

Nov 19, 2022 – 01:48 PM EST

PDB ID	:	3B5U
EMDB ID	:	EMD-1088
Title	:	Actin filament model from extended form of acromsomal bundle in the Limulus
		sperm
Authors	:	Cong, Y.; Topf, M.; Sali, A.; Matsudaira, P.; Dougherty, M.; Chiu, W.;
		Schmid, M.F.
Deposited on	:	2007-10-26
Resolution	:	9.50 Å(reported)
Based on initial model	:	?

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 (i)) were used in the production of this report:

MolProbity : 4.02b-467	
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2	(019)
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: $ELECTRON\ CRYSTALLOGRAPHY$

The reported resolution of this entry is 9.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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 chair	1	
1	٨	077	93%		
1	A	377	57%	36%	5% ••
			89%		
1	В	377	58%	34%	6% ••
			88%		l
1	С	377	66%	27%	6% •
			92%		
1	D	377	57%	33%	9% ••
			91%		
1	Ε	377	60%	29%	9% ••
			90%		-
1	\mathbf{F}	377	58%	34%	6% ••
			93%		
1	G	377	65%	29%	6% •
			97%		
1	Н	377	69%	27%	• ••



Conti	naea fron	i previous	puye		
Mol	Chain	Length	Quality of chain		
			98%		
1	Ι	377	61%	33%	• ••
			95%		
1	J	377	60%	31%	6% ••
			96%		
1	Κ	377	61%	31%	6% ••
			95%		
1	L	377	56%	36%	6% ••
			92%		
1	М	377	64%	28%	6% ••
			92%		
1	Ν	377	57%	32%	9% ••



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 41062 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	Δ	375	Total	С	Ν	0	S	0	0
	Л	515	2933	1854	493	565	21	0	0
1	В	375	Total	С	Ν	0	S	0	0
	D	515	2933	1854	493	565	21	0	0
1	С	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
1	U	515	2933	1854	493	565	21	0	0
1	П	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
		515	2933	1854	493	565	21	0	0
1	E	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
		515	2933	1854	493	565	21	0	0
1	F	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	1	515	2933	1854	493	565	21	0	0
1	G	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
		515	2933	1854	493	565	21	0	0
1	н	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	11	510	2933	1854	493	565	21	0	0
1	Т	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
-	1	510	2933	1854	493	565	21	0	0
1	J	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
-		310	2933	1854	493	565	21		0
1	K	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
		510	2933	1854	493	565	21	0	0
1	L	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
		510	2933	1854	493	565	21	0	0
1	М	375	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	111	510	2933	1854	493	565	21	0	0
1	N	375	Total	С	Ν	Ο	\mathbf{S}	0	0
	11	010	2933	1854	493	565	21		U U

• Molecule 1 is a protein called Actin, alpha skeletal muscle.



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: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle







E364 A365 G366 G366 B367 S368 H371 H371 H371 H371 C374 K373 C374 K375

 \bullet Molecule 1: Actin, alpha skeletal muscle

Chain C:	66%	38%	27%	6% •	
MET MET D1 D2 D3 D3 D3 D3 D3 D3 D3 D3 D3 D3 D3 D3 D3	D11 N12 C13 C13 C15 C15 C15 C15 C15 C15 C15 C15 C15 C10 C10 C10 C10 C10 C10 C10 C10 C10 C10	F21 A22 C23 C23 C23 A26 A26 C2 C28 A29 V30	F31 P32 S33 S33 C36 C36 C36 R37 P38	R39 H40 Q41 C42 V43 V45 C46 C46	49 49 750 753 753 753 753 755 852 857 855 857 855 758
Q59 R62 G63 G63 G63 G63 L65 L65 K68 Y69 Y69 Y70 T71	E72 4 H73 6 G74 6 175 1 177 1 N78 1 N78 1 N79 0 B80 1 D80 1 D80 1	R82 E83 K84 K84 H87 H88 F90 F90 Y91	N92 E93 L94 R95 V96 A97 A97	H101 F102 F103 L104 L105 F106 A108 P109 P109	NIII PI12 KI13 A114 RI16 E117 E117 M119 T120
q121 1122 M123 F124 E126 F126 F126 V129 V129 V129 V129 V129 V123 V123	V134 A135 1136 Q137 A138 A138 X139 S141 L142 S141	1143 1149 1149 0150 1151 1151 1153 1153 1153 1154	G156 0 D157 0 C158 0 V159 0 T160 0 H161 0 N162 0	V163 P164 P165 P165 P165 P167 Q169 A170 L171 P172	H173 A174 1175 N176 L178 D178 L180 A181 A181 A181 C182
R183 D184 L185 T186 D187 Y188 M190 K191 L193 L193	1194 E195 R196 G197 Y198 Y198 Y201 Y201 T202 T203	A204 R205 R206 R206 R206 V209 N211 D211 1212 R210 R213	K215 K215 C217 V219 V219 A220	D222 F223 F223 E224 N225 E226 M227 A228 A229	A231 S232 S234 S234 S235 S235 L236 L236 K228 S229 Y240 F241 F241 L242
P243 P244 C245 C245 C245 C245 C245 C245 C245 C	P265 P265 P266 P266 P568 P568 P568 P569 P260 P261 P261 P262 P262 P263	P.564 8.266 1267 1267 0268 M.269 8.271 8.271 8.271 6.273 6.273	1274 H275 E276 E276 T277 Y279 Y279 N280	2.221 1282 M283 K284 C285 D286 D286 D288 D288 D288	K281 K281 K281 K281 K293 K293 N297 N297 N298 S200 S200
T304 M305 M305 P307 C308 C308 A310 D311 T317 T318 T318	L320 A321 P322 S323 S323 C326 M326 K326 K326 K328	1329 1332 1333 1333 1333 1335 1336 1336 1336 1336	C342 C342 C343 C344 C345 L346 A347 A347 S348	L349 S350 F382 F382 F382 Q364 Q364 M365 M365 M365 1357	T358 K359 Q360 Q360 D363 D363 A365 C366 C366 C366 C366 C366 C366 C366 C



