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PDB ID	:	7TMM
EMDB ID	:	EMD-25996
Title	:	Complete V1 Complex from Saccharomyces cerevisiae
Authors	:	Vasanthakumar, T.; Keon, K.A.; Bueler, S.A.; Jaskolka, M.C.; Rubinstein,
		J.L.
Deposited on	:	2022-01-19
Resolution	:	3.50 Å(reported)

This is a 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 70
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)	:	2.36

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.



Matria	Whole archive	EM structures
Metric	$(\# { m Entries})$	$(\# { m Entries})$
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 $\geq=3, 2, 1$ 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 $\leq=5\%$ 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	639	76% 1	7% 7%
1	С	639	78%	15% 7%
1	Е	639	72% 18%	10%
2	В	517	73% 17%	10%
2	D	517	71% 18%	11%
2	F	517	72% 17%	11%
3	G	233	88%	7% 6%
3	Ι	233	84%	10% 6%



Conti	nuea _I ron	<i>i</i> previous	page		
Mol	Chain	Length	Quality of chain		
3	K	233	77%	14%	9%
4	Н	114	89%		6% •
4	J	114	90%		• 5%
4	L	114	82%	•	13%
5	М	256	77%	6%	16%
6	Ν	118	86%	8	3% 6%
7	О	392	89%		• 8%
8	Р	478	91%		• 8%



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 33713 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	AltConf	Trace			
1	А	593	Total 4150	C 2690	N 720	O 722	S 18	0	0
1	С	592	Total 3985	C 2578	N 704	O 687	S 16	0	0
1	Е	576	Total 4006	C 2595	N 703	O 693	S 15	0	0

• Molecule 1 is a protein called H(+)-transporting two-sector ATPase.

There are 66	discrepancies	between	the modelled	and	reference sequences	3:
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Chain	Residue	Modelled	Actual	Comment	Reference
А	617	ASP	-	expression tag	UNP A0A6L0YX77
А	618	TYR	-	expression tag	UNP A0A6L0YX77
А	619	LYS	-	expression tag	UNP A0A6L0YX77
А	620	ASP	-	expression tag	UNP A0A6L0YX77
А	621	HIS	-	expression tag	UNP A0A6L0YX77
А	622	ASP	-	expression tag	UNP A0A6L0YX77
А	623	GLY	-	expression tag	UNP A0A6L0YX77
А	624	ASP	-	expression tag	UNP A0A6L0YX77
А	625	TYR	-	expression tag	UNP A0A6L0YX77
А	626	LYS	-	expression tag	UNP A0A6L0YX77
А	627	ASP	-	expression tag	UNP A0A6L0YX77
А	628	HIS	-	expression tag	UNP A0A6L0YX77
А	629	ASP	-	expression tag	UNP A0A6L0YX77
А	630	ILE	-	expression tag	UNP A0A6L0YX77
А	631	ASP	-	expression tag	UNP A0A6L0YX77
А	632	TYR	-	expression tag	UNP A0A6L0YX77
А	633	LYS	-	expression tag	UNP A0A6L0YX77
А	634	ASP	-	expression tag	UNP A0A6L0YX77
А	635	ASP	-	expression tag	UNP A0A6L0YX77
А	636	ASP	-	expression tag	UNP A0A6L0YX77
А	637	ASP	-	expression tag	UNP A0A6L0YX77
A	638	LYS	-	expression tag	UNP A0A6L0YX77
C	617	ASP	-	expression tag	UNP A0A6L0YX77
C	618	TYR	-	expression tag	UNP A0A6L0YX77



Continu	ea from pre	vious page			
Chain	Residue	Modelled	Actual	Comment	Reference
C	619	LYS	-	expression tag	UNP A0A6L0YX77
C	620	ASP	-	expression tag	UNP A0A6L0YX77
C	621	HIS	-	expression tag	UNP A0A6L0YX77
С	622	ASP	-	expression tag	UNP A0A6L0YX77
С	623	GLY	-	expression tag	UNP A0A6L0YX77
С	624	ASP	-	expression tag	UNP A0A6L0YX77
С	625	TYR	-	expression tag	UNP A0A6L0YX77
С	626	LYS	-	expression tag	UNP A0A6L0YX77
С	627	ASP	-	expression tag	UNP A0A6L0YX77
С	628	HIS	-	expression tag	UNP A0A6L0YX77
С	629	ASP	-	expression tag	UNP A0A6L0YX77
С	630	ILE	-	expression tag	UNP A0A6L0YX77
С	631	ASP	-	expression tag	UNP A0A6L0YX77
С	632	TYR	-	expression tag	UNP A0A6L0YX77
С	633	LYS	-	expression tag	UNP A0A6L0YX77
С	634	ASP	-	expression tag	UNP A0A6L0YX77
С	635	ASP	-	expression tag	UNP A0A6L0YX77
С	636	ASP	-	expression tag	UNP A0A6L0YX77
С	637	ASP	-	expression tag	UNP A0A6L0YX77
С	638	LYS	-	expression tag	UNP A0A6L0YX77
Е	617	ASP	-	expression tag	UNP A0A6L0YX77
Е	618	TYR	-	expression tag	UNP A0A6L0YX77
Е	619	LYS	-	expression tag	UNP A0A6L0YX77
Е	620	ASP	-	expression tag	UNP A0A6L0YX77
Е	621	HIS	-	expression tag	UNP A0A6L0YX77
Е	622	ASP	-	expression tag	UNP A0A6L0YX77
Е	623	GLY	-	expression tag	UNP A0A6L0YX77
Е	624	ASP	-	expression tag	UNP A0A6L0YX77
Е	625	TYR	-	expression tag	UNP A0A6L0YX77
E	626	LYS	-	expression tag	UNP A0A6L0YX77
Е	627	ASP	-	expression tag	UNP A0A6L0YX77
Е	628	HIS	-	expression tag	UNP A0A6L0YX77
Е	629	ASP	-	expression tag	UNP A0A6L0YX77
Е	630	ILE	-	expression tag	UNP A0A6L0YX77
Е	631	ASP	-	expression tag	UNP A0A6L0YX77
Е	632	TYR	-	expression tag	UNP A0A6L0YX77
Е	633	LYS	-	expression tag	UNP A0A6L0YX77
Е	634	ASP	-	expression tag	UNP A0A6L0YX77
Е	635	ASP	-	expression tag	UNP A0A6L0YX77
Е	636	ASP	-	expression tag	UNP A0A6L0YX77
Е	637	ASP	-	expression tag	UNP A0A6L0YX77
Е	638	LYS	-	expression tag	UNP A0A6L0YX77



Mol	Chain	Residues		At	AltConf	Trace			
9	В	464	Total	С	Ν	0	\mathbf{S}	0	0
2	D	404	3375	2175	599	591	10	0	0
9	Л	450	Total	С	Ν	0	S	0	0
2	D	409	3266	2123	583	549	11	0	0
9	F	450	Total	С	Ν	0	S	0	0
	Ľ	409	3276	2116	584	567	9	0	U

• Molecule 2 is a protein called Vacuolar proton pump subunit B.

• Molecule 3 is a protein called V-ATPase subunit E.

Mol	Chain	Residues		At	oms	AltConf	Trace		
2	3 G	220	Total	С	Ν	0	S	0	0
0			1322	844	239	238	1	0	0
2	Т	220	Total	С	Ν	0	S	0	0
0	1	220	1313	834	241	237	1	0	0
2	K	919	Total	С	Ν	0	S	0	0
J	Γ	212	1288	829	236	222	1	0	0

• Molecule 4 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
4	л п	100	Total	С	Ν	Ο	0	0
4	11	105	578	353	113	112	0	0
4	т	108	Total	С	Ν	Ο	0	0
4	J	100	570	350	111	109	0	0
4	т	00	Total	С	Ν	Ο	0	0
4		99	522	321	101	100	0	0

• Molecule 5 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace	
5	М	214	Total 1341	C 852	N 252	0 234	${ m S} { m 3}$	0	0

• Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
6	Ν	111	Total 610	C 384	N 114	O 112	0	0

• Molecule 7 is a protein called V-type proton ATPase subunit C.



