

Nov 19, 2022 – 11:53 PM EST

PDB ID	:	3IZM
EMDB ID	:	EMD-5249
Title	:	Mm-cpn wildtype with ATP
Authors	:	Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.;
		Chiu, W.; Frydman, J.
Deposited on	:	2010-10-30
Resolution	:	7.20 Å(reported)
This is	a I	Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev 43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 7.20 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.



Motric	Whole archive	EM structures
IVIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	513	95%	•••
1	В	513	95%	•••
1	С	513	95%	•••
1	D	513	96%	•••
1	Е	513	95%	•••
1	F	513	96%	
1	G	513	95%	
1	Н	513	95%	•••



Mol	Chain	Length	Quality of chain	
			70%	
1	Ι	513	95% • •	
	_		70%	
1	J	513	95% ••	
			70%	
1	K	513	95% • •	
	_		70%	
1	L	513	95% • •	
			70%	
1	М	513	95% • •	
			70%	
1	Ν	513	96% • •	•
	_		70%	
1	0	513	95% • •	
			70%	
1	P	513	96% • •	•



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 61632 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.

Mol	Chain	Residues		At	oms		AltConf	Trace		
1	Δ	513	Total	С	Ν	0	S	0	0	
1	11	010	3852	2391	664	772	25	0	0	
1	В	513	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	
1	D	515	3852	2391	664	772	25	0	0	
1	С	513	Total	С	Ν	Ο	S	0	0	
1	U	515	3852	2391	664	772	25	0	0	
1	Л	513	Total	С	Ν	Ο	S	0	0	
1	D	515	3852	2391	664	772	25	0	0	
1	F	513	Total	С	Ν	Ο	S	0	0	
1	Ľ	515	3852	2391	664	772	25	0	0	
1	F	513	Total	С	Ν	0	S	0	0	
1	T,	515	3852	2391	664	772	25	0	0	
1	C	512	Total	С	Ν	0	S	0	0	
1	G	515	3852	2391	664	772	25	0	0	
1	и	512	Total	С	Ν	0	S	0	0	
1	11	515	3852	2391	664	772	25	0	0	
1	т	512	Total	С	Ν	0	S	0	0	
1	1	515	3852	2391	664	772	25	0	0	
1	т	512	Total	С	Ν	0	S	0	0	
1	1	515	3852	2391	664	772	25	0	0	
1	V	519	Total	С	Ν	0	S	0	0	
1	n	515	3852	2391	664	772	25	0	0	
1	т	519	Total	С	Ν	0	S	0	0	
1	L	515	3852	2391	664	772	25	0	0	
1	м	519	Total	С	Ν	0	S	0	0	
1	1/1	515	3852	2391	664	772	25	0	0	
1	N	519	Total	С	Ν	0	S	0	0	
1	IN	515	3852	2391	664	772	25	0	0	
1	0	519	Total	С	Ν	0	S	0	0	
	U	616	3852	2391	664	772	25	U	U	
1	р	519	Total	С	Ν	0	S	0	0	
	Г	519	3852	2391	664	772	25	U	0	

• Molecule 1 is a protein called Chaperonin.



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Chaperonin



• Molecule 1: Chaperonin

Chain B:

95%

70%













\bullet Molecule 1: Chaperonin





















Chain J:	70% 95%		
*****		** ****** ****	*** ** ** * ***
V4618 L4619 P4620 E4621 N4622	M4623 K4626 Y4626 M4627 M4627 G4628 D4631 D4631 A4634 M4632 R4632 R4633 R4633 R4635 F4635 I4642 I4642 I4644 F4644 F4644 F4644	V4646 R4650 L4650 C4651 C4653 R4655 M4655 M4655 D4655 L4665 C4665 C4665 C4665 C4665 C4665	44668 14668 14669 14679 14674 14674 14677 14674 14681 14681 14684 14685
K4687 M4688 ♦ L4689 ♦ E4691 ♦ V4692 ♦	T4695 T4695 E4697 K4698 E4699 V4700 G4701 A4707 V4706 A4707 V4709 V4715 E4713 E4713 E4713 E4713 E4713 K4717 K4717	A4718 E4710 E4720 E4721 L4722 L4722 D4724 Q4725 H4727 P4728 H4727 P4728 T4729 T4729 C4734	Y4735 q4736 A4737 A4737 A4739 Q4740 Q4740 Q4740 E4744 L4746 K4747 T4748 I4748 A4750
C4751 E4752 V4753 G4754 A4755	P4756 P4757 K4759 E4750 L4761 L4761 R4762 K4767 R4771 E4775 K4776 K4776 K4776 K4776 K4776 K4776 K4776 K4776 K4776 K4776 K4776 K4776 K4776 L4781 L4781 E4783	V4786 E4787 A4788 V4789 S4790 S4791 V4792 V4792 D4795 E4795 E4796 C4797 K4798 V4798 V4798	D4802 L4803 L4804 K4805 F4807 E4807 C4811 A4812 A4812 C4813 L4814 D4815 D4815 D4815 C4813 C4
L4819 14820 K4821 G4822 V4823	K4927 E4228 R4829 A4822 Q4833 Q4833 P4835 P4835 P4835 P4835 P4835 P4835 P4835 A4841 K4842 L4845 A4841 K4842 L4846 A4849 L4846 F4867 F4846 F4867	14362 K4853 E4854 E4855 E4856 E4856 E4856 A4859 A4859 A4859 E4860 I4861 R4862 I4861 P4865 P4865 P4865 P4865 A4857	K4968 H4870 E4871 E4871 E4874 E4877 E4877 K4879 K4879 K4881 K4881 A4885
E4886 14887 K4888 A4889 S4890	A4932 N4932 F4936 F4937 F4937 F4930 D4903 D4903 L4904 A4910 K4911 E4913 C4913 C4913 C4913 C4913 A4916	V4920 K4921 K4921 K4922 K4925 K4926 K4926 K4926 K4926 K4936 K4934 K4934 K4934 K4934 K4934 V4936 V4935	14307 14938 14939 14940 14942 14943 84944 44945 94945 04945 04945 04945 04945 04945 04945 04945
G4952 L4953 E4956 R4957	14959 84960 64961 94962 94963 94965 14965 84973 84971 94973 84973 84973 84973 84973 84973 14975 14973 14975 14973	E4985 H4986 V4987 V4987 E4989 E4999 A4994 A4993 A4995 A4995 A4995 A4996 C4996 C4998 C4998 C4998	V5002 T5005 T5005 E5007 D5008 R5010 R5010 S5017 T5018 E5021 E5021 L5022