• Molecule 1: Actin, alpha skeletal muscle



A365 G366 1369 H371 R372 K372 K373 C374 F375

 \bullet Molecule 1: Actin, alpha skeletal muscle

Ch	air	n E	D:								6	50%	,			9	1%									29%	6				ç	9%		•													
T. S	••		•	••			-	•	•	0	4	0	. 2	α σ		2	р Ю	<u>ب</u>	9	2		0 0			•	4	<u>о</u> с	0	•	6	0 -		0 2	4	<u>م</u> 9	•	00	0	0 1	5	• •			÷-	► ●		
CY ME	D1	DG	E4	T T D T	A7	La	2° 5		IN	G1	10 E					A2			A2	P2	R2	A2	P3	E CL	S	EI	N3	3 2	PG	R3	H	G	Λd	M	64 64	M	G	60	DE	SE	YE		DE	B	A	3	
S60 V61	R62	тес	L67	K68 V60	P70	171	E72	H/3 G74	175	176	T77	N78 W70	D80	D81	M82	E83	K84 +05	981	H87	H88	T89	F90	Y91 N92	E93	L94	R95	796 197	P98	E99	E100	P102	T103	L104	L105 T106	E107	A108	P109	L110	P112	K113	A114	N115	R116 E117	K118	M119	T120	TZTN
	c 4	25	26		67	2 E	22 02	80 s	55 55	98	87			1	1 5	6	14 14	ci di		18	19			• •	4	• •		<u>هم</u>	60	<mark>0000000000000000000000000000000000000</mark>		•	34	05 0			6				74 •	2	24 24		6		
113 M	E E	E	EL EL	11.		A10	M1:	Y1:		110	Q1:	A10	L1	S1,	L1,	γLΥ	A1,		R1	TI	11,	15		L1	D1(S10	D10	G11	V1!	II.		V10	P1(11(E1	G1(Y10	TA .		.TH	A1		M1. R1	EI.	D1.	L1	TH
G182	h163	L185	T186 D187	Y188	L189 M100	K191	I 192	L193 T104	1194 F105	R196	G197	1130 S199	F200	V201	T202	T203	A 204 E.205	R206	E207	1208	V 209	R210	1212	K213	E214	K215	L216	Y218	V219	A220	L221	F223	E224	N225	E226	A228	Т229	A230	A231	8232	S234	S235	L236	K238	S 239	Y240	E241
••	•••	••	••				•				•				•	•						•	•	•			•	•			•	•	••			•					••	•4			•		•
L242 D243	P 243 D244	G245	Q246 V247	1248	T249	G251	N252	E253	R254	R256	C257	P258	E259 TO60	1.261 L.261	F262	<mark>q263</mark>	P264	S265	F266 T267	1202	M269	E270	S271	A272	G273	<u>1274</u> но75	E276	T277	T278	Y279	S281	1282	M283	K284	D286	1287	D288	1289 R 290	K291	D292	L293	Y294	N296	N297	V298	M299 S200	G301



G302 T303 T304 T305 T317 T317 T315 T315 T315 T315 T315 T316 T317 T318 T317 T318 T317 T318 T317 T318 T317 T318 T317 T318 T3216 T3217 T3218 T3219 T3216 T3217 T3218 T3219 T3216 T3217 T3218 T3219 T3210 T3211 T3212

Y362 D363 E364 A365 A365 C366 C366 C366 C366 C366 B368 C366 H371 H371 H371 C374 C374 C374

• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle



PROTEIN DATA BANK









 K359
 K369

 E361
 E364

 F362
 B365

 P365
 B365

 P365
 B365

 P365
 B365

 P367
 B370

 P371
 H371

 H372
 H372

 H372
 C374

 F375
 C374

• Molecule 1: Actin, alpha skeletal muscle



DB DATA BANK • Molecule 1: Actin, alpha skeletal muscle



Y362 D363 E364 A365 P365 P367 S368 P367 S368 H371 H371 H371 S368 C374 F375

• Molecule 1: Actin, alpha skeletal muscle



G302 G303 1303 1303 1305 9305 9305 9305 9306 9305 9307 6308 6308 6308 6309 6311 8313 1313 1331 1331 8313 1314 8314 8314 8315 8325 8316 8333 8317 1331 8333 1331 8334 1332 8335 8333 8336 8333 8333 1332 8334 1332 8335 8333 8336 8333 8336 8333 8336 8334 8335 8334 8336 8334 8337 8344 8338 8334 8339 8334 8336 8335 8345 8345 8356</t

Y362 D363 E364 A365 A365 A365 A365 A365 A365 A375 B369 B374 W370 W370 W371 C374 C374 C375 C375 C376 C377 C3

• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, $a=$ Not provided Å, $b=$ Not	Depositor
	provided Å, $c=$ Not provided Å, $\alpha=$ Not	
	provided°, β =Not provided°, γ =Not	
	provided°, space group=Not provided	
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	
Microscope	JEOL 4000EX	Depositor
Voltage (kV)	400	Depositor
Electron dose $(e^-/\text{\AA}^2)$	15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	977.199	Depositor
Minimum map value	-974.403	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	215.097	Depositor
Recommended contour level	430.0	Depositor
Map size (Å)	255.99936, 148.00015, 765.7977	wwPDB
Map dimensions	576, 192, 112	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33333, 1.32143, 1.32951	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).