Mol	Chain	Residues	Atoms			AltConf	Trace	
7	0	359	Total 1873	C 1147	N 362	0 364	0	0

• Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms			AltConf	Trace	
8	Р	441	Total 2211	C 1329	N 441	O 441	0	0

• Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
9	А	1	Total	C 10	N	0	P o	0
			21	10	9	10	Z	



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.





Chain E:	72%	18%	10%
MET ALA GIY GIY JILE ILE ALA ALA ARG CIU ILY STLE ILYS ILE ILYS STRE ARG	LEU LEU ALP ALS ALS ALS ALS ALS CIU CIU CIU CIU CIU CIU CIU CIU CIU CIU	(143 K50 V51 V51 V51 V50 V52 L63 L63 L63 L63 L769 T769	971 972 477 477 877 84 83 83
V85 186 192 198 198 198 104 1110 1110 1111	R126 A132 V161 V161 V161 F170 F176 F176 F176 F176 F176 F176 F176 F176	T210 L211 V215 V216 V216 V223 V223 L233 L233 L233 L233 L240	L243 C246 T252 P255 GLY ALA PHE
GLY CYS CYS CYS CYS CYS CYS SS6 CSS CSS CSS CSS CSS CSS CSS CSS CS	L294 L294 P310 R311 R314 R313 R313 R313 R313 R313 R320 R320 R323 R333 R333	Y334 1337 1338 1338 1338 1338 1334 1353 1353 1353 356	R365 9378 P381 A382 R394
V399 T407 V410 V410 V416 V416 V416 P417 P416 C17 C17 C17 C17 C17 C17 C17 C17 C17 C17	P426 P426 P426 F437 F439 W439 W439 W439 F436 H450 H450 H450 H450 F45 F470	E477 L481 L481 M485 M485 M485 V499 K504 V517	F526 L526 M546 M647 F550 H554
V581 V581 E60 L603 L603 L603 A8P A8P LVS LVS A8P A8P	ASP ASP TYR ASP TYR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP		
• Molecule 2: Vacuol	ar proton pump subunit B		
Chain B:	73%	17%	10%
MET VAL LEU SER ASP ASP CASP CASP CASP CASP CASP CASP C	14 1 14 1 15 1 15 2 15 2 15 5 15 5 15 6 15 6 16 6 17 0 17 0 17 0 17 0	191 192 193 193 193 193 193 109 1110 1110 1111 1111	P147 P147 150 1153 0154 0155 8155 8155 8156 1158
0159 1160 1160 1160 1160 1163 0168 0168 0168 1175 1175	L193 L193 P196 THR LYS LYS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	F312 A213 A214 A214 A214 233 5234 1236 1236 1236 1236 1236 1236 1236 1236	A263 F264 Y265 Q269 Q269 V274 L275 M281
R302 7306 7306 7306 7316 7319 1329 1329 1332	L335 P345 L346 L349 L349 L349 L346 N360 N360 N360 N361 N372 S380 S380	L382 A386 1387 1387 1387 1387 1387 1387 1387 1387	L425 K438 F443 R452 A461
L464 1467 1467 1467 1467 1467 1475 ASP ASP ASP ASP ASP ASP	GLU GLU GLU GLU GLU GLU ASP PRO PRO PRO PRO PRO CLU SER SER SER SER SER SER SER SER SER SER	GLU SER LLEU ILLE	
• Molecule 2: Vacuol	ar proton pump subunit B		
Chain D:	71%	18%	11%
MET VAL LEU LEU ASP ASP LEU ALA ALA ALA ALA ALA ALA ALA ALA	V22 V28 V28 V35 V39 V39 V39 V39 V39 V39 V39 V39 V53 V53 V53 V53 V53 V53 V53 V53 V53 V53	064 066 066 170 170 170 177 176 177 176 177 176 177 176 176	T96 1102 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103 1103
R111 P124 F127 F127 F127 R149 R149 F148 F148 F148 F148 F148 F148 F148 F148	1156 1156 1156 1156 1176 1178 1178 1178 1178 1178 1178 117	THR LIYS ASP ASP ASP ASP ASP ALU GLU A213 A214 A214 A214 A214 A214 A214 A214 A214	1250 1253 1253 1255 1255 1256 1258 1262
L266 1270 E271 E271 1279 1279 A287 L288 R288 R288 R286 E290	E296 E317 F316 F316 F316 F316 F316 F318 A318 A318 A331 F336 F334 F334 F334 F335 F334 F334 F335 F335	P347 E355 1358 R362 R362 A386 M391 D395	H396 V399 1402 1403 1404 A404 A406 K406
M416 V419 V420 F439 A461 L464 A85 A86 A86 A86 A86 A86 A86 A86	ASP ASP ASP ASP ASP ASP GLU GLU GLU CLU SER SER SER SER SER SER SER SER SER SER	ASP ALA SER GLU GLU CLU CLU LEU LLEU LLEU	

WORLDWIDE PROTEIN DATA BANK

• Molecule 2: Vacu	uolar proton pump subunit B		
Chain F:	72%	17%	11%
MET VAL LEU SER SER SER SER CIU CEU CEU CEU CEU CEU CEU CEU CEU CEU CE	115 115 115 157 152 157 152 157 152 157 156 170 170 170 170 170 170 170 170	V104 M108 G110 G110 114 1120 1142 Y142 Y142 Y145	M150 1151 2152 2153 2163 2163 1164
P171 5174 1178 1183 1183 1183 1183 1183 1183 1183	A191 L192 V194 V194 V194 V194 V194 L193 A194 A194 A115 A115 A115 A115 A115 A115 A115 A11	V11/ 1235 1238 1238 1238 1235 1242 1253 1253 1253 1255	R257 L258 A263 1276 1276 1277 1277 1277
Y284 R302 P305 Y309 Y309 C323 E323	1332 1334 1335 1335 1336 1336 1336 1336 1336 1349 1349 1349 1369 1369 1369 1369 1369 1369	L382 L382 R393 R393 R393 D395 C402 C403 Y404 K411	F443 T445 T445 D451 A461 L464 L465
R466 N474 R475 R475 A8P A8P A8P A8P A8P A8P A8P A8P	ASF GLU GLU GLU GLU GLU ASP ASP ASP ASP CLY SER ALA ALA ALA ALA ALA CLU GLU GLU SER	ILE	
• Molecule 3: V-A	TPase subunit E		
Chain G:	88%		7% 6%
MET SER SER ALA ALA ALA ALA ALA CHU CHU CHU CHU CHU ASU ASU	T76 179 199 1120 1120 1120 1125 1125 1126 1130 1125 1125 1125 1125 1125 1125	V188 8191 8191 8191 8198 8198 8198 8198	
• Molecule 3: V-A	TPase subunit E		
Chain I:	84%	10%	6%
MET SER SER ALA ALA THR THR FUC ASN ASN ASN	L86 L96 K106 A111 1121 L130 L130 L130 L130 L136 L149 L149 L149 L149 A164	L169 1172 Y178 V188 N192 L197 E198	1218 R219 L222 K230 K230 PHE ASP
• Molecule 3: V-A	TPase subunit E		
Chain K:	77%	14%	9%
MET SER SER SER ALA ILE ILEU THR ALA ILEU ASN ASN ASN VAL	ASN ASN GLU LEU ASN LAS MET MET MET MET 196 L107 L107 L107 L107 L107 L110 T110	L121 2123 2123 1124 1125 1126 1126 1148 1148 1148 1148	1172 1178 1178 1188 1191 1192
E198 1199 N200 N201 L207 L210 L216 L216 L216 L218 R218	L222 F332 ASP		
• Molecule 4: V-ty	ype proton ATPase subunit G		
Chain H:	89%		6% •
MET SER GLN LYS E79 E79 183 183 199	1103 K104 P105 LEU LEU		

