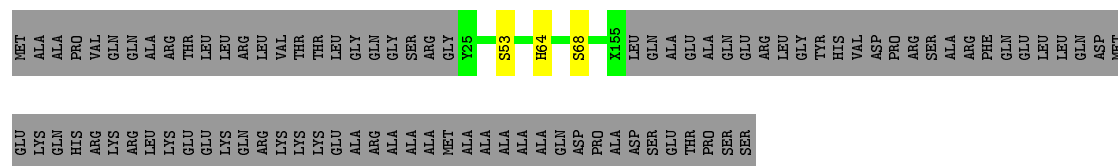
- Molecule 19: MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1

Chain u: 71% 26%



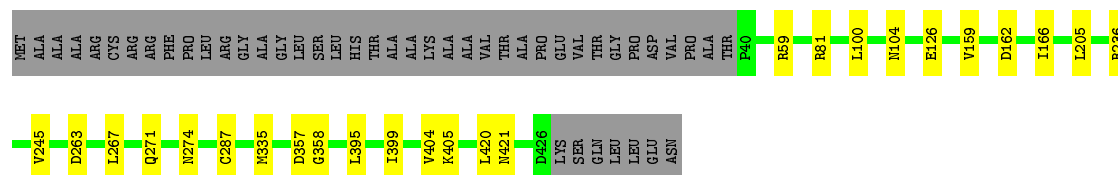
- Molecule 20: MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1

Chain v: 58% 41%



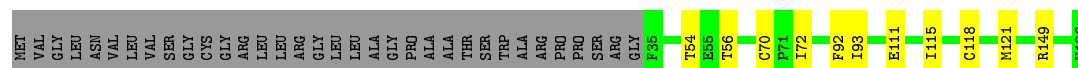
- Molecule 21: MITORIBOSOMAL PROTEIN ML65, MRPS30

Chain w: 84% 6% 11%



- Molecule 22: MITORIBOSOMAL PROTEIN ML66, MRPS18A

Chain x: 77% 6% 17%



- Molecule 23: UNASSIGNED SECONDARY STRUCTURE ELEMENTS

Chain z: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.34	0/3267	0.53	0/4455
10	j	0.34	0/1811	0.56	0/2436
11	k	0.35	0/1070	0.55	0/1448
12	l	0.38	0/1135	0.53	0/1549
13	m	0.30	0/917	0.49	0/1248
14	n	0.44	0/860	0.60	0/1150
15	o	0.39	0/762	0.52	0/1022
16	p	0.34	0/752	0.53	0/1013
17	q	0.29	0/346	0.47	0/463
18	t	0.41	0/798	0.61	0/1073
19	u	0.31	0/1163	0.49	0/1557
2	b	0.36	0/3047	0.55	0/4139
20	v	0.33	0/1022	0.44	0/1382
21	w	0.39	0/3206	0.55	0/4354
22	x	0.36	0/1364	0.62	0/1849
3	c	0.33	0/2464	0.50	0/3330
4	d	0.38	0/853	0.56	1/1153 (0.1%)
5	e	0.37	0/996	0.56	0/1340
6	f	0.38	0/731	0.54	0/990
7	g	0.38	0/1191	0.58	0/1614
8	h	0.35	0/2372	0.53	0/3211
9	i	0.32	0/2034	0.52	0/2759
All	All	0.36	0/32161	0.54	1/43535 (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
10	j	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	n	0	1
2	b	0	1
21	w	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	180	PRO	C-N-CD	-5.25	109.05	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	210	GLU	Peptide
10	j	173	LEU	Peptide
14	n	65	ASN	Peptide
21	w	357	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3173	0	3153	0	0
2	b	2952	0	2840	0	0
3	c	2408	0	2415	0	0
4	d	832	0	828	0	0
5	e	968	0	968	0	0
6	f	852	0	834	0	0
7	g	1167	0	1173	0	0
8	h	2319	0	2332	0	0
9	i	1979	0	1974	0	0
10	j	1775	0	1797	0	0
11	k	1050	0	1044	0	0
12	l	1097	0	1080	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	893	0	878	0	0
14	n	837	0	860	0	0
15	o	747	0	748	0	0
16	p	742	0	749	0	0
17	q	336	0	342	0	0
18	t	780	0	792	0	0
19	u	1208	0	1227	0	0
20	v	1068	0	1034	0	0
21	w	3126	0	3153	0	0
22	x	1325	0	1354	0	0
23	z	282	0	294	0	0
24	x	1	0	0	0	0
All	All	31917	0	31869	0	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 12.

There are no clashes within the asymmetric unit.