Mol	Chain	Bo	ond lengths	E	Sond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.69	0/2996	1.34	21/4058~(0.5%)
1	В	0.68	0/2996	1.35	23/4058~(0.6%)
1	С	0.64	0/2996	1.30	22/4058~(0.5%)
1	D	0.66	0/2996	1.42	33/4058~(0.8%)
1	Е	0.65	0/2996	1.40	30/4058~(0.7%)
1	F	0.64	0/2996	1.34	19/4058~(0.5%)
1	G	0.65	0/2996	1.29	23/4058~(0.6%)
1	Н	0.67	0/2996	1.32	20/4058~(0.5%)
1	Ι	0.67	0/2996	1.29	24/4058~(0.6%)
1	J	1.60	6/2996~(0.2%)	1.32	22/4058~(0.5%)
1	Κ	2.88	3/2996~(0.1%)	1.40	36/4058~(0.9%)
1	L	1.19	5/2996~(0.2%)	1.39	28/4058~(0.7%)
1	М	0.69	0/2996	1.40	27/4058~(0.7%)
1	N	0.69	0/2996	1.39	32/4058~(0.8%)
All	All	1.11	$14/\overline{41944}~(0.0\%)$	1.35	360/56812~(0.6%)

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	8
1	В	0	11
1	С	0	7
1	D	0	11
1	Е	0	10
1	F	0	8
1	G	0	3
1	Н	0	6
1	Ι	0	9
1	J	0	8
1	Κ	0	12



Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	13
1	М	0	7
1	Ν	0	10
All	All	0	123

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Κ	195	GLU	CB-CG	122.37	3.84	1.52
1	Κ	173	HIS	CB-CG	91.74	3.15	1.50
1	J	266	PHE	CG-CD2	38.22	1.96	1.38
1	J	266	PHE	CG-CD1	37.55	1.95	1.38
1	J	266	PHE	CE2-CZ	30.64	1.95	1.37
1	J	266	PHE	CE1-CZ	30.50	1.95	1.37
1	L	112	PRO	CA-CB	30.17	2.13	1.53
1	L	112	PRO	N-CD	28.91	1.88	1.47
1	J	266	PHE	CD2-CE2	28.12	1.95	1.39
1	J	266	PHE	CD1-CE1	27.36	1.94	1.39
1	L	112	PRO	CG-CD	21.76	2.22	1.50
1	L	112	PRO	N-CA	21.55	1.83	1.47
1	L	112	PRO	CB-CG	12.60	2.12	1.50
1	K	173	HIS	CG-CD2	5.44	1.45	1.35

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Κ	173	HIS	CA-CB-CG	16.70	141.98	113.60
1	Е	177	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	М	183	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	D	116	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	Ν	196	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	Е	39	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	Е	196	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	L	112	PRO	CA-N-CD	9.58	125.11	111.70
1	Κ	195	GLU	CA-CB-CG	9.45	134.18	113.40
1	В	356	TRP	CD1-CG-CD2	9.32	113.76	106.30
1	Κ	173	HIS	ND1-CG-CD2	-9.22	93.09	106.00
1	М	39	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	М	79	TRP	CD1-CG-CD2	9.09	113.58	106.30
1	Н	116	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	Ε	196	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	Е	39	ARG	NE-CZ-NH2	-9.04	115.78	120.30



1

М

356

TRP

Mol	Chain	Res	Type	Atoms	Ζ	Observed(^o)	Ideal(°)
1	Ι	28	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	N	116	ARG	NE-CZ-NH2	8.89	124.74	120.30
1	K	79	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	A	356	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	K	28	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	В	356	TRP	CE2-CD2-CG	-8.71	100.34	107.30
1	Е	177	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	L	79	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	Н	356	TRP	CD1-CG-CD2	8.52	113.12	106.30
1	М	86	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	Н	86	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	D	356	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	С	356	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	Е	86	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	Н	356	TRP	CE2-CD2-CG	-8.45	100.54	107.30
1	N	79	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	В	79	TRP	CD1-CG-CD2	8.43	113.05	106.30
1	Е	79	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	М	79	TRP	CE2-CD2-CG	-8.42	100.57	107.30
1	N	79	TRP	CE2-CD2-CG	-8.40	100.58	107.30
1	D	177	ARG	NE-CZ-NH1	-8.40	116.10	120.30
1	С	79	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	Н	79	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	F	356	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	J	79	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	J	356	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	М	37	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	K	86	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	D	356	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	Ν	356	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	С	86	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	K	356	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	G	335	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	G	86	TRP	CD1-CG-CD2	8.21	112.86	106.30
1	G	356	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	J	86	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	А	79	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	В	79	TRP	$CE2-CD2-C\overline{G}$	-8.14	100.79	107.30
1	K	340	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	Ι	79	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	L	356	TRP	CE2-CD2-CG	-8.11	100.81	107.30

Continued from previous page...

Continued on next page...