• Molecule 4: V-type proton ATPase subunit G



Chain J:	90%	• 5%	
MET SER GLN LYS N5 V94 V94	LEU LEU LEU		
• Molecule	4: V-type proton ATPase subunit G		
Chain L:	82%	13%	
MET SER GLN CLYS ASN GLY ALA ALA	LEU LEU LEU EI 193 103 1103 MIL1 LEU		
• Molecule	5: V-type proton ATPase subunit D		
Chain M:	77% 6% 1	.6%	
MET SER GLY N4 Y29 R42 R42	V60 M61 M61 M61 M61 462 V101 V104 V104 V103 V135 V135 V135 V135 V135 V135 V162 V162 V162 V162 V162 V162 V162 V162	GLN ASP ALA SER GLU	VAL ALA ALA ASP GLU
GLU PRO GLN GLV GLU THR LEU VAL	ASP GLU ASP VAL TILE PHE		
• Molecule	6: V-type proton ATPase subunit F		
Chain N:	86% 89	% 6%	I
MET A2 R5 V10 L20	A23 224 225 465 A65 A65 A65 A65 A65 A65 A65 A65 A65 A		
• Molecule	7: V-type proton ATPase subunit C		
Chain O:	89%	• 8%	I
MET ALA THR ALA L5 A3 43	047 155 4155 4156 1176 1176 1176 1177 1177 1176 1177 1176 1177 1178 1	E281 N302	1306 K328 G352 GLY ALA PHE
MET LYS LYS LYS LYS GLY LYS ILE ASM	LYS LYS GLN AGN HIS SER HIR ALA ALA ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU		
• Molecule	8: V-type proton ATPase subunit H		
Chain P:	91%	• 8%	
MET GLY ALA THR K5 K5 K5 K5 K5 K23	824 V25 V25 V25 V25 R32 R33 R33 R33 R33 R47 R41 R41 R41 R41 R41 R41 R41 R41 R41 R41	G154	D223 SER GLN LEU LEU ALA ARG THR THR TLE VAL
ALA THR ASN SER ASN H237 L313	A318 P373 P373 P373 P373 P373 P373 P373 P37		

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	43	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV $(4k \times 4k)$	Depositor
Maximum map value	6.078	Depositor
Minimum map value	-3.634	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	412.0, 412.0, 412.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: 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	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.33	0/4247	0.49	0/5812
1	С	0.31	0/4072	0.48	0/5586
1	Е	0.32	0/4096	0.48	0/5609
2	В	0.35	0/3444	0.52	0/4700
2	D	0.33	0/3334	0.52	0/4559
2	F	0.34	0/3343	0.51	0/4571
3	G	0.26	0/1331	0.43	0/1838
3	Ι	0.26	0/1322	0.43	0/1827
3	Κ	0.26	0/1299	0.44	0/1790
4	Н	0.24	0/579	0.34	0/802
4	J	0.25	0/571	0.34	0/793
4	L	0.24	0/523	0.36	0/728
5	М	0.26	0/1355	0.44	0/1857
6	N	0.24	0/617	0.42	0/859
7	0	0.24	0/1895	0.38	0/2653
8	Р	0.22	0/2217	0.34	0/3099
All	All	0.30	0/34245	0.47	0/47083

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4150	0	3839	67	0
1	С	3985	0	3554	59	0
1	Ε	4006	0	3652	76	0
2	В	3375	0	3240	65	0
2	D	3266	0	3094	68	0
2	F	3276	0	3089	60	0
3	G	1322	0	1061	13	0
3	Ι	1313	0	1014	20	0
3	Κ	1288	0	1034	22	0
4	Н	578	0	363	6	0
4	J	570	0	359	6	0
4	L	522	0	323	4	0
5	М	1341	0	1077	12	0
6	Ν	610	0	381	6	0
7	0	1873	0	961	6	0
8	Р	2211	0	993	4	0
9	А	27	0	12	3	0
All	All	33713	0	28046	446	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 7.

All (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:344:ARG:HG2	1:E:410:VAL:HG23	1.58	0.83
2:F:187:ILE:O	2:F:191:ALA:HB2	1.79	0.81
2:D:40:ILE:HG13	2:D:76:ILE:HG23	1.64	0.78
1:A:51:VAL:HA	1:A:85:VAL:HG12	1.65	0.78
3:K:125:ILE:HG13	3:K:188:VAL:HG21	1.65	0.77
2:B:150:MET:HB2	2:B:386:ALA:HB1	1.66	0.76
5:M:61:MET:HG3	6:N:95:PRO:HD2	1.67	0.76
1:E:27:ILE:HD12	1:E:83:ASP:HB2	1.68	0.75
2:B:210:ILE:HB	2:B:238:THR:HG22	1.68	0.75
1:E:51:VAL:HA	1:E:85:VAL:HG12	1.69	0.74
1:A:262:LYS:NZ	9:A:701:ADP:O1B	2.21	0.74
2:D:296:GLU:O	5:M:207:GLN:NE2	2.22	0.71
1:E:223:VAL:HG12	1:E:344:ARG:HH12	1.55	0.71
1:E:239:VAL:HG22	1:E:526:LEU:HG	1.73	0.71
1:E:283:CYS:SG	1:E:332:SER:OG	2.49	0.71
2:D:144:ARG:NH2	2:D:317:GLU:O	2.25	0.70
1:E:356:SER:H	1:E:415:ALA:HB3	1.56	0.69



	io ao pago	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:161:MET:HE2	2:D:403:LEU:HB3	1.75	0.68
2:F:360:VAL:HG13	2:F:372:PRO:HG2	1.77	0.67
2:D:178:LEU:HD21	2:D:362:ARG:HD3	1.75	0.67
1:E:341:GLU:OE2	1:E:394:ARG:NE	2.28	0.66
2:F:63:ARG:NH1	2:F:82:GLY:O	2.29	0.66
1:C:485:MET:HA	1:C:488:ILE:HG22	1.78	0.65
2:F:376:LEU:HA	2:F:404:TYR:HE1	1.59	0.65
2:F:214:ALA:HB3	2:F:242:LEU:HA	1.80	0.64
2:D:290:GLU:HA	1:E:382:ALA:HB1	1.79	0.64
1:C:232:PRO:HA	1:C:247:VAL:HA	1.79	0.63
2:D:55:LEU:HD22	2:D:93:VAL:HG22	1.80	0.63
1:C:51:VAL:N	1:C:56:LEU:O	2.29	0.63
2:D:109:LEU:O	3:K:85:ARG:NH2	2.31	0.63
1:E:77:ALA:O	1:E:126:ARG:NH1	2.32	0.63
2:F:211:VAL:HG21	2:F:263:ALA:HB2	1.81	0.63
2:B:155:VAL:HG23	2:B:158:ILE:HB	1.82	0.62
1:A:157:ILE:HD13	1:A:171:LYS:HD2	1.81	0.62
1:C:545:ASP:OD1	1:C:548:ARG:NH2	2.33	0.61
2:F:443:PHE:HB2	2:F:464:LEU:HD11	1.80	0.61
2:B:308:MET:HE3	2:B:349:LEU:HD12	1.83	0.61
1:C:152:ILE:HG12	1:C:174:LEU:HD22	1.82	0.60
3:G:125:ILE:HG12	3:G:188:VAL:HG21	1.84	0.60
2:F:376:LEU:HD11	2:F:411:LYS:HG3	1.82	0.60
1:E:449:LYS:HG2	2:F:404:TYR:HD2	1.67	0.60
2:B:55:LEU:HG	2:B:93:VAL:HG22	1.83	0.60
2:B:403:LEU:HD11	2:B:461:ALA:HB1	1.84	0.60
1:A:163:GLU:OE1	1:A:170:HIS:ND1	2.34	0.60
1:E:116:LYS:HD3	2:F:142:TYR:HD2	1.67	0.60
1:A:61:ILE:HD12	1:A:371:LEU:HD11	1.84	0.59
1:C:376:ALA:HB2	1:C:382:ALA:HA	1.83	0.59
2:B:160:THR:HG21	2:B:443:PHE:HZ	1.67	0.59
2:B:160:THR:HG23	2:B:161:MET:HG3	1.83	0.59
2:B:34:VAL:HG13	1:C:45:MET:HE3	1.84	0.59
1:C:51:VAL:HA	1:C:85:VAL:HG13	1.84	0.59
1:C:242:ALA:HA	1:C:478:PHE:HZ	1.68	0.59
1:E:298:PRO:HA	1:E:312:MET:HG2	1.83	0.59
5:M:139:TYR:HB3	6:N:23:ALA:HB2	1.85	0.59
2:D:47:PRO:HG2	2:D:70:ILE:HD11	1.84	0.58
2:F:279:THR:HB	2:F:334:ILE:HD12	1.84	0.58
2:D:215:MET:SD	2:D:256:PRO:HG3	2.43	0.58
1:E:252:THR:HA	1:E:437:VAL:HB	1.85	0.58