K5713 M5714 L5715 15716 E5717 V5718	15721 95722 65723 65724 65725 65725 05728	65729 15732 45733 45733 V5735 V5736 V5736	G5738 E5739 L5740 L5741 R5742 K5743	A5744 E5745 E5746 E5746 L5747 L5748 D5749	N5781 V5752 H5753 P5754 T5755 I5756	K5759 G5760 K5761 A5762 A5763 A5765 A5765 A5765 A5765	K5767 E5770 L5771 L5772 K5773 K5773 T5774 A5776
C5777 E5778 V5779 G5780 G5780 G5780 G5781 Q5782 Q5782	C5783 E5785 E5785 L5786 L5786 T5788 K5783 T5783 T5793	G5797 E5801 K5802 A5802 K5804 E5805	K5806 L5807 A5808 E5809 I5810 I5811	V5812 E5813 A5814 V5815 S5816 A5817 V5818	V5819 D5820 D5821 E5822 G5822 K5824 K5824 V5825	D5826 K5827 D5828 L5829 K5831 F5833 F5833	G837 G5837 S5833 S5833 15840 D5841 D5842 T5843 E5844
L5845 L5846 K5847 G5848 V5849 K5849 K5853	E5884 R5885 A5865 A5865 M5860 M5861 K5862	K5863 V5864 T5865 D5866 A5867 K6868	L5871 L5872 A5875 A5876 E5877 E5877	L5878 K5879 E5880 T5881 E5882 T5883 T5883 D5884	A5885 E5886 I5887 R5888 I5889 T5890 D6891	P5892 A5893 K5894 L5895 M5896 E5897 E5897	q5901 q5902 E5902 E5903 K5904 M5905 M5905 K5904 M5905 M5905 M5905 M5905 M5905 M5905 M5901
E5912 15913 K5914 A5915 A5916 S5916 G5917 A5918	N5919 F5922 C5923 15927 D5928 D5928 D5928	L5936 L5936 A5936 A5936 K5937 E5938 C5939 C5939	I5940 V5941 A5942 A5943 R5944 R5945	V5946 (K5947 (K5948 (K5948 (K5948 (K59595 (K5953 (K595) (K	L5954 A5955 K5956 A5957 T5958 G5959 A5960 A5960	U5962 15963 15964 N5965 N5966 K5967 D5968	A5971 45972 45972 45973 15973 15974 65975 55975 A5977 A5977
C 5978 C 5982 R 5983 K 5984 K 5984 C 5985 C 598	S5986 C5987 D5988 M5990 M5990 15991	C5995 C5996 K5997 H5998 P5999 K6000 A6001	T6003 M6004 L6005 T6009 T6010	E6011 H6012 V6013 E6015 E6015 E6016	A6018 R6019 A6020 V6021 D6022 D6023 A6024	V6025 G6026 V6027 V6028 T6031 T6031 E6033 E6033	De034 R6035 S6043 S6043 S6043 E6044 E6047 E6047
86049 M6050 ♦ K6051 ♦ L6052 R6053 ♦ E6054 ♦	A6056 E6057 G6058 16059 S6060 G6061 A6062 E6063	Q6064 ♦ V6067 ♦ R6068 ♦ A6069 € F6070 ♦ A6071 ♦	A6073 L6074 E6075 V6076 L6077 P6078	T6079 T6080 L6081 A6082 A6082 A6085 G6086	L6087 D6088 E6091 L6092 V6094	A6095 R6097 A6098 A6099 A6101 S6102	06104 06104 N6105 K6106 06107 A6108 N6111 V6112
F6113 T6114 G6115 A6116 V6117 E6118	M61120 C6121 E6122 N6123 G6124 V6125 V6125 E6127	P6128 L6129 R6130 K6131 F6132 Q6134 Q6134	I6136 Q6137 A6140 E6141	E6144 ♦ M6145 ♦ L6147 ♦ R6148 ♦ I6149 ♦	D6151 V6152 16153 A6154 A6155 E6156		
• Molecule	1: Chaperonin	70%					
Chain M:		70%	95%			•••	
V6157 L6158 P6159 E6160 N6161 M6162	Roles Y6165 M6165 M6167 G6167 R6167 A6170 A6170	R6172 M6173 M6174 N6174 I6175 A6177 A6177 G6178	R6179 I6180 I6181 A6182 E6183 E6183 T6184	R6186 L6189 G6190 P6191 P6191	G6193 M6194 D6195 K6196 L6202 G6203	V6205	10213 86216 66217 66220 66223 66223 66223 66225
K6226 M6227 L6228 E6230 V6231	T6234 06235 E6236 K6237 E6238 V6239 V6239 C6240 D6241	65242 T6245 A6246 V6246 V6246 V6249 V6249	G6251 E6252 L6253 L6254 R6255 K6255	A6257 E6258 E6259 L6260 L6261 D6263	N6264 V6265 H6266 P6267 T6268 I6269	K6272 G6273 Y6274 Q6275 A6277 A6277 A6277 A6277 C279	K6280 (E6283 (L6284 (L6284 (K6286 (T6284 (T6288 (A6288 (
C6290 E6291 V6292 G6293 A6294 Q6295	Mc297 K6297 E6298 E6298 E6298 E6300 T6301 K6302	G6310 6314 K6315 A6315 K6317 K6317 E6318	K6319 L6320 A6321 E6322 E6323 I6323	V6325 E6326 A6327 V6328 S6329 A6330 V6331 V6331	V6332 D6333 D6334 E6335 G6335 K6337 V6338	D6339 K6340 D6341 L6342 L6342 K6344 K6344 L6345 F6346	66350 66350 86352 16355 16355 16355 16356 16356 86357
L6358 16359 K6360 G6361 V6362 K6366	E6367 ♦ R6368 ♦ A6371 ♦ Q6372 ♦ M6373 ♦ F6374 ♦	K6376 V6377 T6378 D6379 A6380 K6381 I6382	A6383 L6384 L6385 A6388 A6389 I6389	E6390 16391 K6392 E6393 T6394 E6395 T6395	D6397 A6398 A6401 I6402 T6403 D6404	P6405 A6406 K6407 L6408 M6409 E6410 E6413	06414 E6415 E8415 K6417 M6418 M6418 K6420 D6421 D6424
E6425 E6425 K6427 A6427 S6428 G6430 A6431	N6432 ♦ C6436 ♦ 16440 ♦ D6441 ♦ D6442 ↓ L6443 ♦	Y6447 L6448 A6449 K6450 E6451 G6452	V6454 ♦ A6455 A6456 R6457 R6457 R6457 V6459	K6460 M6464 E6465 K6466 L6467 A6467	K6469 A6470 T6471 66472 A6473 N6474 V6475	16477 16477 16477 16479 16480 16481 16482 56483 56483	Q6485 D6485 L6487 G6488 G6489 A6490 G6491 L6492

• Molecule 1: Chaperonin

Chain O:

95%

70%

. .