106.30

112.77



8.09

CD1-CG-CD2

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Е	340	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	F	86	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	Е	356	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	N	340	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	М	28	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	Ι	356	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	А	356	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	Н	79	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	G	356	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	А	340	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	K	39	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	А	79	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	С	356	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	F	177	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	М	356	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	L	356	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	D	340	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	G	79	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	Е	356	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	K	177	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	Е	79	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	G	340	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	L	86	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	М	340	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Н	340	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	Н	86	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	J	340	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	J	86	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	F	79	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	Н	340	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	J	340	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	В	28	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	Κ	79	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	J	356	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	С	79	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	В	340	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	Ι	340	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	В	340	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	E	86	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	D	86	TRP	CD1-CG-CD2	7.66	112.42	106.30
1	G	79	TRP	CE2-CD2-CG	-7.66	101.18	107.30
1	F	356	TRP	CE2-CD2-CG	-7.65	101.18	107.30



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	F	79	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	D	340	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	L	112	PRO	N-CA-C	7.59	131.83	112.10
1	L	79	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	В	86	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	J	79	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	С	340	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	Κ	356	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	Ι	340	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	С	86	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	L	340	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	Ν	340	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	Е	218	TYR	CB-CG-CD1	-7.46	116.53	121.00
1	Κ	86	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	М	340	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	Κ	340	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	L	340	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	А	340	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	L	72	GLU	CA-C-N	-7.41	100.91	117.20
1	Ι	356	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	Е	340	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	С	335	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	G	86	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	С	340	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	А	86	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	G	340	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	D	254	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	Κ	183	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	L	62	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	F	86	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	D	86	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	Ι	79	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	Ν	86	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	М	86	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	D	147	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	D	79	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	D	79	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	Ι	86	TRP	CD1-CG-CD2	7.14	112.02	106.30
1	F	116	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	D	206	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	Н	356	TRP	$CG-\overline{CD2}-\overline{CE3}$	7.05	$1\overline{40.25}$	133.90
1	G	62	ARG	NE-CZ-NH2	7.05	123.83	120.30



Conti	nued fron	i previ	ous page				
\mathbf{Mol}	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$ $ Ideal(o)
1	Ν	356	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	Ν	39	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	L	112	PRO	CA-C-N	-7.02	101.75	117.20
1	L	86	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	В	86	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	Н	356	TRP	CB-CG-CD1	-6.95	117.96	127.00
1	N	86	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	А	290	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	N	28	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	А	183	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	K	173	HIS	CG-ND1-CE1	6.85	117.78	108.20
1	J	177	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	D	69	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	М	335	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	K	116	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	Н	177	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	F	340	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	F	196	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	Е	335	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	Е	188	TYR	CB-CG-CD2	-6.69	116.98	121.00
1	F	340	TRP	CD1-CG-CD2	6.69	111.66	106.30
1	L	244	ASP	CA-C-N	6.68	129.56	116.20
1	Ι	290	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	N	277	THR	CA-CB-CG2	6.65	121.70	112.40
1	А	62	ARG	O-C-N	-6.64	111.91	123.20
1	K	195	GLU	CB-CG-CD	6.60	132.01	114.20
1	Н	277	THR	N-CA-CB	-6.59	97.77	110.30
1	В	356	TRP	CG-CD2-CE3	6.56	139.80	133.90
1	В	356	TRP	CB-CG-CD1	-6.55	118.49	127.00
1	N	322	PRO	CA-N-CD	-6.54	102.35	111.50
1	J	356	TRP	CG-CD2-CE3	6.52	139.77	133.90
1	K	218	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	В	39	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	335	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	D	28	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	Е	183	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	В	169	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	L	290	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	N	183	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	А	335	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	N	322	PRO	N-CA-C	6.42	128.80	112.10

ARG

206

1

Е

1: α 1 C

Continued on next page...

120.30

123.50



6.41

NE-CZ-NH1

Continued from	n previous	page

Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	L	335	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	Ι	86	TRP	CE2-CD2-CG	-6.38	102.20	107.30
1	D	356	TRP	CB-CG-CD1	-6.34	118.76	127.00
1	С	177	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	А	62	ARG	CA-C-N	6.32	128.84	116.20
1	А	86	TRP	CE2-CD2-CG	-6.30	102.26	107.30
1	L	244	ASP	O-C-N	-6.30	112.49	123.20
1	В	196	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	D	356	TRP	CG-CD2-CE3	6.26	139.54	133.90
1	D	39	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	С	28	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	Ι	356	TRP	CB-CG-CD1	-6.21	118.93	127.00
1	J	177	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	М	37	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	G	356	TRP	CB-CG-CD1	-6.13	119.03	127.00
1	С	28	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	L	356	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	L	147	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	А	277	THR	CA-CB-CG2	6.09	120.93	112.40
1	D	198	TYR	CA-C-N	6.07	130.56	117.20
1	Ν	79	TRP	CG-CD2-CE3	6.07	139.36	133.90
1	G	356	TRP	CG-CD2-CE3	6.07	139.36	133.90
1	Κ	290	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	М	196	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	Н	277	THR	CA-CB-CG2	6.04	120.86	112.40
1	D	202	THR	N-CA-CB	6.03	121.76	110.30
1	J	28	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	K	206	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	В	79	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	Ι	147	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	В	356	TRP	CG-CD1-NE1	-5.97	104.13	110.10
1	D	218	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	N	290	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	В	290	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	K	303	THR	CA-CB-CG2	5.93	120.71	112.40
1	М	177	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	D	188	TYR	CB-CG-CD2	-5.91	117.46	121.00
1	I	356	TRP	CG-CD2-CE3	5.90	139.21	133.90
1	С	356	TRP	CG-CD2-CE3	5.87	139.19	133.90
1	G	155	SER	CA-C-N	-5.85	104.50	116.20
1	J	277	THR	CA-CB-CG2	5.85	120.59	112.40
1	G	290	ARG	NE-CZ-NH2	-5.83	117.39	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	N	303	THR	CA-CB-CG2	5.81	120.53	112.40
1	В	196	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	F	285	CYS	C-N-CA	5.79	136.16	121.70
1	N	147	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	K	244	ASP	N-CA-CB	-5.78	100.19	110.60
1	F	335	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	K	356	TRP	CB-CG-CD1	-5.75	119.53	127.00
1	М	79	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	G	177	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	J	356	TRP	CB-CG-CD1	-5.74	119.54	127.00
1	N	278	THR	CA-CB-CG2	5.73	120.42	112.40
1	D	198	TYR	O-C-N	-5.72	113.54	122.70
1	Е	356	TRP	CG-CD2-CE3	5.72	139.05	133.90
1	М	116	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	Ι	196	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	М	356	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	А	292	ASP	CB-CG-OD1	5.69	123.42	118.30
1	Н	303	THR	CA-CB-CG2	5.68	120.36	112.40
1	В	183	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	С	206	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	177	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	N	177	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	Ι	306	TYR	CB-CG-CD2	-5.62	117.62	121.00
1	В	303	THR	CA-CB-CG2	5.62	120.27	112.40
1	G	120	THR	CA-CB-OG1	-5.62	97.20	109.00
1	С	196	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	K	242	LEU	CA-CB-CG	5.61	128.20	115.30
1	L	116	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	265	SER	N-CA-CB	5.60	118.90	110.50
1	Ν	53	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	Ν	177	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	L	196	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	Н	79	TRP	CG-CD2-CE3	5.55	138.89	133.90
1	K	79	TRP	CG-CD1-NE1	-5.53	104.58	110.10
1	Ε	267	ILE	CA-C-N	5.52	127.25	116.20
1	J	340	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	K	177	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	L	356	TRP	$CB-CG-\overline{CD1}$	-5.50	$119.8\overline{5}$	127.00
1	E	$\overline{79}$	TRP	CG-CD2-CE3	$5.\overline{49}$	138.84	133.90
1	D	277	THR	CA-CB-CG2	5.42	119.98	112.40
1	J	$21\overline{0}$	ARG	CA-CB-CG	$5.4\overline{2}$	$125.3\overline{2}$	113.40
1	L	372	ARG	NE-CZ-NH2	-5.41	117.59	120.30