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:485:MET:HG2	1:C:551:ILE:HD11	1.85	0.58
2:D:147:PRO:HA	2:D:321:ARG:HD3	1.84	0.58
3:K:222:LEU:HD13	4:L:94:VAL:HG21	1.85	0.58
2:B:240:LEU:HD23	2:B:242:LEU:HD21	1.85	0.58
1:C:471:TYR:HE2	1:C:482:ARG:HH12	1.51	0.58
2:D:270:THR:HG21	2:D:272:ARG:HH21	1.68	0.58
1:E:286:ARG:HB2	1:E:289:GLU:HG2	1.86	0.58
1:E:210:THR:HG22	1:E:211:LEU:H	1.67	0.58
2:F:102:ILE:HD12	2:F:258:LEU:HD22	1.86	0.58
1:C:217:VAL:HG12	1:C:334:TYR:HB3	1.86	0.58
2:F:235:LEU:HA	2:F:238:THR:HG22	1.85	0.58
1:A:376:ALA:HB2	1:A:382:ALA:HA	1.86	0.57
1:A:81:VAL:HG23	2:B:70:ILE:HD12	1.87	0.57
1:A:152:ILE:HG12	1:A:174:LEU:HD22	1.86	0.57
1:A:517:VAL:HG11	1:A:554:HIS:HB2	1.85	0.57
2:B:183:ILE:HD11	2:B:372:PRO:HD2	1.85	0.57
3:K:114:ARG:HA	3:K:117:TYR:HB3	1.86	0.57
1:C:226:LYS:HD2	1:C:398:ALA:HB2	1.86	0.57
2:F:376:LEU:HB2	2:F:377:PRO:HD3	1.87	0.57
2:D:319:ALA:HB2	2:D:331:GLN:HE21	1.70	0.57
1:E:139:TRP:HB3	1:E:161:VAL:HG21	1.87	0.56
1:E:426:PRO:HA	1:E:429:THR:HG22	1.88	0.56
1:C:111:PRO:HD3	1:C:132:ALA:HA	1.88	0.56
1:E:81:VAL:HG23	2:F:70:ILE:HD12	1.87	0.56
2:B:153:THR:HG23	2:B:187:ILE:HG23	1.87	0.56
1:C:125:PRO:HG2	1:C:128:ILE:HB	1.86	0.56
7:O:47:ASP:HA	7:O:328:LYS:HA	1.88	0.56
2:F:308:MET:HE3	2:F:349:LEU:HD12	1.87	0.56
2:D:402:GLN:HE21	2:D:406:LYS:HG2	1.71	0.56
2:D:344:HIS:HB3	2:D:347:PRO:HD2	1.88	0.56
1:A:446:ALA:HA	1:A:451:PHE:HE2	1.71	0.56
1:A:49:VAL:HG21	1:A:70:ILE:HD13	1.87	0.56
2:B:212:PHE:HE2	2:B:214:ALA:HB2	1.71	0.55
2:F:376:LEU:HA	2:F:404:TYR:CE1	2.41	0.55
2:B:264:GLU:HA	2:B:329:ILE:HD11	1.88	0.55
1:A:239:VAL:HG23	1:A:526:LEU:HD22	1.88	0.55
1:E:243:LEU:HD11	1:E:485:MET:HE2	1.89	0.55
4:J:99:ILE:O	4:J:103:ILE:HG12	2.05	0.55
1:C:520:LEU:HG	1:C:550:PHE:HE1	1.72	0.55
2:D:149:GLU:HA	2:D:391:MET:HG2	1.89	0.55
3:I:222:LEU:HD13	4:J:94:VAL:HG21	1.88	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1.A.288.ASN.HB2	2:B:355:GLU:OE1	2.07	0.55
2:B:53:VAL:N	2:B:65:GLY:0	2.37	0.55
1:E:104:ILE:HG12	1.E.294.LEU.HD22	1.88	0.55
$2 \cdot B \cdot 147 \cdot PRO \cdot HB3$	2·B·167·GLY·H	1.72	0.55
2:B:129:GLU:OE1	2:B:265:TYR:OH	2.22	0.55
2:F:243:ASN:ND2	2:F:251:GLU:OE1	2.39	0.55
2:D:419:VAL:HG13	2:D:420:VAL:HG13	1.89	0.55
3:I:125:ILE:HG12	3:I:188:VAL:HG21	1.88	0.54
7:0:224:VAL:HA	7:O:234:PHE:HA	1.90	0.54
7:O:155:ALA:HB1	7:O:281:GLU:HA	1.90	0.54
1:E:517:VAL:HG11	1:E:554:HIS:HB2	1.89	0.54
3:K:121:LEU:HD22	3:K:148:LEU:HD22	1.89	0.54
1:C:249:GLY:H	1:C:411:SER:HB3	1.72	0.54
2:D:279:THR:HA	2:D:334:ILE:HB	1.89	0.54
2:F:186:GLN:O	2:F:190:GLN:HG2	2.08	0.54
2:F:466:ARG:HA	2:F:485:TYR:HE1	1.73	0.54
2:B:20:PHE:HE2	4:J:97:ILE:HG12	1.73	0.54
2:B:160:THR:HG21	2:B:443:PHE:CZ	2.43	0.54
2:B:41:LEU:HD11	2:B:93:VAL:HG11	1.91	0.53
2:F:153:THR:HG21	2:F:164:ILE:HD12	1.90	0.53
1:C:294:LEU:HD21	1:C:319:ALA:HB2	1.91	0.53
5:M:42:ARG:NH1	5:M:101:VAL:HG22	2.23	0.53
2:B:161:MET:HE1	2:B:375:VAL:HG11	1.90	0.53
6:N:95:PRO:HG3	6:N:101:TYR:HB3	1.90	0.53
1:A:98:PRO:HB3	1:A:161:VAL:HG21	1.90	0.53
3:K:121:LEU:HD21	3:K:149:ILE:HG12	1.89	0.53
2:B:111:ARG:HH11	2:B:111:ARG:HG2	1.74	0.53
2:B:319:ALA:HB2	2:B:331:GLN:HG3	1.91	0.53
1:E:170:HIS:CE1	1:E:346:GLN:HE22	2.26	0.53
1:E:217:VAL:HB	1:E:334:TYR:HB3	1.90	0.53
2:D:214:ALA:HA	2:D:279:THR:HB	1.91	0.53
2:D:153:THR:HG22	2:D:155:VAL:H	1.75	0.52
2:B:387:ILE:HG23	2:B:396:HIS:HB3	1.90	0.52
2:D:253:ILE:HG13	2:D:287:ALA:HB1	1.91	0.52
2:F:346:ILE:HB	2:F:347:PRO:HD3	1.90	0.52
1:A:232:PRO:HA	1:A:247:VAL:HA	1.92	0.52
2:D:105:SER:O	2:D:108:MET:HG2	2.09	0.52
2:D:439:PHE:HA	2:D:464:LEU:HD21	1.92	0.52
2:B:302:ARG:HB3	2:B:345:PRO:HG2	1.92	0.52
2:B:417:LYS:HB2	2:B:425:LEU:HD11	1.91	0.52
2:D:278:LEU:O	2:D:334:ILE:N	2.41	0.52