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	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
2	b	352/380 (93%)	329 (94%)	23 (6%)	0	100	100
3	c	293/334 (88%)	279 (95%)	14 (5%)	0	100	100
4	d	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
5	e	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
6	f	82/142 (58%)	81 (99%)	1 (1%)	0	100	100
7	g	146/159 (92%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	h	287/332 (86%)	270 (94%)	17 (6%)	0	100	100
9	i	240/312 (77%)	230 (96%)	10 (4%)	0	100	100
10	j	211/279 (76%)	200 (95%)	9 (4%)	2 (1%)	21	65
11	k	125/212 (59%)	119 (95%)	6 (5%)	0	100	100
12	l	131/166 (79%)	127 (97%)	4 (3%)	0	100	100
13	m	107/159 (67%)	101 (94%)	6 (6%)	0	100	100
14	n	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
15	o	92/124 (74%)	87 (95%)	5 (5%)	0	100	100
16	p	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
17	q	35/138 (25%)	33 (94%)	2 (6%)	0	100	100
18	t	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
19	u	137/205 (67%)	130 (95%)	7 (5%)	0	100	100
20	v	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
21	w	385/433 (89%)	363 (94%)	20 (5%)	2 (0%)	34	75
22	x	160/196 (82%)	155 (97%)	4 (2%)	1 (1%)	30	72
All	All	3790/4899 (77%)	3612 (95%)	173 (5%)	5 (0%)	59	89

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	w	159	VAL
22	x	93	ILE
10	j	84	TYR
10	j	151	ARG
21	w	358	GLY

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	348/365 (95%)	332 (95%)	16 (5%)	33	72
2	b	310/328 (94%)	296 (96%)	14 (4%)	34	73
3	c	271/299 (91%)	260 (96%)	11 (4%)	37	75
4	d	92/181 (51%)	87 (95%)	5 (5%)	27	67
5	e	100/108 (93%)	94 (94%)	6 (6%)	24	64
6	f	80/110 (73%)	72 (90%)	8 (10%)	9	38
7	g	128/136 (94%)	113 (88%)	15 (12%)	7	30
8	h	251/284 (88%)	234 (93%)	17 (7%)	20	60
9	i	218/281 (78%)	211 (97%)	7 (3%)	46	80
10	j	190/242 (78%)	180 (95%)	10 (5%)	28	67
11	k	115/181 (64%)	111 (96%)	4 (4%)	43	78
12	l	122/147 (83%)	115 (94%)	7 (6%)	25	65
13	m	103/145 (71%)	101 (98%)	2 (2%)	65	87
14	n	88/113 (78%)	81 (92%)	7 (8%)	15	51
15	o	74/97 (76%)	68 (92%)	6 (8%)	15	51
16	p	79/88 (90%)	78 (99%)	1 (1%)	76	91
17	q	36/114 (32%)	36 (100%)	0	100	100
18	t	75/82 (92%)	67 (89%)	8 (11%)	8	35
19	u	126/169 (75%)	121 (96%)	5 (4%)	38	75
20	v	102/173 (59%)	99 (97%)	3 (3%)	50	82
21	w	340/373 (91%)	318 (94%)	22 (6%)	21	61
22	x	149/173 (86%)	139 (93%)	10 (7%)	20	60
All	All	3397/4189 (81%)	3213 (95%)	184 (5%)	32	67

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	35	VAL
1	a	113	LEU
1	a	151	ASP
1	a	175	THR
1	a	195	HIS
1	a	207	ASN
1	a	210	SER
1	a	225	SER

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Mol	Chain	Res	Type
1	a	248	THR
1	a	268	CYS
1	a	270	VAL
1	a	274	ASN
1	a	277	THR
1	a	335	VAL
1	a	348	ASP
1	a	398	VAL
2	b	53	SER
2	b	143	CYS
2	b	157	LEU
2	b	173	LEU
2	b	209	ASP
2	b	210	GLU
2	b	237	VAL
2	b	267	ARG
2	b	281	PHE
2	b	288	SER
2	b	321	CYS
2	b	324	ASP
2	b	350	TYR
2	b	360	ARG
3	c	56	THR
3	c	106	ASP
3	c	131	ASP
3	c	140	TRP
3	c	149	CYS
3	c	211	LEU
3	c	222	VAL
3	c	272	CYS
3	c	280	VAL
3	c	285	THR
3	c	310	ASN
4	d	99	ARG
4	d	136	ILE
4	d	139	LEU
4	d	150	LEU
4	d	168	LEU
5	e	19	SER
5	e	66	PHE
5	e	78	GLU
5	e	106	THR