Continued from previous page...

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	С	303	THR	CA-CB-CG2	5.38	119.94	112.40
1	F	79	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	D	340	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	J	69	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	Ι	256	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	Κ	340	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	Е	169	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	Κ	340	TRP	CB-CG-CD1	-5.34	120.06	127.00
1	Ν	306	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	J	62	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	М	210	ARG	CA-CB-CG	5.32	125.10	113.40
1	А	340	TRP	CB-CG-CD1	-5.32	120.09	127.00
1	D	53	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	G	169	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	D	340	TRP	CB-CG-CD1	-5.30	120.10	127.00
1	F	282	ILE	CA-C-N	5.30	128.87	117.20
1	Ι	116	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	М	66	THR	CA-C-N	-5.30	105.54	117.20
1	L	340	TRP	CB-CG-CD1	-5.30	120.11	127.00
1	С	356	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	L	147	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	K	62	ARG	CA-CB-CG	5.27	124.98	113.40
1	В	340	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	L	290	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	J	72	GLU	CA-C-N	-5.26	105.63	117.20
1	Κ	356	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	G	222	ASP	N-CA-CB	5.25	120.06	110.60
1	D	202	THR	CA-CB-CG2	5.25	119.75	112.40
1	М	196	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	303	THR	CA-CB-CG2	5.25	119.74	112.40
1	F	306	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	L	79	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	N	79	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	K	39	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	Н	79	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	Н	120	THR	CA-CB-OG1	-5.23	98.01	109.00
1	E	100	GLU	N-CA-CB	-5.22	101.19	110.60
1	М	79	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	G	79	TRP	CG-CD2-CE3	5.22	138.59	133.90
1	Ι	335	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	А	177	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	Ι	177	ARG	NE-CZ-NH1	-5.18	117.71	120.30



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	G	173	HIS	CA-CB-CG	5.17	122.39	113.60
1	N	37	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	А	79	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	G	254	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	Ι	39	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	В	340	TRP	CG-CD2-CE3	5.15	138.54	133.90
1	М	178	LEU	CA-CB-CG	5.15	127.15	115.30
1	Ν	39	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	Ν	356	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	М	86	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	J	37	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	А	79	TRP	CG-CD2-CE3	5.14	138.52	133.90
1	K	340	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	В	306	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	G	147	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	Н	86	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	С	340	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	М	356	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	Ι	356	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	Н	340	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	K	86	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	Е	222	ASP	N-CA-CB	5.10	119.78	110.60
1	А	356	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	Ι	340	TRP	CG-CD2-CE3	5.09	138.48	133.90
1	М	312	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	Ν	197	GLY	CA-C-N	-5.08	106.03	117.20
1	Ι	62	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	Ν	275	HIS	CA-CB-CG	5.08	122.23	113.60
1	Ν	356	TRP	CG-CD1-NE1	-5.08	105.03	110.10
1	С	169	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	D	53	TYR	CA-CB-CG	5.07	123.04	113.40
1	А	62	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	С	198	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	Ε	356	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	Ε	86	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	Е	79	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	E	100	GLU	CA-CB-CG	5.05	124.50	113.40
1	E	237	GLU	N-CA-C	5.04	124.61	111.00
1	L	79	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	С	356	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	K	62	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	G	86	TRP	CG-CD1-NE1	-5.03	105.07	110.10