	ious puge	Interstomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:B:234:SER:O	2:B:238:THR:HG23	2.09	0.52
3:I:121:LEU:HD11	3:I:188:VAL:HG13	1.90	0.52
1:C:43:CYS:HB3	1:C:87:ARG:HD3	1.92	0.51
2:B:105:SER:O	2:B:108:MET:HG3	2.10	0.51
2:F:309:TYR:HB2	2:F:349:LEU:HD13	1.91	0.51
2:B:263:ALA:HB1	2:B:274:VAL:HG11	1.93	0.51
2:D:266:LEU:O	2:D:272:ARG:HG2	2.11	0.51
2:B:20:PHE:CE2	4:J:97:ILE:HG12	2.46	0.51
3:G:76:THR:HA	3:G:79:THR:HG22	1.93	0.51
1:A:358:SER:HB2	1:A:417:SER:H	1.75	0.51
2:B:275:LEU:HD11	2:B:332:ILE:HD11	1.93	0.51
2:B:156:SER:OG	2:B:452:ARG:NE	2.32	0.51
1:C:233:LEU:N	1:C:246:CYS:O	2.37	0.51
2:B:111:ARG:HH12	3:I:86:LEU:HD11	1.75	0.51
1:C:281:VAL:HG23	1:C:354:ALA:HA	1.93	0.51
2:D:346:ILE:HB	2:D:347:PRO:HD3	1.94	0.50
2:F:183:ILE:HD11	2:F:372:PRO:HD2	1.93	0.50
5:M:181:THR:O	5:M:185:ILE:HG12	2.11	0.50
1:E:223:VAL:HG12	1:E:344:ARG:NH1	2.22	0.50
1:E:310:PRO:HD2	1:E:313:LYS:HD2	1.92	0.50
3:I:111:ALA:O	3:I:144:ARG:NH2	2.43	0.50
2:D:35:ASN:HA	1:E:62:ARG:HG3	1.92	0.50
2:B:438:LYS:NZ	2:B:467:ILE:HD11	2.27	0.50
1:E:111:PRO:HD3	1:E:132:ALA:HA	1.94	0.50
3:I:192:ASN:HB2	3:I:197:ILE:HB	1.93	0.50
2:B:127:PHE:HE1	3:I:96:LEU:HD22	1.75	0.50
1:A:375:PRO:HD2	5:M:202:ARG:HG2	1.94	0.50
2:B:175:ALA:HB3	2:B:178:LEU:HG	1.92	0.50
1:E:62:ARG:O	1:E:69:THR:N	2.41	0.50
2:F:150:MET:HB2	2:F:386:ALA:HB1	1.93	0.50
1:A:365:ARG:HD3	2:B:306:GLY:HA3	1.93	0.50
1:E:112:LEU:HD13	2:F:141:PRO:HD2	1.94	0.50
3:G:121:LEU:HD11	3:G:188:VAL:HG13	1.93	0.50
2:D:187:ILE:O	2:D:191:ALA:HB2	2.11	0.49
1:E:288:ASN:HD22	2:F:355:GLU:CD	2.15	0.49
2:D:175:ALA:HB3	2:D:178:LEU:HG	1.94	0.49
1:E:344:ARG:NH1	1:E:345:ASP:OD1	2.44	0.49
1:C:282:GLY:O	1:C:284:GLY:N	2.45	0.49
2:D:253:ILE:O	2:D:256:PRO:HD2	2.11	0.49
2:D:316:TYR:O	2:D:331:GLN:NE2	2.45	0.49
1:C:27:ILE:HD11	1:C:51:VAL:HG13	1.93	0.49