V7 183	L7184	P7185	E7186 N7187	M7 188	K7 189 🔶	R7190	Y7191	G7193	R7194	D7195		R7198	M7 199	N7 200	1 7 2012	A7203	G7204	R7205 I7206	17207	A7208	E7209	V7211	R7212		L7215	P7217	K7218	G7219	M/ 220	K7222	L7228	G7 229	D7230	V7231	V7 233	T7234	N7 235	V7 238	T7 239	01010	KI 242 E7243		V 7 246	P7249	A7 251
K7252	M7253	L7254	E7256	V7257	T7260	Q7261	E7262	K7263 E7764	V7265	G7266	D7267	G7268	T7271	A7272	V7273	V1275	A7276	G7277	E/2/8	L7280	R7281	K7282	A/283 E7284	E7285	L7286	L7287 D7288	Q7289	N7290	V7291	H7293	T7294	I7295	K7298	G7299	1/300	A7302	A7303	A7304	K7306		E7309		K7312	1/313 17314	A7315
C7316	E7317 🔶	V7318	67319 A7320	07321	D7322	K7323	E7324 T7325	L7326	T7327	KI 328	T7 332	2222	000 15	E7340	K7341	K7343	E7344	K7345	L/ 346 A7 347	E7348	I7349	I7350	V/351 E7352	A7353	V7354	S7355	A7 356 V7 357	V7 358	D7359	D/360	G7362	K7363	V/ 304 D7365	K7366	D7367	L/ 300 17369	K7370	17371	E7372	G7376	A7377	57378 17379	D7380	D7381	E7383
L7384	I7385	K7386	G7387 V7388		K7392	E7393		A7 397	Q7398	P7400	K7401	K7402	V7 403	T7404	01405	K7407	17408	A7409			A7414	1/415 E7/16		K7418	E7419	T/ 420 E7 421	T7 422	D7423	A7424	R7 427	I7428	T7429	P7431	A7432	K7433 L7434	M7 435	E7436	E7439	Q7 440	E7441	E7442	M7 444	L7445	D7 447	A7450
E7451	I7452	K7453	A / 404 S 7 4 55	G7456	A7457	N7458	C7462	112400	1/466 D7467	D7468	L7469	¥7473	L7474	A7475	K7476 E7477	G7478	I7479	V7480	A/481 A7482	R7483	R7484	V7485	K / 486	M7490	E7491	L7493	A7494	K7495	T7497	G7498	A7499 N7500	V7501	17502	T7503	I7505	K7506	L7508	S7509	A7510	Q7511	D7512 1.7513	G7514	D7515	A/516 G7517	L7518
	E7521	R7522	17524	S7525	G7526	D/ 52/ S7528	M7529	I7530	E7533	E7534	C7535	K7536 H7537	P7538	K7539	A7540	V7541	M7543	L7544	T7548	T7549	E7550	H7551	V7553	E7554	E7555	V7556	R7558	A7559	V7560	D7562	A7563	07565	V7566	V7567	T7570	17571	E/5/2	G7574	R7575		S7582 T7583		E7586	S7588	
K7590	L7591	R7592	E/ 393	A7595	E7596	G7597	27599	G7 60 0	R7601	E/ 602		V7606	R7607 A7608	F7609	A7610	D7611	L7613 🔶	E7614		P7617	R7618	T7619	L/ 620		A7624	G7625	D7627		E7630	L7632	V7633	K/ 634 V7 635	R7636	A7637	A 638 H7 639	A7640	S7641	N7642 G7643	N7644	K7 645 🔶	C7646	A7647	N7 650	V / 551 F7652	T7 653
G7654	A7655	V7656	E7657	M7659	C7660	E7661	G7663	V7664	V7665	P7667	L7668	R7669	K7671	T7672	Q7673 🔶	A7674	07676		A7679	E7680	E7683	M7684		R7687	17688	D7689	V7691	17692	A7693	E7695															

C	ha	in	P): •											709	%			96	%															•	•												
V7 69 6	L7697	P7698	E7 699	M7701	K7702	R7703	M7705	G7706	R7707	D7708	A7709	R7711	M7712	N7713	I7714	L7715	G7717	R7718	I7719	I7720	A/ /21	T7723	V7724	R7725	0.777	G7729	P7730	K7731	G7732	M7733	N 134 K7735		G7742	D7743	V7744	V7745	V//40	N7748		V7751	T7752	R7755	E7756	H	V7759	P7762	A7763	A7764
K7765	M7766	L7767	E7769	V7770	T7773	Q7774	E1775	E7777	V7778	G7779	D7780	G7781	T7784	A7785	V7786	V7787	V7788	A7789 G7790	E7791	L7792	L7793	K1794	A7796	E7797	E77 98	L7799		07802	N7803	V7804	H7805	T7807	17808	K7811	G7812	Y7813	Q7814	A7815	A7816 🕈 A7817	Q7818	K7819		E7822	L7823 L7824	K7825	T7826	17827 A7838	0701W
C7829	E7830	V7831	G7832 A 7033	A (833 D 7834	D7835	K7836	E/ 83/ 17838	L7839	T7840	K/841	T7845		G7849	E7853	K7854	A7855	K7856	E7857 V7869	L7859	A7860	E7861	17862	V7864	E7865	A7866	V7867	S7868	A7869 V7870	V7871 🔶	D7872	D7873	E/8/4 G7875	K7876	V7877	D7879	D7880	L7881	17882	K7883	17884	E7885	G7889	A7890	S7891	L r 09 Z	D7894	T7895	E7896
L7897	I7898	K7 899	G7900	TOGIA	K7 905	E7906 R7907		A7910	U7911	D7013	K7914	K7915	V7916	T7917	D7918	A7919	NI 920	L7923	L7924	1001	A/ 92/	E7929	I7930	K7931	E7932	T7933	E/ 934	D7936	A7937	E7938	L/ 939 R7940	I7941	T7942	D7943	P/ 944 A7945	K7946	L7947	M7 948	E7949	E7952	Q7953	E7 954	E/955	M7957	L7958	K7959	D'r 960	A7 963