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Mol	Chain	Res	Type
5	e	111	HIS
5	e	127	GLN
6	f	44	ASN
6	f	59	VAL
6	f	64	SER
6	f	72	THR
6	f	103	LEU
6	f	120	LYS
6	f	122	ARG
6	f	131	ARG
7	g	6	THR
7	g	9	ARG
7	g	14	VAL
7	g	21	ARG
7	g	28	ARG
7	g	33	LEU
7	g	34	SER
7	g	39	SER
7	g	70	CYS
7	g	94	VAL
7	g	108	SER
7	g	112	VAL
7	g	114	ARG
7	g	126	ILE
7	g	138	THR
8	h	33	LYS
8	h	51	LEU
8	h	78	ARG
8	h	88	LEU
8	h	98	ILE
8	h	133	SER
8	h	148	LEU
8	h	167	CYS
8	h	171	ARG
8	h	181	SER
8	h	191	LEU
8	h	192	ARG
8	h	211	THR
8	h	216	ARG
8	h	232	TRP
8	h	288	THR
8	h	301	LEU

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Mol	Chain	Res	Type
9	i	81	THR
9	i	100	LEU
9	i	134	ILE
9	i	151	CYS
9	i	165	THR
9	i	215	ARG
9	i	258	SER
10	j	55	ARG
10	j	145	ASP
10	j	231	VAL
10	j	255	VAL
10	j	262	ASP
10	j	264	LEU
10	j	265	LYS
10	j	274	ARG
10	j	276	LEU
10	j	277	LEU
11	k	77	VAL
11	k	98	TYR
11	k	151	THR
11	k	162	LEU
12	l	89	SER
12	l	90	ARG
12	l	93	ASN
12	l	99	ASP
12	l	100	ILE
12	l	101	THR
12	l	141	ASN
13	m	90	ILE
13	m	121	MET
14	n	46	ARG
14	n	56	VAL
14	n	66	PHE
14	n	92	ILE
14	n	98	VAL
14	n	101	ARG
14	n	105	ASP
15	o	40	TYR
15	o	43	LEU
15	o	44	THR
15	o	48	ASP
15	o	65	ARG

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Mol	Chain	Res	Type
15	o	76	ARG
16	p	60	SER
18	t	9	ARG
18	t	25	ARG
18	t	45	ASN
18	t	49	LEU
18	t	51	ARG
18	t	82	PHE
18	t	86	ARG
18	t	101	TRP
19	u	79	SER
19	u	97	LYS
19	u	123	LYS
19	u	137	GLU
19	u	140	ARG
20	v	53	SER
20	v	64	HIS
20	v	68	SER
21	w	59	ARG
21	w	81	ARG
21	w	100	LEU
21	w	104	ASN
21	w	126	GLU
21	w	162	ASP
21	w	166	ILE
21	w	205	LEU
21	w	236	ARG
21	w	245	VAL
21	w	263	ASP
21	w	267	LEU
21	w	271	GLN
21	w	274	ASN
21	w	287	CYS
21	w	335	MET
21	w	395	LEU
21	w	399	ILE
21	w	404	VAL
21	w	405	LYS
21	w	420	LEU
21	w	421	ASN
22	x	54	THR
22	x	56	THR

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Mol	Chain	Res	Type
22	x	70	CYS
22	x	72	ILE
22	x	92	PHE
22	x	111	GLU
22	x	115	ILE
22	x	118	CYS
22	x	121	MET
22	x	149	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	96	HIS
1	a	108	HIS
1	a	156	ASN
1	a	223	HIS
1	a	274	ASN
1	a	289	HIS
1	a	343	GLN
1	a	360	ASN
1	a	420	HIS
2	b	220	ASN
2	b	224	HIS
2	b	266	HIS
2	b	308	GLN
2	b	320	GLN
3	c	281	HIS
3	c	294	GLN
3	c	305	HIS
3	c	310	ASN
6	f	44	ASN
6	f	121	HIS
6	f	130	HIS
7	g	17	ASN
7	g	120	HIS
7	g	131	HIS
8	h	94	ASN
8	h	177	GLN
8	h	260	GLN
9	i	115	ASN
9	i	157	HIS
9	i	193	GLN

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Mol	Chain	Res	Type
9	i	196	GLN
9	i	217	HIS
9	i	274	GLN
11	k	61	HIS
11	k	177	ASN
12	l	93	ASN
12	l	141	ASN
13	m	107	ASN
14	n	69	HIS
14	n	122	ASN
14	n	124	HIS
15	o	63	GLN
16	p	72	HIS
16	p	93	HIS
18	t	34	ASN
18	t	45	ASN
18	t	85	HIS
19	u	103	HIS
19	u	145	ASN
21	w	101	ASN
21	w	104	ASN
21	w	173	GLN
21	w	228	ASN
21	w	233	ASN
21	w	234	GLN
21	w	367	GLN
21	w	385	ASN
22	x	164	ASN
22	x	184	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 1 ligands modelled in this entry, 1 is 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.