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:I:125:ILE:HG21	3:I:156:ILE:HD13	1.93	0.49
1:C:356:SER:H	1:C:415:ALA:HB3	1.78	0.49
1:E:217:VAL:HG12	1:E:338:THR:HG21	1.94	0.49
1:E:365:ARG:HA	1:E:381:PRO:HD3	1.95	0.49
3:G:99:ILE:HD13	4:H:91:LYS:HZ3	1.78	0.49
5:M:42:ARG:HH11	5:M:101:VAL:HG22	1.76	0.49
1:A:321:THR:OG1	1:A:324:MET:HG3	2.13	0.49
1:E:52:GLY:HA2	1:E:83:ASP:HB3	1.95	0.49
1:A:166:LEU:HD23	1:A:314:ARG:HB3	1.94	0.49
1:A:485:MET:HG3	1:A:551:ILE:HD11	1.95	0.49
2:B:443:PHE:HB2	2:B:464:LEU:HD11	1.95	0.49
1:E:72:VAL:HG21	1:E:76:THR:HB	1.95	0.49
1:A:266:SER:HB3	1:A:353:ILE:HG21	1.95	0.48
2:D:150:MET:HB2	2:D:386:ALA:HB1	1.94	0.48
3:G:191:SER:HA	3:G:198:GLU:HA	1.95	0.48
2:D:52:ILE:O	2:D:96:THR:OG1	2.20	0.48
5:M:29:TYR:HB2	5:M:173:ILE:HG21	1.94	0.48
1:A:270:SER:HA	1:A:278:ILE:HD13	1.94	0.48
2:B:81:GLU:HG3	2:B:248:PRO:HG2	1.95	0.48
1:E:30:VAL:HG13	1:E:35:VAL:HG22	1.94	0.48
1:C:103:THR:HG23	1:C:105:TYR:CE2	2.49	0.48
1:C:28:TYR:OH	2:D:71:ARG:NH2	2.46	0.48
1:A:330:GLU:HG3	1:A:360:TRP:NE1	2.28	0.48
3:I:145:ASP:O	3:I:149:ILE:HG12	2.13	0.48
3:G:206:ARG:NH2	4:H:105:PRO:HB3	2.28	0.48
2:F:305:PRO:HG2	2:F:308:MET:HB2	1.96	0.48
1:E:399:VAL:HG22	1:E:407:THR:HG22	1.96	0.47
1:C:344:ARG:HG3	1:C:409:SER:N	2.28	0.47
1:E:581:VAL:HG12	1:E:603:LEU:HD21	1.96	0.47
3:K:191:SER:HA	3:K:198:GLU:HA	1.95	0.47
1:A:270:SER:HB3	1:A:353:ILE:HD12	1.96	0.47
2:D:173:PHE:N	2:D:358:ILE:O	2.47	0.47
1:E:485:MET:SD	1:E:547:MET:HG3	2.53	0.47
1:E:525:PHE:HD2	1:E:526:LEU:HD12	1.78	0.47
3:I:192:ASN:N	3:I:197:ILE:O	2.41	0.47
7:O:169:ASP:O	7:O:173:ARG:N	2.45	0.47
1:C:171:LYS:HB2	1:C:346:GLN:HG2	1.95	0.47
1:E:477:GLU:O	1:E:481:LEU:HD13	2.14	0.47
1:C:333:ILE:HG12	1:C:360:TRP:CD1	2.50	0.47
2:D:127:PHE:HE1	3:K:96:LEU:HD22	1.79	0.47
2:F:211:VAL:HG23	2:F:276:THR:HG23	1.97	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:281:VAL:HG12	1:C:318:VAL:HB	1.96	0.47
2:F:178:LEU:HD13	2:F:360:VAL:HG12	1.97	0.47
2:F:402:GLN:OE1	2:F:475:ARG:HB2	2.15	0.47
3:G:120:ILE:HD12	4:H:104:LYS:H	1.79	0.47
1:A:269:LEU:HD22	1:A:353:ILE:HD11	1.97	0.47
1:C:297:PHE:HD2	1:C:317:LEU:HD11	1.79	0.47
1:A:278:ILE:HB	1:A:315:THR:HG22	1.97	0.47
1:E:233:LEU:N	1:E:246:CYS:O	2.41	0.46
1:A:33:PRO:HD2	1:A:370:ARG:HG3	1.97	0.46
2:D:403:LEU:HD11	2:D:461:ALA:HB1	1.96	0.46
1:E:232:PRO:HG3	1:E:470:PHE:CE2	2.50	0.46
1:A:193:LEU:HD23	1:A:212:TYR:HB3	1.97	0.46
1:A:264:VAL:HG11	9:A:701:ADP:C5	2.50	0.46
2:B:34:VAL:HG22	1:C:45:MET:CE	2.45	0.46
2:D:213:ALA:HB3	2:D:278:LEU:HD23	1.97	0.46
1:E:320:ASN:ND2	1:E:329:ARG:HA	2.30	0.46
8:P:49:SER:HA	8:P:53:LYS:HA	1.96	0.46
2:B:335:LEU:HD11	2:B:346:ILE:HG22	1.97	0.46
1:C:288:ASN:HD22	2:D:147:PRO:HD3	1.81	0.46
3:K:215:LEU:HA	3:K:218:ILE:HG22	1.97	0.46
1:A:107:GLY:HA2	1:A:332:SER:HB3	1.97	0.46
1:E:63:ILE:HA	1:E:68:ALA:HA	1.98	0.46
2:F:114:ASP:HA	2:F:120:ILE:HD11	1.98	0.46
1:A:56:LEU:HD21	1:A:126:ARG:HB3	1.98	0.46
2:F:171:PRO:HB3	2:F:333:PRO:HG2	1.97	0.46
1:C:284:GLY:HA2	1:C:329:ARG:HD2	1.97	0.46
1:E:43:CYS:SG	1:E:60:VAL:HG21	2.56	0.46
1:C:101:MET:HA	1:C:316:THR:HG22	1.97	0.46
2:F:174:SER:O	2:F:336:THR:HA	2.16	0.46
2:F:215:MET:CE	2:F:256:PRO:HB3	2.46	0.46
1:C:32:GLY:O	1:C:76:THR:HG21	2.16	0.45
1:E:49:VAL:HG12	1:E:87:ARG:HA	1.96	0.45
3:I:106:LYS:HD3	4:J:99:ILE:HG13	1.97	0.45
4:L:103:ILE:O	4:L:105:PRO:HD3	2.16	0.45
1:A:344:ARG:HG3	1:A:409:SER:N	2.31	0.45
2:B:34:VAL:HG22	1:C:45:MET:HE3	1.97	0.45
2:B:110:GLY:HA2	2:B:235:LEU:O	2.16	0.45
1:C:281:VAL:HG11	1:C:336:GLY:HA3	1.98	0.45
7:O:196:VAL:HA	7:O:257:PRO:HA	1.97	0.45
2:B:269:GLN:O	3:I:230:LYS:N	2.49	0.45
2:F:257:ARG:NH1	2:F:315:ILE:HD11	2.31	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:L:80:LEU:O	4:L:83:ILE:HG22	2.16	0.45
1:A:395:ALA:HB2	1:A:412:ILE:HG13	1.98	0.45
2:D:416:MET:O	2:D:420:VAL:HG22	2.17	0.45
2:B:58:PRO:HD3	2:B:91:THR:HG22	1.98	0.45
2:D:53:VAL:N	2:D:65:GLY:O	2.37	0.45
3:K:124:LEU:HD23	4:L:105:PRO:HG3	1.98	0.45
2:F:57:LEU:HD12	2:F:61:THR:OG1	2.17	0.45
2:F:168:GLN:HB2	2:F:382:LEU:HD12	1.98	0.45
1:A:109:GLN:HG2	1:A:132:ALA:HB1	1.99	0.45
2:B:127:PHE:HD2	3:I:219:ARG:HD2	1.82	0.45
2:B:178:LEU:HD13	2:B:360:VAL:HG12	1.99	0.45
3:G:139:VAL:HG21	3:G:172:ILE:HD11	1.99	0.45
1:C:291:ALA:HB2	2:D:144:ARG:HB3	1.98	0.45
2:F:403:LEU:HD11	2:F:461:ALA:HB1	1.97	0.45
1:A:330:GLU:HG3	1:A:360:TRP:HE1	1.81	0.45
1:A:446:ALA:HA	1:A:451:PHE:CE2	2.50	0.45
1:C:238:ARG:NH1	1:C:538:CYS:SG	2.90	0.45
2:D:111:ARG:NH2	2:D:124:PRO:O	2.44	0.45
1:A:141:PHE:CE1	1:A:159:GLY:HA3	2.52	0.44
3:K:107:LEU:HD12	3:K:207:LEU:HD22	1.99	0.44
5:M:60:VAL:HA	5:M:63:THR:HG22	1.98	0.44
2:F:27:ASN:HB2	3:G:198:GLU:HG2	2.00	0.44
2:B:168:GLN:NE2	2:B:382:LEU:HB2	2.33	0.44
1:C:267:GLN:O	1:C:271:LYS:HG2	2.18	0.44
1:E:43:CYS:HB3	1:E:63:ILE:HD12	1.99	0.44
2:D:127:PHE:CE2	3:K:219:ARG:HG3	2.52	0.44
1:A:378:GLN:HB3	1:A:426:PRO:HG2	2.00	0.44
1:C:477:GLU:O	1:C:481:LEU:HD23	2.17	0.44
1:A:197:ILE:HG13	1:A:211:LEU:HG	2.00	0.44
1:C:62:ARG:HG2	1:C:69:THR:HB	1.99	0.44
1:A:495:LEU:HB3	1:A:515:LEU:HD21	1.99	0.44
1:E:232:PRO:HB3	1:E:467:LEU:HD21	2.00	0.44
1:A:358:SER:O	1:A:362:GLU:HG3	2.18	0.44
1:E:288:ASN:ND2	2:F:355:GLU:OE2	2.50	0.44
3:G:106:LYS:HE2	3:G:106:LYS:HB2	1.79	0.44
1:E:378:GLN:HB3	1:E:426:PRO:HG3	2.00	0.43
3:I:130:LEU:HD22	3:I:164:ALA:HB2	1.99	0.43
5:M:104:VAL:HG21	5:M:162:VAL:HG21	1.99	0.43
2:B:281:MET:HG2	2:B:316:TYR:OH	2.17	0.43
1:C:224:THR:HB	1:C:399:VAL:HG13	1.98	0.43
2:B:156:SER:O	2:B:160:THR:HG22	2.18	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
2·B·178·LEU·HD21	2·B·362·ABG·HE	1.82	0.43
1:E:266:SEB:HA	1:E:353:ILE:HD13	2.01	0.43
1:A:56:LEU:HD22	1:A:74:GLU:CB	2.48	0.43
2:B:51:GLU:O	2:B:53:VAL:HG23	2.18	0.43
2:D:55:LEU:CD2	2:D:93:VAL:HG22	2.47	0.43
2:D:253:ILE:HD11	2:D:288:LEU:HA	2.01	0.43
1:C:297:PHE:CD2	1:C:317:LEU:HD21	2.53	0.43
2:D:293:ALA:HB3	1:E:382:ALA:HB2	2.00	0.43
1:A:238:ARG:O	1:A:242:ALA:HB3	2.18	0.43
2:B:209:SER:O	2:B:274:VAL:HA	2.18	0.43
3:K:215:LEU:O	3:K:218:ILE:HG22	2.19	0.43
1:A:220:PRO:HB3	1:A:394:ARG:HD2	2.00	0.43
2:D:22:VAL:CG2	3:K:210:LEU:HD12	2.49	0.43
2:D:67:VAL:HA	2:D:77:VAL:HA	2.01	0.43
1:E:302:THR:HG21	1:E:314:ARG:NH1	2.33	0.43
2:F:277:ILE:HD13	2:F:332:ILE:HB	2.01	0.43
3:I:143:GLU:HA	3:I:178:TYR:CD2	2.53	0.43
2:D:108:MET:HE3	2:D:262:THR:HG23	2.00	0.43
2:D:250:ILE:HD12	2:D:250:ILE:H	1.83	0.43
1:E:484:ARG:O	1:E:488:ILE:HG12	2.19	0.43
3:K:192:ASN:N	3:K:197:ILE:O	2.48	0.43
2:B:212:PHE:CE2	2:B:214:ALA:HB2	2.52	0.43
1:C:100:LEU:HD12	1:C:316:THR:HG21	2.00	0.43
1:C:471:TYR:CD2	1:C:479:PRO:HG3	2.54	0.43
2:D:28:TYR:CE1	2:D:44:VAL:HA	2.53	0.43
2:D:160:THR:O	2:D:396:HIS:NE2	2.48	0.43
2:D:335:LEU:HD11	2:D:346:ILE:HG22	2.01	0.43
1:E:160:SER:HA	1:E:171:LYS:HA	2.00	0.43
1:E:290:MET:O	1:E:294:LEU:HG	2.19	0.43
1:C:337:ILE:HB	1:C:391:PHE:HE1	1.84	0.43
1:C:528:GLN:HE21	1:C:536:ALA:HA	1.83	0.43
1:E:176:PRO:HG2	1:E:215:TRP:CZ3	2.53	0.43
2:F:302:ARG:HH11	2:F:302:ARG:HG2	1.84	0.42
1:A:115:ILE:HG12	1:A:128:ILE:HG21	2.01	0.42
2:B:127:PHE:CD2	3:I:219:ARG:HD2	2.55	0.42
2:D:102:ILE:CG2	2:D:258:LEU:HD22	2.49	0.42
4:H:79:GLU:O	4:H:83:ILE:HG12	2.19	0.42
3:I:218:ILE:HD11	4:J:98:LEU:HD21	2.01	0.42
2:B:163:SER:O	2:B:380:SER:OG	2.21	0.42
1:C:138:LYS:HB3	1:C:190:GLU:CG	2.49	0.42
1:E:439:TRP:HB3	1:E:454:ILE:HD12	2.00	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
8:P:405:LYS:O	8:P:409:GLY:N	2.52	0.42
1:A:388:LEU:O	1:A:392:TYR:HD2	2.03	0.42
1:A:364:LEU:HD11	1:A:387:LYS:HD3	2.01	0.42
2:D:38:LEU:HD23	2:D:76:ILE:CG2	2.49	0.42
2:F:253:ILE:HA	2:F:284:TYR:HE1	1.85	0.42
3:G:99:ILE:HD13	4:H:91:LYS:NZ	2.34	0.42
3:K:106:LYS:O	3:K:110:ILE:N	2.48	0.42
5:M:42:ARG:HH12	5:M:102:SER:CB	2.32	0.42
1:A:233:LEU:N	1:A:246:CYS:O	2.48	0.42
2:D:64:GLN:HB3	2:D:80:PHE:CD2	2.55	0.42
1:E:302:THR:HG21	1:E:314:ARG:HH12	1.85	0.42
2:F:215:MET:HB2	2:F:279:THR:O	2.20	0.42
1:A:95:GLU:OE1	1:A:135:ARG:NH2	2.51	0.42
1:E:92:LEU:HD23	1:E:217:VAL:HG21	2.01	0.42
1:E:445:LEU:HD12	1:E:450:HIS:ND1	2.34	0.42
6:N:10:VAL:HA	6:N:68:LEU:HB2	2.02	0.42
1:A:35:VAL:N	1:A:70:ILE:O	2.47	0.42
1:A:485:MET:HB3	1:A:485:MET:HE2	1.71	0.42
1:C:135:ARG:O	1:C:192:THR:OG1	2.37	0.42
1:C:320:ASN:HD21	1:C:329:ARG:HA	1.83	0.42
1:E:35:VAL:N	1:E:70:ILE:O	2.51	0.42
3:I:169:LEU:HD23	3:I:172:ILE:HB	2.01	0.42
3:K:143:GLU:HA	3:K:178:TYR:CE1	2.55	0.42
1:A:196:LYS:HA	1:A:210:THR:HG22	2.01	0.42
2:D:102:ILE:HG21	2:D:258:LEU:HD22	2.01	0.42
1:E:98:PRO:HG2	1:E:193:LEU:HD21	2.02	0.42
1:E:283:CYS:SG	1:E:333:ILE:HG12	2.60	0.42
8:P:372:PRO:N	8:P:373:PRO:HD2	2.35	0.42
1:A:255:PRO:HG2	1:A:438:PHE:HE1	1.84	0.42
2:B:193:LEU:HD23	2:B:196:PRO:HA	2.00	0.42
1:C:320:ASN:ND2	1:C:329:ARG:HA	2.35	0.41
1:E:32:GLY:O	1:E:76:THR:HG21	2.20	0.41
1:E:182:ILE:O	1:E:182:ILE:HG13	2.20	0.41
2:F:43:LYS:HB3	2:F:43:LYS:HE3	1.84	0.41
3:G:130:LEU:HD11	3:G:163:LYS:HD2	2.02	0.41
5:M:152:LEU:HD23	5:M:152:LEU:HA	1.90	0.41
7:O:302:ASN:O	7:O:306:ILE:HG12	2.20	0.41
1:A:329:ARG:HD2	1:A:363:ALA:HB2	2.02	0.41
1:A:451:PHE:CD1	9:A:701:ADP:C4	3.08	0.41
1:E:485:MET:HE2	1:E:485:MET:HB3	1.93	0.41
2:F:152:SER:N	2:F:192:GLY:O	2.54	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	(\dot{A})
1·A·537·PHE·O	1·A·589·PBO·HG3	2 20	0.41
2:F:150:MET:SD	2:F:163:SER:HB2	2.61	0.41
2:F:214:ALA:HB1	2:F:217:VAL:HG22	2.03	0.41
1:A:320:ASN:HA	1:A:324:MET:HE3	2.03	0.41
1:A:335:THR:O	1:A:339:LEU:HG	2.21	0.41
2:B:27:ASN:HB2	3:I:198:GLU:HG2	2.01	0.41
2:D:127:PHE:CE1	3:K:96:LEU:HD22	2.55	0.41
1:E:334:TYR:HA	1:E:337:ILE:HG22	2.02	0.41
1:E:499:VAL:HG13	1:E:504:LYS:CB	2.51	0.41
1:E:546:MET:HG3	1:E:600:PHE:CZ	2.56	0.41
2:F:334:ILE:H	2:F:334:ILE:HG13	1.74	0.41
1:C:104:ILE:HD12	1:C:294:LEU:HD22	2.02	0.41
2:D:376:LEU:HA	2:D:404:TYR:CE2	2.55	0.41
2:F:331:GLN:HG2	2:F:333:PRO:HD3	2.02	0.41
6:N:5:ARG:O	6:N:65:ALA:HB2	2.19	0.41
2:B:111:ARG:NH1	3:I:86:LEU:HD11	2.36	0.41
1:E:240:LEU:HD21	1:E:454:ILE:HG13	2.02	0.41
2:F:279:THR:HA	2:F:334:ILE:HB	2.02	0.41
3:K:169:LEU:HD23	3:K:172:ILE:HB	2.02	0.41
8:P:313:LEU:HA	8:P:318:ALA:HB3	2.03	0.41
1:A:255:PRO:HA	1:A:416:VAL:O	2.20	0.41
2:B:416:MET:O	2:B:420:VAL:HG22	2.21	0.41
1:C:110:ARG:HB2	1:C:115:ILE:HD11	2.03	0.41
2:D:153:THR:HG23	2:D:187:ILE:HG12	2.03	0.41
2:D:161:MET:CE	2:D:403:LEU:HB3	2.47	0.41
2:F:145:ILE:HD11	2:F:323:GLU:HA	2.02	0.41
1:A:174:LEU:HG	1:A:175:PRO:HD2	2.02	0.41
2:B:156:SER:HB2	2:B:452:ARG:HH21	1.86	0.41
2:B:401:ASN:HB3	2:B:475:ARG:HH11	1.84	0.41
1:C:100:LEU:HD11	1:C:343:PHE:CZ	2.56	0.41
1:E:100:LEU:HD13	1:E:339:LEU:HD22	2.03	0.41
1:E:525:PHE:HB2	1:E:550:PHE:CE2	2.56	0.41
2:F:393:ARG:HG3	2:F:395:ASP:H	1.86	0.41
3:G:169:LEU:HD23	3:G:172:ILE:HB	2.03	0.41
4:H:99:ILE:O	4:H:103:ILE:HG12	2.20	0.41
3:K:86:LEU:HD23	3:K:86:LEU:HA	1.89	0.41
2:D:104:VAL:HG21	2:D:132:LEU:HD13	2.03	0.41
2:F:52:ILE:O	2:F:96:THR:OG1	2.23	0.41
2:F:104:VAL:HA	2:F:108:MET:HE3	2.03	0.41
6:N:20:LEU:HD12	6:N:25:ILE:HG21	2.02	0.41
1:C:30:VAL:O	2:D:70:ILE:HG22	2.21	0.40