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	J	79	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	С	340	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	J	340	TRP	CB-CG-CD1	-5.02	120.47	127.00
1	Κ	62	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	F	356	TRP	CB-CG-CD1	-5.02	120.48	127.00
1	F	183	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	Ι	340	TRP	CB-CG-CD1	-5.01	120.48	127.00
1	D	79	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	188	TYR	Sidechain
1	А	210	ARG	Sidechain
1	А	269	MET	Peptide
1	А	290	ARG	Sidechain
1	А	337	TYR	Sidechain
1	А	37	ARG	Sidechain
1	А	62	ARG	Sidechain
1	А	91	TYR	Sidechain
1	В	116	ARG	Sidechain
1	В	133	TYR	Sidechain
1	В	147	ARG	Sidechain
1	В	169	TYR	Sidechain
1	В	206	ARG	Sidechain
1	В	272	ALA	Peptide
1	В	28	ARG	Sidechain
1	В	285	CYS	Peptide
1	В	37	ARG	Sidechain
1	В	53	TYR	Sidechain
1	В	62	ARG	Sidechain
1	С	166	TYR	Sidechain
1	С	206	ARG	Sidechain
1	С	256	ARG	Sidechain
1	С	279	TYR	Sidechain
1	С	290	ARG	Sidechain
1	С	303	THR	Peptide
1	С	53	TYR	Sidechain
1	D	116	ARG	Sidechain
1	D	169	TYR	Sidechain
1	D	196	ARG	Sidechain



	j = j	- P	F = J	
Mol	Chain	Res	Type	Group
1	D	198	TYR	Sidechain
1	D	206	ARG	Sidechain
1	D	233	SER	Peptide
1	D	337	TYR	Sidechain
1	D	37	ARG	Sidechain
1	D	53	TYR	Sidechain
1	D	60	SER	Peptide
1	D	65	LEU	Peptide
1	Е	111	ASN	Peptide
1	Е	147	ARG	Sidechain
1	Е	188	TYR	Sidechain
1	Е	198	TYR	Sidechain
1	Е	232	SER	Peptide
1	Е	290	ARG	Sidechain
1	Е	337	TYR	Sidechain
1	Е	362	TYR	Sidechain
1	Е	39	ARG	Sidechain
1	Е	62	ARG	Sidechain
1	F	233	SER	Peptide
1	F	240	TYR	Sidechain
1	F	280	ASN	Peptide
1	F	281	SER	Peptide
1	F	282	ILE	Peptide
1	F	37	ARG	Sidechain
1	F	44	MET	Peptide
1	F	91	TYR	Sidechain
1	G	198	TYR	Sidechain
1	G	337	TYR	Sidechain
1	G	91	TYR	Sidechain
1	Н	116	ARG	Sidechain
1	Н	143	TYR	Sidechain
1	Н	147	ARG	Sidechain
1	Н	335	ARG	Sidechain
1	Н	337	TYR	Sidechain
1	Н	62	ARG	Sidechain
1	Ι	116	ARG	Sidechain
1	Ι	147	ARG	Sidechain
1	Ι	166	TYR	Sidechain
1	Ι	197	GLY	Peptide
1	Ι	252	ASN	Peptide
1	Ι	335	ARG	Sidechain
1	Ι	337	TYR	Sidechain



Mol	Chain	Res	Type	Group
1	Ι	37	ARG	Sidechain
1	Ι	53	TYR	Sidechain
1	J	111	ASN	Peptide
1	J	196	ARG	Sidechain
1	J	202	THR	Peptide
1	J	205	GLU	Peptide
1	J	206	ARG	Sidechain
1	J	272	ALA	Peptide
1	J	290	ARG	Sidechain
1	J	306	TYR	Sidechain
1	Κ	116	ARG	Sidechain
1	K	147	ARG	Sidechain
1	K	166	TYR	Sidechain
1	K	206	ARG	Sidechain
1	K	218	TYR	Sidechain
1	K	240	TYR	Sidechain
1	К	290	ARG	Sidechain
1	K	303	THR	Peptide
1	K	337	TYR	Sidechain
1	K	37	ARG	Sidechain
1	К	53	TYR	Sidechain
1	K	91	TYR	Sidechain
1	L	116	ARG	Sidechain
1	L	169	TYR	Sidechain
1	L	179	ASP	Peptide
1	L	239	SER	Peptide
1	L	284	LYS	Peptide
1	L	289	ILE	Peptide
1	L	303	THR	Peptide
1	L	322	PRO	Peptide
1	L	337	TYR	Sidechain
1	L	39	ARG	Sidechain
1	L	53	TYR	Sidechain
1	L	62	ARG	Sidechain
1	L	65	LEU	Peptide
1	М	147	ARG	Sidechain
1	М	272	ALA	Peptide
1	М	337	TYR	Sidechain
1	М	39	ARG	Sidechain
1	М	53	TYR	Sidechain
1	М	62	ARG	Sidechain
1	М	91	TYR	Sidechain

Continued from previous page...



Mol	Chain	Res	Type	Group
1	Ν	143	TYR	Sidechain
1	Ν	147	ARG	Sidechain
1	Ν	196	ARG	Sidechain
1	Ν	254	ARG	Sidechain
1	N	275	HIS	Sidechain
1	Ν	306	TYR	Sidechain
1	Ν	37	ARG	Sidechain
1	Ν	53	TYR	Sidechain
1	Ν	62	ARG	Sidechain
1	N	91	TYR	Sidechain

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	2933	0	2894	113	0
1	В	2933	0	2894	110	0
1	С	2933	0	2894	98	0
1	D	2933	0	2894	241	0
1	Е	2933	0	2894	109	0
1	F	2933	0	2894	270	0
1	G	2933	0	2894	67	0
1	Н	2933	0	2894	85	0
1	Ι	2933	0	2894	76	0
1	J	2933	0	2894	105	0
1	K	2933	0	2894	120	0
1	L	2933	0	2894	114	0
1	М	2933	0	2894	69	0
1	Ν	2933	0	2894	82	0
All	All	41062	0	40516	1305	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 16.

