

wwPDB EM Validation Summary Report (i)

Nov 14, 2022 - 09:17 AM EST

PDB ID	:	7K58
EMDB ID	:	EMD-22677
Title	:	Structure of outer-arm dyneins bound to microtubule with microtubule binding state 1(MTBS-1)
Authors	:	Qinhui, R.; Kai, Z.
Deposited on	:	2020-09-16
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
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)	:	2.31.2

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 3.50 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 $(\#Entries)$	${ m EM~structures}\ (\#{ m Entries})$
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	4615	19%	9% •
2	С	3943	90%	10% •
3	Q	192	95%	5%
4	В	4588	85%	12% •••
5	Ι	106	26%	18% •
6	Н	91	30%	9% •
7	G	96	31%	14%
8	F	110	25%	17% ·

Continued on next page...



20100				
Mol	Chain	Length	Quality of chain	
			17%	
9	Ν	114	87%	12%
	11	111	310/	15 //
10	0	100	51%	
10	0	120	81%	17% ••
			28%	
11	E	557	87%	11% •
			18%	
10	Л	505		
12	D		82%	14% • •
			41%	
13	Р	112	88%	9% •
			45%	
14	L	98	86%	12%
			32%	1270
1 5	17	00	5270	
15	K	90	96%	•
			25%	
16	J	95	95%	5%
			23%	
17	м	87		170/
1 1	IVI	01	82%	1/% •

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2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 117936 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 Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	4443	Total 33894	C 21519	N 5788	O 6429	S 158	0	0

• Molecule 2 is a protein called gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	С	3943	Total 30436	C 19390	N 5162	O 5735	S 149	0	0

• Molecule 3 is a protein called Dynein light chain 1.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
3	Q	192	Total 1002	C 607	N 202	O 193	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	2	ALA	SER	conflict	UNP Q1HGH9

• Molecule 4 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues		Α	AltConf	Trace			
4	В	4516	Total	C	N	0	S	0	0
			34604	21978	5928	6547	151		

• Molecule 5 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ι	106	Total 827	C 526	N 134	0 161	S 6	0	0

• Molecule 6 is a protein called Dynein light chain.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	Н	91	Total 750	C 483	N 124	O 139	$\frac{S}{4}$	0	0

• Molecule 7 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	G	96	Total 749	C 471	N 129	0 148	S 1	0	0

• Molecule 8 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues		At	AltConf	Trace			
8	F	110	Total 863	С 544	N 152	0 165	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 9 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	Ν	114	Total 855	C 543	N 143	0 166	${ m S} { m 3}$	0	0

• Molecule 10 is a protein called Dynein light chain 2A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	О	120	Total 986	C 634	N 172	0 177	${ m S} { m 3}$	0	0

• Molecule 11 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues		At	AltConf	Trace			
11	Е	555	Total 4423	C 2786	N 759	O 856	S 22	0	0

• Molecule 12 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues		At	AltConf	Trace			
12	D	579	Total 4664	C 2964	N 787	0 883	S 30	0	0

• Molecule 13 is a protein called Thioredoxin.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
13	Р	109	Total 541	C 323	N 109	O 109	0	0

• Molecule 14 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms	AltConf	Trace		
14	L	98	Total 783	C 511	N 132	0 137	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	K	90	Total 754	C 489	N 124	0 137	$\frac{S}{4}$	0	0

• Molecule 16 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	J	95	Total 806	$\begin{array}{c} \mathrm{C} \\ 527 \end{array}$	N 135	O 140	${f S}$ 4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	ALA	CYS	conflict	UNP Q22R86

• Molecule 17 is a protein called Dynein light chain.