EMD-25996,	7TMM
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Continued from pree	ious puge		-
Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$\begin{tabular}{ c c c c c } \hline Interatomic \\ distance (Å) \\ \hline 2.61 \\ \hline 2.03 \\ \hline 2.21 \\ \hline 2.55 \\ \hline 2.03 \\ \hline 2.01 \\ \hline 2.03 \\ \hline 2.01 \\ \hline 2.03 \\ \hline 2.21 \\ \hline 1.94 \\ \hline 2.22 \\ \hline 2.21 \\ \hline 2.03 \\ \hline 2.04 \\ \hline 2.04 \\ \hline 2.37 \\ \hline 2.22 \\ \hline 2.21 \\ \hline 2.20 \\ \hline 2.04 \\ \hline 2.$	overlap (Å)
1:C:253:CYS:SG	1:C:416:VAL:HB	2.61	0.40
1:C:286:ARG:HD3	2:D:355:GLU:HG2	2.03	0.40
2:F:190:GLN:OE1	2:F:451:ASP:HA	2.21	0.40
2:F:474:ASN:OD1	2:F:474:ASN:N	2.55	0.40
3:K:199:ILE:HG22	3:K:201:ASN:HB2	2.03	0.40
1:A:279:ILE:HB	1:A:352:MET:HG2	2.01	0.40
1:A:499:VAL:HG21	1:A:507:LEU:HD11	2.03	0.40
1:A:558:GLN:O	1:A:561:VAL:HG12	2.21	0.40
2:D:315:ILE:HD13	2:D:315:ILE:HA	1.94	0.40
2:D:395:ASP:O	2:D:399:VAL:HG23	2.22	0.40
2:F:110:GLY:HA2	2:F:235:LEU:O	2.21	0.40
1:A:217:VAL:HB	1:A:334:TYR:HB3	2.03	0.40
1:A:262:LYS:HB3	1:A:415:ALA:HB1	2.04	0.40
2:B:81:GLU:HA	2:B:248:PRO:HB3	2.04	0.40
2:D:257:ARG:NH1	2:D:315:ILE:HD11	2.37	0.40
2:F:369:ILE:HG23	2:F:445:THR:OG1	2.22	0.40
1:A:296:GLU:O	1:A:300:LEU:HG	2.21	0.40
1:E:33:PRO:O	1:E:72:VAL:HG22	2.20	0.40
3:K:123:SER:HA	3:K:126:VAL:HG12	2.04	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	entiles
1	А	591/639~(92%)	561 (95%)	30~(5%)	0	100	100
1	С	590/639~(92%)	559~(95%)	31~(5%)	0	100	100
1	Е	570/639~(89%)	542 (95%)	28~(5%)	0	100	100
2	В	460/517~(89%)	434 (94%)	26 (6%)	0	100	100
2	D	455/517~(88%)	429 (94%)	26~(6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	\mathbf{F}	455/517~(88%)	439~(96%)	16 (4%)	0	100	100
3	G	218/233~(94%)	215 (99%)	3~(1%)	0	100	100
3	Ι	218/233~(94%)	215~(99%)	3~(1%)	0	100	100
3	Κ	210/233~(90%)	205~(98%)	5(2%)	0	100	100
4	Н	107/114~(94%)	104 (97%)	3~(3%)	0	100	100
4	J	106/114~(93%)	104 (98%)	2(2%)	0	100	100
4	L	97/114~(85%)	97 (100%)	0	0	100	100
5	М	212/256~(83%)	208 (98%)	4 (2%)	0	100	100
6	Ν	109/118~(92%)	105 (96%)	4 (4%)	0	100	100
7	Ο	355/392~(91%)	345~(97%)	10 (3%)	0	100	100
8	Р	435/478 (91%)	430 (99%)	5 (1%)	0	100	100
All	All	5188/5753~(90%)	4992 (96%)	196 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	356/537~(66%)	356~(100%)	0	100	100
1	С	306/537~(57%)	305 (100%)	1 (0%)	92	97
1	Е	331/537~(62%)	331 (100%)	0	100	100
2	В	313/444~(70%)	313 (100%)	0	100	100
2	D	282/444~(64%)	282 (100%)	0	100	100
2	F	289/444~(65%)	289 (100%)	0	100	100
3	G	74/208~(36%)	74 (100%)	0	100	100
3	Ι	67/208~(32%)	67~(100%)	0	100	100
3	K	68/208~(33%)	68 (100%)	0	100	100
4	Н	13/94~(14%)	13 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
4	J	13/94~(14%)	13 (100%)	0	100	100	
4	L	12/94~(13%)	12 (100%)	0	100	100	
5	М	76/221~(34%)	76 (100%)	0	100	100	
6	Ν	17/104~(16%)	17 (100%)	0	100	100	
7	Ο	26/348~(8%)	26 (100%)	0	100	100	
8	Р	9/439~(2%)	9 (100%)	0	100	100	
All	All	2252/4961~(45%)	2251 (100%)	1 (0%)	100	100	