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D8	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	11.011	Depositor
Minimum map value	-5.521	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.15	Depositor
Map size (Å)	255.36002, 255.36002, 255.36002	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bo	ond lengths	В	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	В	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	С	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	D	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	Е	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	F	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	G	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	Н	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	Ι	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	J	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	Κ	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	L	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	М	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	Ν	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	0	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
1	Р	0.88	2/3875~(0.1%)	0.78	2/5214~(0.0%)
All	All	0.88	32/62000~(0.1%)	0.78	32/83424~(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	А	0	3
1	В	0	3
1	С	0	3
1	D	0	3
1	Е	0	3
1	F	0	3
1	G	0	3
1	Н	0	3
1	Ι	0	3

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	Κ	0	3
1	L	0	3
1	М	0	3
1	Ν	0	3
1	0	0	3
1	Р	0	3
All	All	0	48

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	М	6160	GLU	C-O	-5.76	1.12	1.23
1	0	7186	GLU	C-O	-5.75	1.12	1.23
1	А	4	GLU	C-O	-5.72	1.12	1.23
1	С	1030	GLU	C-O	-5.72	1.12	1.23
1	Е	2056	GLU	C-O	-5.72	1.12	1.23
1	G	3082	GLU	C-O	-5.72	1.12	1.23
1	Κ	5134	GLU	C-O	-5.72	1.12	1.23
1	В	517	GLU	C-O	-5.72	1.12	1.23
1	D	1543	GLU	C-O	-5.72	1.12	1.23
1	F	2569	GLU	C-O	-5.72	1.12	1.23
1	Н	3595	GLU	C-O	-5.72	1.12	1.23
1	J	4621	GLU	C-O	-5.72	1.12	1.23
1	L	5647	GLU	C-O	-5.72	1.12	1.23
1	N	6673	GLU	C-O	-5.72	1.12	1.23
1	Р	7699	GLU	C-O	-5.72	1.12	1.23
1	Ι	4108	GLU	C-O	-5.71	1.12	1.23
1	А	4	GLU	C-N	5.45	1.46	1.34
1	С	1030	GLU	C-N	5.45	1.46	1.34
1	Е	2056	GLU	C-N	5.45	1.46	1.34
1	G	3082	GLU	C-N	5.45	1.46	1.34
1	Ν	6673	GLU	C-N	5.43	1.46	1.34
1	Р	7699	GLU	C-N	5.43	1.46	1.34
1	В	517	GLU	C-N	5.41	1.46	1.34
1	D	1543	GLU	C-N	5.41	1.46	1.34
1	F	2569	GLU	C-N	5.41	1.46	1.34
1	Н	3595	GLU	C-N	5.41	1.46	1.34
1	Ι	4108	GLU	C-N	5.40	1.46	1.34
1	J	4621	GLU	C-N	5.40	1.46	1.34
1	Κ	5134	GLU	C-N	5.40	1.46	1.34
1	L	5647	GLU	C-N	5.40	1.46	1.34

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
1	М	6160	GLU	C-N	5.40	1.46	1.34
1	0	7186	GLU	C-N	5.40	1.46	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	229	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	С	1255	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	Е	2281	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	G	3307	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	Ι	4333	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	Κ	5359	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	М	6385	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	0	7411	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	В	742	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	D	1768	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	F	2794	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	Н	3820	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	N	6898	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	Р	7924	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	J	4846	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	L	5872	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	В	978	ALA	CB-CA-C	5.11	117.77	110.10
1	D	2004	ALA	CB-CA-C	5.11	117.77	110.10
1	F	3030	ALA	CB-CA-C	5.11	117.77	110.10
1	Н	4056	ALA	CB-CA-C	5.11	117.77	110.10
1	А	465	ALA	CB-CA-C	5.11	117.76	110.10
1	С	1491	ALA	CB-CA-C	5.11	117.76	110.10
1	Е	2517	ALA	CB-CA-C	5.11	117.76	110.10
1	G	3543	ALA	CB-CA-C	5.11	117.76	110.10
1	Κ	5595	ALA	CB-CA-C	5.11	117.76	110.10
1	М	6621	ALA	CB-CA-C	5.10	117.75	110.10
1	N	7134	ALA	CB-CA-C	5.09	117.74	110.10
1	Р	8160	ALA	CB-CA-C	5.09	117.74	110.10
1	J	5082	ALA	CB-CA-C	5.08	117.73	110.10
1	L	6108	ALA	CB-CA-C	5.08	117.73	110.10
1	Ι	4569	ALA	CB-CA-C	5.07	117.70	110.10
1	0	7647	ALA	CB-CA-C	5.06	117.69	110.10

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	119	GLN	Mainchain
1	А	138	ALA	Mainchain
1	А	475	GLU	Mainchain
1	В	632	GLN	Mainchain
1	В	651	ALA	Mainchain
1	В	988	GLU	Mainchain
1	С	1145	GLN	Mainchain
1	С	1164	ALA	Mainchain
1	С	1501	GLU	Mainchain
1	D	1658	GLN	Mainchain
1	D	1677	ALA	Mainchain
1	D	2014	GLU	Mainchain
1	Е	2171	GLN	Mainchain
1	Е	2190	ALA	Mainchain
1	Ε	2527	GLU	Mainchain
1	F	2684	GLN	Mainchain
1	F	2703	ALA	Mainchain
1	F	3040	GLU	Mainchain
1	G	3197	GLN	Mainchain
1	G	3216	ALA	Mainchain
1	G	3553	GLU	Mainchain
1	Н	3710	GLN	Mainchain
1	Н	3729	ALA	Mainchain
1	Н	4066	GLU	Mainchain
1	Ι	4223	GLN	Mainchain
1	Ι	4242	ALA	Mainchain
1	Ι	4579	GLU	Mainchain
1	J	4736	GLN	Mainchain
1	J	4755	ALA	Mainchain
1	J	5092	GLU	Mainchain
1	Κ	5249	GLN	Mainchain
1	K	5268	ALA	Mainchain
1	Κ	5605	GLU	Mainchain
1	L	5762	GLN	Mainchain
1	L	5781	ALA	Mainchain
1	L	6118	GLU	Mainchain
1	М	6275	GLN	Mainchain
1	М	6294	ALA	Mainchain
1	М	6631	GLU	Mainchain
1	N	6788	GLN	Mainchain
1	N	6807	ALA	Mainchain
1	N	7144	GLU	Mainchain
1	0	7301	GLN	Mainchain