Mol	Chain	Residues		At	oms			AltConf	Trace
17	М	87	Total 735	С 477	N 123	O 130	${S \atop 5}$	0	0

• Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





Mol	Chain	Residues	Atoms					AltConf
18	Δ	1	Total	С	Ν	Ο	Р	0
10	Л	T	54	20	10	20	4	0
18	Δ	1	Total	С	Ν	Ο	Р	0
10	Π	T	54	20	10	20	4	0
18	С	1	Total	С	Ν	Ο	Р	0
10		1	54	20	10	20	4	0
18	C	1	Total	\mathbf{C}	Ν	Ο	Р	0
10	U	I	54	20	10	20	4	0
18	В	1	Total	С	Ν	Ο	Р	0
10	D	I	54	20	10	20	4	0
18	В	1	Total	С	Ν	Ο	Р	0
10			54	20	10	20	4	

• Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues	Atoms					AltConf
10	Λ	1	Total	С	Ν	Ο	Р	0
19	Л	T	31	10	5	13	3	0
10	10 C	1	Total	С	Ν	Ο	Р	0
	U		31	10	5	13	3	0
10	В	1	Total	С	Ν	Ο	Р	0
19	D		31	10	5	13	3	0

 $\bullet\,$ Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
20	А	3	Total Mg 3 3	0
20	С	3	Total Mg 3 3	0
20	В	3	Total Mg 3 3	0



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: Dynein heavy chain, outer arm protein









K2722 12723 12723 12725 12725 12725 12725 12775 12775 12775 12775 12775 12776 12775 12776 12779 12789 12
V28 66 T29 55 K29 95 K29 95 K29 900 D29 05 K29 900 D29 05 K29 33 L29 35 K29 33 K29 33 K29 34 K29 35 K29 35 K29 36 K29 35 K29 35 K29 36 K29 36 K29 36 K29 36 K29 36 K29 36 K29 37 K29 36 K29 40 K29 55 K29 56 K29 56 K29 56 K29 56 K29 56 K29 57 K29 56 K29 57 K29 56 K29 57 K29 56 K29 57 K29 57 K29 56 K29 57 K29 58 K29 59 K29 59 K29 50 <td< td=""></td<>
D2989 P2989 D2989 C3005 P2999 C3005 P2005 C3005 P3005 C3005 P3111 C3115 P3125 C3125 P3125 C3125 P3125 C3125 P3125 C3125 P3126 C3125 P3127 C3125 P3126 C3125 P3127 C3125 P3
I3132 I3132 I3132 I3145 K3139 I3145 I3145 I3145 I3145 I3145 I3145 I3145 I3145 I3146 I3145 I3146 I3147 I3215 I3216 I3220 I32215 I32215 I32215 I32215 I32225 I32225 I32232 I32232 I32232 I32232 I32232 I32232 I32233 I32233 I32233 I32334
Y3235 13236 13236 13236 13240 13241 13242 13246 13246 13246 13256 13261 13265 13266 13266 13266 13266 13266 13266 13266 13266 132267 132268 132269
D3 315 D3 315 A3 322 T13 323 K3 324 K3 325 K3 425 K3 426 <
13600 13510 13510 13511 13511 13511 13511 13511 13511 13511 13511 13511 13511 13511 13511 13551
Q3606 P3606 F3607 9 V3610 A V3611 C V3611 C A3611 C A3611 C A3611 C A3611 C A3611 C A3615 C A3615 C A3616 C A3617 C A3627 C A3641 C A3642 C A3641 C A3642 C A3641 C A3642 C A3641 C A3641 C A3642 C A3641 C A3642 C A3641 C A3642<
Ti3710 E3711 H3713 M3713 M3715 H3715 H3715 H3715 H3715 H3715 H3715 H3715 H3715 H3715 H3715 H3745 H
P3 891 P3 895 P3 994 P3 995 P3 995 P3 995 P3 995 P3 994 P3 995 P3
E4055 14056 14053 14063 14065 14065 14073 14073 14073 14073 14073 14113 14073 14125 141555 141555 141555 1415555 1415555555555
Y4236 N4229 N4229 V4240 D4241 CLY SER D4245 SER CLY SER CLY SER CLY SER CLY SER CLY CLY CLY CLY CL
R4 377 H4 377 R4 334 H4 336 R4 335 H4 336 R4 336 H4 336 R4 336 H4 405 R4 403 H4 405 R4 403 H4 405 R4 436 H4 436 R4 436 H4 436 R4 436 H4 436 R4 436 H4 436 R4 437 H4 437 R4 436 H4 437 R4 436 H4 437 R4 436 H4 437 R4 486 H4 438 R4 487 H4 436 R4 486 H4 486 R4 486 H4 486 <t< td=""></t<>