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
1	С	323	ASN	

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
2	В	344	HIS
2	D	331	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)

1 ligand is modelled in this entry.

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	ths	B	ond ang	les
INIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	А	701	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)

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
9	ADP	А	701	-	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	А	701	ADP	C5-C4	2.36	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
9	А	701	ADP	PA-O3A-PB	-3.92	119.37	132.83
9	А	701	ADP	N3-C2-N1	-3.03	123.95	128.68
9	А	701	ADP	C3'-C2'-C1'	2.72	105.07	100.98
9	А	701	ADP	C4-C5-N7	-2.51	106.78	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	А	701	ADP	C5'-O5'-PA-O3A
9	А	701	ADP	C5'-O5'-PA-O1A
9	А	701	ADP	C3'-C4'-C5'-O5'
9	А	701	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	А	701	ADP	3	0

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)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25996. 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.

Orthogonal projections (i) 6.1

6.1.1Primary map



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

6.2Central slices (i)

6.2.1Primary map



X Index: 200

Y Index: 200



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: 193

Y Index: 205

Z Index: 231

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 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 385 nm^3 ; this corresponds to an approximate mass of 347 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 0.286 $\mathrm{\AA^{-1}}$



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-25996 and PDB model 7TMM. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.42 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 (0.42).



9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9550	0.4850	
A	0.9550	0.5370	
В	0.9530	0.5390	1 0
С	0.9620	0.5160	
D	0.9550	0.5350	
Е	0.9600	0.5260	
F	0.9560	0.5420	
G	0.9760	0.4600	
Н	0.9780	0.3520	
Ι	0.9820	0.4720	
J	0.9790	0.3730	
K	0.9840	0.4770	0.0
L	0.9810	0.3770	<0.0
М	0.9430	0.4640	
N	0.9650	0.4160	
0	0.9040	0.3300	
Р	0.9170	0.2970	1