		1	1 0	
Mol	Chain	\mathbf{Res}	Type	Group
1	0	7320	ALA	Mainchain
1	0	7657	GLU	Mainchain
1	Р	7814	GLN	Mainchain
1	Р	7833	ALA	Mainchain
1	Р	8170	GLU	Mainchain

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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	А	3852	0	3996	13	0
1	В	3852	0	3993	13	0
1	С	3852	0	3993	13	0
1	D	3852	0	3993	12	0
1	Ε	3852	0	3993	13	0
1	F	3852	0	3993	12	0
1	G	3852	0	3993	13	0
1	Н	3852	0	3993	13	0
1	Ι	3852	0	3993	14	0
1	J	3852	0	3993	13	0
1	Κ	3852	0	3993	13	0
1	L	3852	0	3993	13	0
1	М	3852	0	3993	13	0
1	Ν	3852	0	3993	12	0
1	0	3852	0	3993	13	0
1	Р	3852	0	3993	12	0
All	All	61632	0	63891	189	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 2.

All (189) 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:4:GLU:O	1:A:5:ASN:HB2	1.96	0.65
1:B:517:GLU:O	1:B:518:ASN:HB2	1.96	0.65

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:5134:GLU:O	1:K:5135:ASN:HB2	1.96	0.65
1:L:5647:GLU:O	1:L:5648:ASN:HB2	1.96	0.65
1:C:1030:GLU:O	1:C:1031:ASN:HB2	1.96	0.65
1:H:3595:GLU:O	1:H:3596:ASN:HB2	1.96	0.65
1:J:4621:GLU:O	1:J:4622:ASN:HB2	1.96	0.65
1:D:1543:GLU:O	1:D:1544:ASN:HB2	1.96	0.64
1:M:6160:GLU:O	1:M:6161:ASN:HB2	1.96	0.64
1:N:6673:GLU:O	1:N:6674:ASN:HB2	1.96	0.64
1:I:4108:GLU:O	1:I:4109:ASN:HB2	1.96	0.64
1:G:3082:GLU:O	1:G:3083:ASN:HB2	1.96	0.64
1:P:7699:GLU:O	1:P:7700:ASN:HB2	1.96	0.64
1:F:2569:GLU:O	1:F:2570:ASN:HB2	1.96	0.64
1:O:7186:GLU:O	1:O:7187:ASN:HB2	1.96	0.64
1:E:2056:GLU:O	1:E:2057:ASN:HB2	1.96	0.64
1:E:2287:ILE:H	1:E:2287:ILE:HD12	1.65	0.62
1:O:7417:ILE:H	1:O:7417:ILE:HD12	1.65	0.62
1:C:1261:ILE:HD12	1:C:1261:ILE:H	1.65	0.61
1:M:6391:ILE:H	1:M:6391:ILE:HD12	1.65	0.61
1:G:3313:ILE:H	1:G:3313:ILE:HD12	1.65	0.61
1:I:4339:ILE:HD12	1:I:4339:ILE:H	1.65	0.61
1:N:6904:ILE:H	1:N:6904:ILE:HD12	1.65	0.60
1:J:5051:ILE:HB	1:J:5052:PRO:HD3	1.83	0.60
1:K:5564:ILE:HB	1:K:5565:PRO:HD3	1.84	0.60
1:A:434:ILE:HB	1:A:435:PRO:HD3	1.84	0.60
1:H:4025:ILE:HB	1:H:4026:PRO:HD3	1.84	0.60
1:D:1774:ILE:H	1:D:1774:ILE:HD12	1.65	0.60
1:L:6077:ILE:HB	1:L:6078:PRO:HD3	1.83	0.60
1:B:947:ILE:HB	1:B:948:PRO:HD3	1.84	0.60
1:M:6590:ILE:HB	1:M:6591:PRO:HD3	1.84	0.60
1:D:1973:ILE:HB	1:D:1974:PRO:HD3	1.84	0.60
1:E:2486:ILE:HB	1:E:2487:PRO:HD3	1.84	0.60
1:O:7616:ILE:HB	1:0:7617:PRO:HD3	1.84	0.60
1:F:2800:ILE:H	1:F:2800:ILE:HD12	1.65	0.60
1:F:2999:ILE:HB	1:F:3000:PRO:HD3	1.84	0.60
1:C:1460:ILE:HB	1:C:1461:PRO:HD3	1.84	0.60
1:A:235:ILE:H	1:A:235:ILE:HD12	1.65	0.60
1:J:4852:ILE:H	1:J:4852:ILE:HD12	1.65	0.60
1:N:7103:ILE:HB	1:N:7104:PRO:HD3	1.84	0.60
1:P:8129:ILE:HB	1:P:8130:PRO:HD3	1.84	0.60
1:G:3512:ILE:HB	1:G:3513:PRO:HD3	1.84	0.60
1:K:5365:ILE:HD12	1:K:5365:ILE:H	1.65	0.60