FI 546 El 5548 El 5548 El 5548 NI 564 NI 564 R1 558 R1 568 R1 568 R1 568 R1 568 R1 568 R1 568 R1 668 P1 613 P1 643 P1 643 P1 643	E1672
L1673 L1674 A1760 A1700 A1700 A1700 A1700 D1702 F1704 K1707 M1705 K1707 M1705 K1707 M1705 K1707 V1718 K1707 V1718 F1705	ul/66 I1767 E1768
N1 77.1 N1 77.1 N1 77.5 N1 77.5 N1 77.5 N1 77.6 N1 77.6 N1 77.6 N1 77.6 N1 78.5 N1 78.4 N1 78.5 N1 78.4 N1 78.5 N1 78.4 N1 78.6 N1 78.6 N1 78.6 N1 80.1 N1 78.6 N1 80.1 N1 80.6 N1	11883 C1884
L1 881 L1 881 L1 881 L1 882 L1 884 L1 885 L1 885 L1 886 L1 886 L1 886 L1 900 L1 900 L1 900 L1 900 L1 900 L1 910 L1 944 L1 944 L1 946 L1	V2002
P2005 82006 82006 L2007 L2008 R2041 F2043 R2041 F2043 R2041 F2043 R2041 F2043 R2041 F2043 R2065 R205 R2065 R205 R205 R205 R205 R205 R205 R205 R20	
F2145 F2145 F2156 F2157 F2156 F2233 F2233 F2234 F2245 F2245 F2246 F2245 F2245 F2246 F2245 F2245 F2245 F2245 F2245 F2246 F2245 F2245 F2245 F2246 F2245 F2246 F2245 F2245<	01071
02335 02335 02335 02335 02335 02335 02335 02335 02335 02355 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02365 02451 02451 02452 02451 02452 02452 02452 02452 02452 02452 02452 02454 02452 02454 02454 02454 02455 02454	P2466 D2467 T2468
R26 01 R26 02 R26 03 R26 03	F2641
A2642 + A2643 + A2644 + A2644 + A2644 + A2644 + A2654 + A2655 + A2705	A2724
12727 12728 12739 12739 12739 12739 12739 12739 12739 12739 12739 12739 12739 12739 12739 12769 12769 12769 12769 12769 12769 12769 12769 12769 12769 12769 12769 12779 12789 12799 12799 12799 12799 12799 12799 12799 12799 12799 12799 12799 12799	
P2800 P2801 (2802 (2806 (2806 (2806 (2806 (2814) A2806 A2806 A2806 A2806 A2810 (2814 V2816 V2816 V2816 V2816 V2816 V2816 V2816 V2826 V2866 V2826 V28666 V2866 V2866 V2866 V2866 V2866 V2866 V2866 V2866 V286	
K2941 K2941 K2941 K2943 K2943 K2943 K2943 K2945 K2	L3034 R3035 L3036
G33037 S3035 R3042 R3042 R3042 R3042 R3042 R3042 R3042 R3042 R3042 R3042 R3042 R3042 R3055 R3055 R30554 R3055 A3055 R3055 A3055 R3056 R30554 R3056 A30555 R3056 A30565 R3056 A3065 R3056 A3065 R3071 A3065 R3071 A3065 R3072 A3065 R3073 A3065 R3073 A3065 R3073 A3065 R3073 A3065 R3073 R3073 R3073 R3073 R3073 R3073 R3073 R3073 R3073 R3073 R3073 R3094 R3074 R3095 R3073 R3095 R3075 R3	I3115 E3118 A3119