All (1305) 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:D:44:MET:CG	1:F:293:LEU:CD2	1.79	1.58
1:J:266:PHE:CZ	1:J:266:PHE:CE2	1.95	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CE1	1.94	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CG	1.95	1.52
1:J:266:PHE:CZ	1:J:266:PHE:CE1	1.95	1.51
1:J:266:PHE:CE2	1:J:266:PHE:CD2	1.95	1.51
1:D:44:MET:CG	1:F:293:LEU:HD21	1.06	1.50
1:J:266:PHE:CG	1:J:266:PHE:CD2	1.96	1.49
1:D:44:MET:SD	1:F:293:LEU:CD1	2.01	1.49
1:D:61:LYS:NZ	1:F:291:LYS:HD2	1.19	1.41
1:D:43:VAL:CB	1:F:166:TYR:HD1	1.34	1.39
1:L:112:PRO:N	1:L:112:PRO:CA	1.83	1.39
1:A:62:ARG:HH21	1:C:287:ILE:CD1	1.33	1.39
1:D:57:GLU:OE1	1:F:291:LYS:HE3	1.24	1.38
1:L:112:PRO:N	1:L:112:PRO:CD	1.88	1.35
1:A:62:ARG:NH2	1:C:287:ILE:HD11	1.37	1.34
1:D:65:LEU:N	1:F:287:ILE:HD11	1.39	1.33
1:D:64:ILE:C	1:F:287:ILE:HD11	1.45	1.32
1:B:64:ILE:CG2	1:C:267:ILE:HB	1.59	1.31
1:D:44:MET:HG3	1:F:293:LEU:CD2	1.45	1.31
1:D:61:LYS:NZ	1:F:291:LYS:CD	1.91	1.31
1:F:45:VAL:HG21	1:H:166:TYR:CE1	1.64	1.31
1:D:44:MET:SD	1:F:293:LEU:HD11	1.62	1.31
1:B:64:ILE:HG23	1:C:267:ILE:CB	1.63	1.26
1:L:112:PRO:CG	1:L:112:PRO:CB	2.12	1.25
1:L:112:PRO:CA	1:L:112:PRO:CB	2.13	1.25
1:A:62:ARG:HD2	1:C:287:ILE:CD1	1.68	1.23
1:D:43:VAL:HB	1:F:166:TYR:CD1	1.73	1.22
1:D:43:VAL:CB	1:F:166:TYR:CD1	2.25	1.18
1:D:65:LEU:N	1:F:287:ILE:CD1	2.06	1.18
1:L:112:PRO:CD	1:L:112:PRO:CG	2.22	1.18
1:F:45:VAL:CG2	1:H:166:TYR:CE1	2.24	1.18
1:D:44:MET:HG3	1:F:293:LEU:HD22	1.23	1.16
1:F:45:VAL:HA	1:H:167:GLU:CB	1.78	1.13
1:D:43:VAL:CG1	1:F:166:TYR:HD1	1.62	1.13
1:D:44:MET:SD	1:F:293:LEU:HD13	1.74	1.12
1:D:57:GLU:OE1	1:F:291:LYS:CE	1.97	1.12
1:F:45:VAL:HA	1:H:167:GLU:HB2	1.23	1.12
1:F:45:VAL:HG11	1:H:166:TYR:CE1	1.83	1.12
1:D:44:MET:HG2	1:F:293:LEU:CD2	1.56	1.11
1:D:65:LEU:HD23	1:F:287:ILE:HG13	1.22	1.10
1:B:50:LYS:HD3	1:B:53:TYR:OH	1.52	1.10



EMD-1088, 3B	5U
--------------	----

	Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:F:45:VAL:CG1	1:H:166:TYR:CE1	2.35	1.09
1:A:62:ARG:HD2	1:C:287:ILE:HD13	1.30	1.09
1:D:43:VAL:HG12	1:F:166:TYR:CD1	1.87	1.09
1:E:267:ILE:HD12	1:F:287:ILE:O	1.53	1.08
1:F:45:VAL:HG11	1:H:166:TYR:CZ	1.89	1.08
1:A:243:PRO:O	1:C:323:SER:N	1.86	1.08
1:D:43:VAL:HB	1:F:166:TYR:HD1	1.09	1.06
1:D:43:VAL:CG1	1:F:166:TYR:CD1	2.37	1.05
1:F:45:VAL:CG2	1:H:166:TYR:CD1	2.41	1.04
1:J:266:PHE:CZ	1:K:173:HIS:CG	2.46	1.02
1:J:266:PHE:CD1	1:K:173:HIS:CG	2.48	1.02
1:J:266:PHE:CE1	1:K:173:HIS:CG	2.47	1.02
1:J:266:PHE:CE2	1:K:173:HIS:CG	2.47	1.02
1:J:266:PHE:CG	1:K:173:HIS:CG	2.48	1.01
1:J:266:PHE:CD2	1:K:173:HIS:CG	2.48	1.00
1:D:45:VAL:HA	1:F:165:ILE:O	1.63	0.99
1:E:112:PRO:HB2	1:E:115:ASN:HB3	1.44	0.99
1:F:45:VAL:HG21	1:H:166:TYR:CD1	1.97	0.99
1:D:57:GLU:CD	1:F:291:LYS:HE3	1.85	0.97
1:F:45:VAL:CG1	1:H:166:TYR:CZ	2.50	0.95
1:D:64:ILE:HD11	1:F:286:ASP:HA	1.47	0.93
1:D:43:VAL:HG11	1:F:169:TYR:HD1	1.32	0.93
1:J:266:PHE:CD2	1:K:173:HIS:CB	2.52	0.92
1:D:64:ILE:HG13	1:F:287:ILE:HG12	1.49	0.92
1:D:45:VAL:HG13	1:F:165:ILE:HB	1.51	0.92
1:B:45:VAL:HG21	1:D:289:ILE:HD13	1.50	0.91
1:D:45:VAL:HG22	1:F:164:PRO:HA	1.52	0.91
1:F:45:VAL:HG11	1:H:166:TYR:OH	1.68	0.91
1:J:266:PHE:CG	1:K:173:HIS:CB	2.53	0.91
1:D:61:LYS:HZ2	1:F:291:LYS:CD	1.65	0.91
1:J:266:PHE:CE2	1:K:173:HIS:CB	2.54	0.91
1:J:266:PHE:CE1	1:K:173:HIS:CB	2.54	0.91
1:F:45:VAL:HG22	1:H:166:TYR:CD1	2.05	0.90
1:J:266:PHE:CZ	1:K:173:HIS:CB	2.55	0.90
1:D:61:LYS:HZ1	1:F:291:LYS:CD	1.76	0.89
1:F:45:VAL:HG21	1:H:166:TYR:HE1	1.12	0.89
1:J:266:PHE:CD2	1:K:173:HIS:HB2	2.06	0.89
1:J:266:PHE:CD1	1:K:173:HIS:CB	2.54	0.89
1:D:64:ILE:CA	1:F:287:ILE:HD11	2.02	0.89
1:K:192:ILE:HA	1:L:112:PRO:HG3	1.54	0.88
1:B:39:ARG:HD3	1:B:66:THR:HG23	1.55	0.87