	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:P:7930:ILE:HD12	1:P:7930:ILE:H	1.65	0.60
1:H:3826:ILE:HD12	1:H:3826:ILE:H	1.65	0.59
1:I:4538:ILE:HB	1:I:4539:PRO:HD3	1.84	0.59
1:L:5878:ILE:HD12	1:L:5878:ILE:H	1.65	0.59
1:B:748:ILE:HD12	1:B:748:ILE:H	1.65	0.59
1:A:163:LYS:HE3	1:A:163:LYS:HA	1.90	0.54
1:K:5293:LYS:HE3	1:K:5293:LYS:HA	1.90	0.54
1:I:4267:LYS:HA	1:I:4267:LYS:HE3	1.90	0.54
1:F:2728:LYS:HA	1:F:2728:LYS:HE3	1.90	0.54
1:G:3241:LYS:HA	1:G:3241:LYS:HE3	1.90	0.54
1:C:1189:LYS:HE3	1:C:1189:LYS:HA	1.90	0.54
1:M:6319:LYS:HA	1:M:6319:LYS:HE3	1.90	0.53
1:P:7858:LYS:HE3	1:P:7858:LYS:HA	1.90	0.53
1:H:3754:LYS:HA	1:H:3754:LYS:HE3	1.90	0.53
1:J:4780:LYS:HA	1:J:4780:LYS:HE3	1.90	0.53
1:L:5806:LYS:HE3	1:L:5806:LYS:HA	1.90	0.53
1:B:676:LYS:HA	1:B:676:LYS:HE3	1.90	0.53
1:E:2215:LYS:HA	1:E:2215:LYS:HE3	1.90	0.53
1:O:7345:LYS:HE3	1:0:7345:LYS:HA	1.90	0.53
1:E:2555:LEU:C	1:E:2555:LEU:HD23	2.30	0.53
1:O:7685:LEU:C	1:O:7685:LEU:HD23	2.30	0.53
1:C:1529:LEU:C	1:C:1529:LEU:HD23	2.30	0.52
1:D:2042:LEU:C	1:D:2042:LEU:HD23	2.29	0.52
1:M:6659:LEU:C	1:M:6659:LEU:HD23	2.30	0.52
1:N:7172:LEU:C	1:N:7172:LEU:HD23	2.29	0.52
1:L:6146:LEU:C	1:L:6146:LEU:HD23	2.29	0.52
1:B:1016:LEU:C	1:B:1016:LEU:HD23	2.29	0.52
1:G:3581:LEU:HD23	1:G:3581:LEU:C	2.30	0.52
1:I:4607:LEU:HD23	1:I:4607:LEU:C	2.30	0.52
1:D:1702:LYS:HE3	1:D:1702:LYS:HA	1.90	0.52
1:F:3068:LEU:C	1:F:3068:LEU:HD23	2.29	0.52
1:P:8198:LEU:HD23	1:P:8198:LEU:C	2.29	0.52
1:N:6832:LYS:HE3	1:N:6832:LYS:HA	1.90	0.52
1:J:5120:LEU:C	1:J:5120:LEU:HD23	2.29	0.51
1:H:4094:LEU:C	1:H:4094:LEU:HD23	2.29	0.51
1:K:5633:LEU:C	1:K:5633:LEU:HD23	2.30	0.51
1:A:503:LEU:C	1:A:503:LEU:HD23	2.30	0.51
1:G:3082:GLU:O	1:G:3083:ASN:CB	2.60	0.50
1:I:4108:GLU:O	1:I:4109:ASN:CB	2.60	0.50
1:F:2569:GLU:O	1:F:2570:ASN:CB	2.60	0.49
1:H:3826:ILE:HD12	1:H:3826:ILE:N	2.27	0.49

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:4852:ILE:HD12	1:J:4852:ILE:N	2.27	0.49
1:J:4621:GLU:O	1:J:4622:ASN:CB	2.60	0.49
1:P:7699:GLU:O	1:P:7700:ASN:CB	2.60	0.49
1:H:3595:GLU:O	1:H:3596:ASN:CB	2.60	0.49
1:C:1030:GLU:O	1:C:1031:ASN:CB	2.60	0.49
1:M:6160:GLU:O	1:M:6161:ASN:CB	2.60	0.49
1:B:517:GLU:O	1:B:518:ASN:CB	2.60	0.49
1:B:748:ILE:HD12	1:B:748:ILE:N	2.27	0.49
1:L:5878:ILE:HD12	1:L:5878:ILE:N	2.27	0.49
1:L:5647:GLU:O	1:L:5648:ASN:CB	2.60	0.49
1:N:6673:GLU:O	1:N:6674:ASN:CB	2.60	0.49
1:D:1543:GLU:O	1:D:1544:ASN:CB	2.60	0.49
1:E:2056:GLU:O	1:E:2057:ASN:CB	2.60	0.49
1:I:4339:ILE:HD12	1:I:4339:ILE:N	2.27	0.49
1:G:3313:ILE:HD12	1:G:3313:ILE:N	2.27	0.49
1:K:5134:GLU:O	1:K:5135:ASN:CB	2.60	0.49
1:A:4:GLU:O	1:A:5:ASN:CB	2.60	0.48
1:O:7186:GLU:O	1:O:7187:ASN:CB	2.60	0.48
1:A:235:ILE:HD12	1:A:235:ILE:N	2.27	0.48
1:C:1261:ILE:HD12	1:C:1261:ILE:N	2.27	0.48
1:M:6391:ILE:HD12	1:M:6391:ILE:N	2.27	0.48
1:K:5365:ILE:HD12	1:K:5365:ILE:N	2.27	0.48
1:N:6904:ILE:HD12	1:N:6904:ILE:N	2.27	0.48
1:D:1774:ILE:HD12	1:D:1774:ILE:N	2.27	0.48
1:E:2287:ILE:HD12	1:E:2287:ILE:N	2.27	0.48
1:F:2800:ILE:HD12	1:F:2800:ILE:N	2.27	0.48
1:O:7417:ILE:HD12	1:O:7417:ILE:N	2.27	0.48
1:P:7930:ILE:HD12	1:P:7930:ILE:N	2.27	0.47
1:D:2047:ASP:HB3	1:E:2092:LYS:HD2	1.98	0.45
1:O:7690:ASP:HB3	1:P:7735:LYS:HD2	1.98	0.45
1:E:2560:ASP:HB3	1:F:2605:LYS:HD2	1.98	0.45
1:M:6664:ASP:HB3	1:N:6709:LYS:HD2	1.98	0.45
1:C:1534:ASP:HB3	1:D:1579:LYS:HD2	1.98	0.45
1:N:7177:ASP:HB3	1:O:7222:LYS:HD2	1.99	0.45
1:F:3073:ASP:HB3	1:G:3118:LYS:HD2	1.98	0.45
1:B:1021:ASP:HB3	1:C:1066:LYS:HD2	1.98	0.45
1:I:4144:LYS:HD2	1:P:8203:ASP:HB3	1.99	0.44
1:I:4612:ASP:HB3	1:J:4657:LYS:HD2	1.98	0.44
1:L:6151:ASP:HB3	1:M:6196:LYS:HD2	1.99	0.44
1:G:3586:ASP:HB3	1:H:3631:LYS:HD2	1.98	0.44
1:K:5638:ASP:HB3	1:L:5683:LYS:HD2	1.98	0.44