PROTEIN DATA BANK



• Molecule 7: Dynein light chain roadblock







 \bullet Molecule 12: Dynein intermediate chain 2









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	11.012	Depositor
Minimum map value	0.000	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	530.5338, 477.21387, 449.22086	wwPDB
Map dimensions	398, 358, 337	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3329996, 1.3329996, 1.3329996	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: MG, ATP, ADP

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	Bond angles		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.69	0/34464	0.78	1/46623~(0.0%)	
2	С	0.68	0/31038	0.77	1/42003~(0.0%)	
3	Q	0.86	0/1005	0.84	0/1388	
4	В	0.69	1/35205~(0.0%)	0.80	3/47647~(0.0%)	
5	Ι	0.69	0/838	0.77	0/1131	
6	Н	0.67	0/767	0.76	0/1031	
7	G	0.69	0/755	0.77	0/1018	
8	F	0.68	0/875	0.77	0/1178	
9	N	0.69	0/867	0.79	0/1179	
10	0	0.67	0/1004	0.80	0/1349	
11	Е	0.67	0/4522	0.78	0/6114	
12	D	0.66	0/4772	0.78	1/6458~(0.0%)	
13	Р	0.87	0/538	0.86	0/746	
14	L	0.66	0/800	0.76	0/1076	
15	Κ	0.66	0/776	0.73	0/1038	
16	J	0.63	0/831	0.74	0/1118	
17	М	0.65	0/752	0.76	0/1006	
All	All	0.69	1/119809~(0.0%)	0.78	6/162103~(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	2
2	С	0	3
4	В	0	4
11	Е	0	1
All	All	0	10



All (1) bond length outliers are listed below:	
--	--

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	В	730	LEU	C-O	5.23	1.33	1.23

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	3248	PRO	N-CA-CB	-6.26	95.71	102.60
4	В	533	ARG	CB-CA-C	6.19	122.77	110.40
4	В	1127	ASN	CB-CA-C	5.71	121.82	110.40
12	D	397	ASP	CB-CA-C	5.18	120.76	110.40
1	А	1016	PHE	CB-CA-C	5.13	120.66	110.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	35	GLU	Peptide
1	А	4250	ARG	Peptide
2	С	2717	ALA	Peptide
2	С	2746	PRO	Peptide
2	С	528	GLU	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	А	33894	0	32288	250	0
2	С	30436	0	29392	239	0
3	Q	1002	0	501	6	0
4	В	34604	0	33094	332	0
5	Ι	827	0	829	17	0
6	Н	750	0	735	7	0
7	G	749	0	772	10	0
8	F	863	0	881	9	0
9	N	855	0	800	12	0
10	0	986	0	1002	12	0
11	Е	4423	0	4291	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	4664	0	4484	57	0
13	Р	541	0	220	2	0
14	L	783	0	811	10	0
15	K	754	0	716	3	0
16	J	806	0	772	1	0
17	М	735	0	738	9	0
18	А	54	0	24	2	0
18	В	54	0	24	0	0
18	С	54	0	24	3	0
19	А	31	0	12	0	0
19	В	31	0	12	1	0
19	С	31	0	12	0	0
20	А	3	0	0	0	0
20	В	3	0	0	0	0
20	С	3	0	0	0	0
All	All	117936	0	112434	961	0

Continued from previous page...

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 4.

The worst 5 of 961 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)
4:B:764:GLN:O	4:B:765:PHE:C	1.73	1.26
4:B:764:GLN:O	4:B:766:ILE:N	1.79	1.12
4:B:750:PRO:O	4:B:752:ILE:N	1.89	1.05
4:B:3255:THR:OG1	4:B:3337:CYS:SG	2.13	1.02
2:C:2826:VAL:O	2:C:2829:ASP:N	1.96	0.97

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	entiles
1	А	4381/4615~(95%)	4081 (93%)	257~(6%)	43~(1%)	15	54
2	С	3915/3943~(99%)	3583~(92%)	283~(7%)	49 (1%)	12	48
3	Q	190/192~(99%)	163 (86%)	24 (13%)	3(2%)	9	43
4	В	4488/4588~(98%)	4019 (90%)	382 (8%)	87 (2%)	8	40
5	Ι	104/106~(98%)	95~(91%)	8 (8%)	1 (1%)	15	54
6	Н	89/91~(98%)	83 (93%)	6 (7%)	0	100	100
7	G	92/96~(96%)	87~(95%)	5(5%)	0	100	100
8	F	108/110~(98%)	96~(89%)	11 (10%)	1 (1%)	17	56
9	Ν	112/114~(98%)	92~(82%)	17 (15%)	3(3%)	5	33
10	Ο	118/120 (98%)	104 (88%)	9~(8%)	5 (4%)	3	23
11	Ε	551/557~(99%)	496 (90%)	51 (9%)	4 (1%)	22	61
12	D	569/595~(96%)	510 (90%)	51 (9%)	8 (1%)	11	46
13	Р	103/112~(92%)	86 (84%)	11 (11%)	6 (6%)	1	16
14	L	96/98~(98%)	91~(95%)	4 (4%)	1 (1%)	15	54
15	K	88/90~(98%)	79~(90%)	9 (10%)	0	100	100
16	J	93/95~(98%)	84 (90%)	8 (9%)	1 (1%)	14	52
17	М	85/87~(98%)	72 (85%)	11 (13%)	2 (2%)	6	35
All	All	15182/15609~(97%)	13821 (91%)	1147 (8%)	214 (1%)	15	46

5 of 214 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	125	PRO
1	А	197	ILE
1	А	871	LEU
1	А	973	ASP
1	А	3251	ILE

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	3420/4191~(82%)	3338~(98%)	82 (2%)	49	76
2	С	3149/3501~(90%)	3095~(98%)	54 (2%)	60	82
3	Q	10/176~(6%)	10 (100%)	0	100	100
4	В	3497/4138~(84%)	3399~(97%)	98~(3%)	43	72
5	Ι	91/91~(100%)	87~(96%)	4 (4%)	28	62
6	Н	82/82~(100%)	81~(99%)	1 (1%)	71	87
7	G	86/87~(99%)	85~(99%)	1 (1%)	71	87
8	F	93/93~(100%)	86~(92%)	7 (8%)	13	43
9	Ν	85/102~(83%)	84 (99%)	1 (1%)	71	87
10	Ο	106/108~(98%)	99~(93%)	7 (7%)	16	49
11	Ε	484/496~(98%)	467 (96%)	17 (4%)	36	67
12	D	507/545~(93%)	482~(95%)	25~(5%)	25	59
14	L	87/87~(100%)	83~(95%)	4(5%)	27	61
15	Κ	80/80~(100%)	79~(99%)	1 (1%)	69	86
16	J	81/81 (100%)	79~(98%)	2 (2%)	47	75
17	М	78/78~(100%)	74 (95%)	4 (5%)	24	57
All	All	11936/13936~(86%)	11628 (97%)	308 (3%)	49	74

5 of 308 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	В	4540	LYS
12	D	392	ASN
6	Н	68	PHE
11	Е	193	MET
14	L	86	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such side chains are listed below:

Mol	Chain	Res	Type
4	В	4176	ASN
7	G	129	GLN
11	Е	481	GLN
2	С	1428	ASN
2	С	1300	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)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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

Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	ADP	C	4801	20	24,29,29	0.65	0	29,45,45	0.87	2 (6%)
18	ADP	В	5501	20	24,29,29	0.70	0	$29,\!45,\!45$	0.96	2 (6%)
18	ADP	С	4401	20	24,29,29	0.69	1 (4%)	$29,\!45,\!45$	1.04	2 (6%)
18	ADP	А	4701	20	24,29,29	0.69	0	$29,\!45,\!45$	0.77	1 (3%)
19	ATP	В	4701	20	26,33,33	0.66	0	31,52,52	0.92	1 (3%)
18	ADP	А	4901	-	24,29,29	0.66	0	29,45,45	0.80	1 (3%)
19	ATP	А	4801	20	26,33,33	0.65	0	31,52,52	0.86	1 (3%)
19	ATP	С	4201	20	26,33,33	0.69	0	31,52,52	0.94	2 (6%)
18	ADP	В	5601	20	24,29,29	0.66	0	29,45,45	0.72	1 (3%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ADP	С	4801	20	-	3/12/32/32	0/3/3/3
18	ADP	В	5501	20	-	5/12/32/32	0/3/3/3
18	ADP	С	4401	20	-	5/12/32/32	0/3/3/3
18	ADP	А	4701	20	-	5/12/32/32	0/3/3/3
19	ATP	В	4701	20	-	2/18/38/38	0/3/3/3
18	ADP	А	4901	-	-	1/12/32/32	0/3/3/3
19	ATP	А	4801	20	-	5/18/38/38	0/3/3/3
19	ATP	С	4201	20	-	4/18/38/38	0/3/3/3
18	ADP	В	5601	20	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
18	С	4401	ADP	C8-N7	-2.07	1.31	1.34

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
18	С	4401	ADP	C1'-N9-C4	2.72	131.41	126.64
19	С	4201	ATP	PA-O3A-PB	-2.45	124.44	132.83
19	В	4701	ATP	C5-C6-N6	2.42	124.04	120.35
19	А	4801	ATP	C5-C6-N6	2.22	123.73	120.35
18	С	4801	ADP	C5-C6-N6	2.20	123.69	120.35

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	А	4701	ADP	PA-O3A-PB-O3B
18	С	4401	ADP	C5'-O5'-PA-O1A
18	С	4401	ADP	C5'-O5'-PA-O2A
18	С	4801	ADP	O4'-C4'-C5'-O5'
18	В	5501	ADP	PB-O3A-PA-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	С	4801	ADP	2	0
18	С	4401	ADP	1	0

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Jerry					
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	А	4701	ADP	1	0
19	В	4701	ATP	1	0
18	А	4901	ADP	1	0

Continued from previous page...

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	С	13
1	А	6
4	В	2
12	D	2
13	Р	1
7	G	1

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	С	3277:MET	С	3380:MET	N	42.35
1	С	809:ARG	С	818:ILE	N	14.24
1	А	1235:PRO	С	1246:MET	N	12.91
1	С	665:ILE	С	670:SER	N	11.42
1	С	449:TYR	С	453:THR	N	10.61



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22677. 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: 199



Y Index: 179



Z Index: 168



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: 222

Y Index: 223

Z Index: 191

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 0.8. 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 1003 nm^3 ; this corresponds to an approximate mass of 906 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



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-22677 and PDB model 7K58. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.8 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 (0.8).



9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 59% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5895	0.3570
А	0.6015	0.3820
В	0.6170	0.3590
\mathbf{C}	0.5698	0.3380
D	0.5985	0.3420
Ε	0.5229	0.3550
F	0.5182	0.3830
G	0.4553	0.3710
Н	0.4857	0.3550
Ι	0.5256	0.3180
J	0.5367	0.3860
Κ	0.4752	0.3630
L	0.4137	0.3650
М	0.5180	0.3810
N	0.5697	0.2740
0	0.5115	0.2540
Р	0.5564	0.1490
Q	0.7986	0.3230