	i as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:40:LYS:HD2	1:H:4099:ASP:HB3	1.98	0.44
1:A:508:ASP:HB3	1:B:553:LYS:HD2	1.98	0.43
1:M:6335:GLU:HA	1:M:6336:GLY:HA3	1.81	0.43
1:J:5125:ASP:HB3	1:K:5170:LYS:HD2	1.99	0.43
1:C:1205:GLU:HA	1:C:1206:GLY:HA3	1.81	0.43
1:F:2836:LYS:O	1:F:2836:LYS:HD3	2.19	0.43
1:P:7966:LYS:O	1:P:7966:LYS:HD3	2.19	0.43
1:B:609:GLU:HG2	1:B:946:VAL:HB	2.01	0.43
1:E:2323:LYS:O	1:E:2323:LYS:HD3	2.19	0.43
1:F:2661:GLU:HG2	1:F:2998:VAL:HB	2.01	0.43
1:N:6940:LYS:O	1:N:6940:LYS:HD3	2.19	0.43
1:0:7453:LYS:O	1:O:7453:LYS:HD3	2.19	0.43
1:P:7791:GLU:HG2	1:P:8128:VAL:HB	2.01	0.43
1:D:1635:GLU:HG2	1:D:1972:VAL:HB	2.01	0.43
1:D:1810:LYS:O	1:D:1810:LYS:HD3	2.19	0.43
1:L:5739:GLU:HG2	1:L:6076:VAL:HB	2.01	0.43
1:N:6765:GLU:HG2	1:N:7102:VAL:HB	2.01	0.43
1:G:3349:LYS:O	1:G:3349:LYS:HD3	2.19	0.42
1:I:4375:LYS:O	1:I:4375:LYS:HD3	2.19	0.42
1:J:4619:LEU:HA	1:J:4620:PRO:HD3	1.91	0.42
1:L:5862:LYS:HA	1:L:5862:LYS:HE2	2.02	0.42
1:A:219:LYS:HA	1:A:219:LYS:HE2	2.02	0.42
1:H:3593:LEU:HA	1:H:3594:PRO:HD3	1.91	0.42
1:H:3687:GLU:HG2	1:H:4024:VAL:HB	2.01	0.42
1:H:3862:LYS:O	1:H:3862:LYS:HD3	2.19	0.42
1:J:4713:GLU:HG2	1:J:5050:VAL:HB	2.01	0.42
1:K:5349:LYS:HE2	1:K:5349:LYS:HA	2.02	0.42
1:A:2:LEU:HA	1:A:3:PRO:HD3	1.91	0.42
1:A:271:LYS:O	1:A:271:LYS:HD3	2.19	0.42
1:C:1297:LYS:O	1:C:1297:LYS:HD3	2.19	0.42
1:J:4888:LYS:O	1:J:4888:LYS:HD3	2.19	0.42
1:K:5132:LEU:HA	1:K:5133:PRO:HD3	1.91	0.42
1:K:5401:LYS:O	1:K:5401:LYS:HD3	2.19	0.42
1:M:6427:LYS:O	1:M:6427:LYS:HD3	2.19	0.42
1:M:6252:GLU:HG2	1:M:6589:VAL:HB	2.01	0.42
1:B:732:LYS:HA	1:B:732:LYS:HE2	2.02	0.42
1:C:1122:GLU:HG2	1:C:1459:VAL:HB	2.01	0.42
1:C:1245:LYS:HE2	1:C:1245:LYS:HA	2.02	0.42
1:N:6888:LYS:HE2	1:N:6888:LYS:HA	2.02	0.42
1:M:6375:LYS:HA	1:M:6375:LYS:HE2	2.02	0.42
1:O:7361:GLU:HA	1:O:7362:GLY:HA3	1.81	0.42

		International	Clash
Atom-1	Atom-2		
		distance (A)	overlap (A)
1:A:96:GLU:HG2	1:A:433:VAL:HB	2.01	0.42
1:D:1758:LYS:HA	1:D:1758:LYS:HE2	2.02	0.42
1:J:4836:LYS:HA	1:J:4836:LYS:HE2	2.02	0.42
1:K:5226:GLU:HG2	1:K:5563:VAL:HB	2.01	0.42
1:0:7278:GLU:HG2	1:O:7615:VAL:HB	2.01	0.42
1:B:784:LYS:O	1:B:784:LYS:HD3	2.19	0.42
1:H:3810:LYS:HA	1:H:3810:LYS:HE2	2.02	0.42
1:E:2148:GLU:HG2	1:E:2485:VAL:HB	2.01	0.41
1:L:5914:LYS:O	1:L:5914:LYS:HD3	2.19	0.41
1:I:4200:GLU:HG2	1:I:4537:VAL:HB	2.01	0.41
1:E:2231:GLU:HA	1:E:2232:GLY:HA3	1.81	0.41
1:E:2271:LYS:HE2	1:E:2271:LYS:HA	2.02	0.41
1:0:7401:LYS:HE2	1:O:7401:LYS:HA	2.02	0.41
1:G:3174:GLU:HG2	1:G:3511:VAL:HB	2.01	0.41
1:I:4323:LYS:HA	1:I:4323:LYS:HE2	2.02	0.41
1:G:3297:LYS:HA	1:G:3297:LYS:HE2	2.02	0.41
1:P:7914:LYS:HA	1:P:7914:LYS:HE2	2.02	0.41
1:G:3080:LEU:HA	1:G:3081:PRO:HD3	1.91	0.41
1:I:4106:LEU:HA	1:I:4107:PRO:HD3	1.91	0.41
1:F:2784:LYS:HA	1:F:2784:LYS:HE2	2.02	0.41
1:B:515:LEU:HA	1:B:516:PRO:HD3	1.91	0.40
1:I:4283:GLU:HA	1:I:4284:GLY:HA3	1.81	0.40
1:L:5645:LEU:HA	1:L:5646:PRO:HD3	1.91	0.40

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	Perce	ntiles
1	А	511/513~(100%)	497~(97%)	13 (2%)	1 (0%)	47	81
1	В	511/513~(100%)	497 (97%)	13 (2%)	1 (0%)	47	81

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	\mathbf{C}	511/513~(100%)	497~(97%)	13~(2%)	1 (0%)	47	81
1	D	511/513~(100%)	497~(97%)	13~(2%)	1 (0%)	47	81
1	Е	511/513~(100%)	497~(97%)	13 (2%)	1 (0%)	47	81
1	F	511/513~(100%)	497~(97%)	13~(2%)	1 (0%)	47	81
1	G	511/513~(100%)	497~(97%)	13 (2%)	1 (0%)	47	81
1	Н	511/513~(100%)	497~(97%)	13 (2%)	1 (0%)	47	81
1	Ι	511/513~(100%)	497~(97%)	13 (2%)	1 (0%)	47	81
1	J	511/513~(100%)	497~(97%)	13~(2%)	1 (0%)	47	81
1	Κ	511/513~(100%)	497~(97%)	13 (2%)	1 (0%)	47	81
1	L	511/513~(100%)	497~(97%)	13~(2%)	1 (0%)	47	81
1	М	511/513~(100%)	497~(97%)	13 (2%)	1 (0%)	47	81
1	Ν	511/513~(100%)	497~(97%)	13~(2%)	1 (0%)	47	81
1	Ο	511/513~(100%)	497 (97%)	13 (2%)	1 (0%)	47	81
1	Р	511/513~(100%)	497 (97%)	13 (2%)	1 (0%)	47	81
All	All	8176/8208~(100%)	7952 (97%)	208 (2%)	16 (0%)	50	81

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	5	ASN
1	В	518	ASN
1	С	1031	ASN
1	D	1544	ASN
1	Е	2057	ASN
1	F	2570	ASN
1	G	3083	ASN
1	Н	3596	ASN
1	Ι	4109	ASN
1	J	4622	ASN
1	K	5135	ASN
1	L	5648	ASN
1	М	6161	ASN
1	N	6674	ASN
1	0	7187	ASN
1	Р	7700	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	414/414~(100%)	409~(99%)	5 (1%)	71	83
1	В	414/414~(100%)	409 (99%)	5 (1%)	71	83
1	С	414/414~(100%)	409~(99%)	5 (1%)	71	83
1	D	414/414~(100%)	409 (99%)	5 (1%)	71	83
1	Ε	414/414~(100%)	409~(99%)	5 (1%)	71	83
1	F	414/414~(100%)	409 (99%)	5 (1%)	71	83
1	G	414/414~(100%)	409~(99%)	5 (1%)	71	83
1	Н	414/414~(100%)	409 (99%)	5 (1%)	71	83
1	Ι	414/414~(100%)	409 (99%)	5 (1%)	71	83
1	J	414/414~(100%)	409 (99%)	5 (1%)	71	83
1	Κ	414/414 (100%)	409 (99%)	5 (1%)	71	83
1	L	414/414 (100%)	409 (99%)	5 (1%)	71	83
1	М	414/414 (100%)	409 (99%)	5 (1%)	71	83
1	Ν	414/414 (100%)	409 (99%)	5 (1%)	71	83
1	Ο	414/414 (100%)	409 (99%)	5 (1%)	71	83
1	Р	414/414 (100%)	409 (99%)	5 (1%)	71	83
All	All	6624/6624~(100%)	6544 (99%)	80 (1%)	72	83

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	36	LYS
1	А	72	LEU
1	А	144	LEU
1	А	163	LYS
1	А	419	ARG
1	В	549	LYS
1	В	585	LEU
1	В	657	LEU

Mol	Chain	Res	Type
1	В	676	LYS
1	В	932	ARG
1	С	1062	LYS
1	С	1098	LEU
1	С	1170	LEU
1	С	1189	LYS
1	С	1445	ARG
1	D	1575	LYS
1	D	1611	LEU
1	D	1683	LEU
1	D	1702	LYS
1	D	1958	ARG
1	Е	2088	LYS
1	Е	2124	LEU
1	Е	2196	LEU
1	Е	2215	LYS
1	Е	2471	ARG
1	F	2601	LYS
1	F	2637	LEU
1	F	2709	LEU
1	F	2728	LYS
1	F	2984	ARG
1	G	3114	LYS
1	G	3150	LEU
1	G	3222	LEU
1	G	3241	LYS
1	G	3497	ARG
1	Н	3627	LYS
1	Н	3663	LEU
1	Н	3735	LEU
1	Н	3754	LYS
1	Н	4010	ARG
1	Ι	4140	LYS
1	I	4176	LEU
1	Ι	4248	LEU
1	Ι	4267	LYS
1	Ι	4523	ARG
1	J	4653	LYS
1	J	4689	LEU
1	J	4761	LEU
1	J	4780	LYS
1	J	5036	ARG

Mol	Chain	Res	Type
1	K	5166	LYS
1	K	5202	LEU
1	K	5274	LEU
1	K	5293	LYS
1	K	5549	ARG
1	L	5679	LYS
1	L	5715	LEU
1	L	5787	LEU
1	L	5806	LYS
1	L	6062	ARG
1	М	6192	LYS
1	М	6228	LEU
1	М	6300	LEU
1	М	6319	LYS
1	М	6575	ARG
1	N	6705	LYS
1	N	6741	LEU
1	N	6813	LEU
1	Ν	6832	LYS
1	N	7088	ARG
1	0	7218	LYS
1	0	7254	LEU
1	0	7326	LEU
1	0	7345	LYS
1	0	7601	ARG
1	Р	7731	LYS
1	Р	7767	LEU
1	Р	7839	LEU
1	Р	7858	LYS
1	Р	8114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	18	ASN
1	А	79	GLN
1	В	531	ASN
1	В	592	GLN
1	С	1044	ASN
1	С	1105	GLN
1	D	1557	ASN
1	D	1618	GLN

Mol	Chain	Res	Type
1	Е	2070	ASN
1	Е	2131	GLN
1	F	2583	ASN
1	F	2644	GLN
1	G	3096	ASN
1	G	3157	GLN
1	Н	3609	ASN
1	Н	3670	GLN
1	Ι	4122	ASN
1	Ι	4183	GLN
1	J	4635	ASN
1	J	4696	GLN
1	J	4907	HIS
1	K	5148	ASN
1	К	5209	GLN
1	L	5661	ASN
1	L	5722	GLN
1	М	6174	ASN
1	М	6235	GLN
1	Ν	6687	ASN
1	N	6748	GLN
1	0	7200	ASN
1	0	7261	GLN
1	Р	7713	ASN
1	Р	7774	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5249. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map

The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 96

Y Index: 96

Z Index: 96

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 74

Y Index: 74

Z Index: 104

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

The images above show the 3D surface view of the map at the recommended contour level 4.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)

The volume at the recommended contour level is 307 nm^3 ; this corresponds to an approximate mass of 278 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

*Reported resolution corresponds to spatial frequency of 0.139 \AA^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5249 and PDB model 3IZM. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)

The images above show the 3D surface view of the map at the recommended contour level 4.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.15).

9.4 Atom inclusion (i)

At the recommended contour level, 36% of all backbone atoms, 27% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.2712	0.0630	
А	0.2723	0.0630	
В	0.2697	0.0650	1 0
С	0.2723	0.0660	
D	0.2700	0.0670	
Е	0.2723	0.0660	
F	0.2700	0.0650	
G	0.2726	0.0630	
Н	0.2700	0.0620	
Ι	0.2723	0.0600	
J	0.2702	0.0610	
K	0.2723	0.0600	0.0
L	0.2702	0.0620	<0.0
М	0.2723	0.0610	
N	0.2702	0.0610]
0	0.2726	0.0610	
Р	0.2702	0.0610	