EMD-1088,	3B5U
-----------	------

	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:45:VAL:HG13	1:D:171:LEU:HB2	1.56	0.87
1:D:45:VAL:HG11	1:F:142:LEU:HD13	1.56	0.87
1:D:64:ILE:CD1	1:F:286:ASP:HA	2.05	0.87
1:D:65:LEU:H	1:F:287:ILE:CD1	1.84	0.87
1:A:357:ILE:HG13	1:A:370:VAL:HG22	1.55	0.86
1:D:44:MET:CE	1:F:293:LEU:HD13	2.06	0.86
1:D:43:VAL:HA	1:F:166:TYR:CE1	2.10	0.86
1:D:44:MET:O	1:F:165:ILE:N	2.09	0.85
1:K:195:GLU:CB	1:L:112:PRO:N	2.39	0.85
1:E:267:ILE:HG23	1:F:290:ARG:HB2	1.59	0.85
1:B:63:GLY:HA3	1:C:267:ILE:HA	1.58	0.84
1:N:102:PRO:HB3	1:N:131:ALA:HB3	1.58	0.84
1:F:154:ASP:HB3	1:F:161:HIS:HB2	1.59	0.84
1:J:266:PHE:CD1	1:K:173:HIS:HB3	2.12	0.84
1:B:102:PRO:HB3	1:B:131:ALA:HB3	1.59	0.84
1:L:160:THR:HB	1:L:178:LEU:HB3	1.59	0.83
1:A:62:ARG:CD	1:C:287:ILE:CD1	2.54	0.83
1:A:62:ARG:HG3	1:C:286:ASP:HB2	1.58	0.83
1:D:44:MET:HB2	1:F:289:ILE:CG2	2.10	0.82
1:A:243:PRO:HB2	1:C:322:PRO:HB2	1.62	0.82
1:K:195:GLU:CG	1:L:112:PRO:N	2.43	0.82
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.62	0.81
1:A:257:CYS:SG	1:A:258:PRO:HD3	2.20	0.81
1:J:19:ALA:HB3	1:J:29:ALA:HB3	1.61	0.81
1:D:61:LYS:HZ3	1:F:291:LYS:HD2	1.40	0.81
1:K:195:GLU:CG	1:L:112:PRO:CA	2.59	0.81
1:C:160:THR:HB	1:C:178:LEU:HB2	1.62	0.81
1:K:195:GLU:CB	1:L:112:PRO:CD	2.59	0.81
1:B:63:GLY:H	1:C:268:GLY:H	1.25	0.81
1:A:62:ARG:HD2	1:C:287:ILE:HD11	1.64	0.80
1:D:47:MET:O	1:F:166:TYR:HD2	1.65	0.79
1:E:267:ILE:CD1	1:F:287:ILE:O	2.30	0.79
1:K:195:GLU:CG	1:L:112:PRO:CD	2.61	0.79
1:E:267:ILE:CG2	1:F:290:ARG:HB2	2.14	0.78
1:G:257:CYS:SG	1:G:258:PRO:HD3	2.24	0.78
1:H:164:PRO:HG3	1:H:174:ALA:HB3	1.64	0.78
1:L:19:ALA:HB3	1:L:29:ALA:HB3	1.65	0.78
1:D:64:ILE:N	1:F:287:ILE:HD13	1.99	0.77
1:N:36:GLY:HA2	1:N:66:THR:HB	1.64	0.77
1:D:64:ILE:N	1:F:287:ILE:CD1	2.48	0.77
1:D:65:LEU:H	1:F:287:ILE:HD12	1.49	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:44:MET:SD	1:F:293:LEU:CD2	2.71	0.77
1:K:195:GLU:CB	1:L:112:PRO:CA	2.62	0.77
1:D:47:MET:O	1:F:166:TYR:CD2	2.38	0.77
1:D:43:VAL:CA	1:F:166:TYR:CD1	2.69	0.76
1:F:45:VAL:HG13	1:H:167:GLU:HG2	1.68	0.76
1:M:160:THR:HB	1:M:178:LEU:HB2	1.68	0.76
1:E:206:ARG:HG3	1:F:264:PRO:HB2	1.68	0.75
1:D:44:MET:CG	1:F:293:LEU:HD22	1.90	0.75
1:B:63:GLY:N	1:C:268:GLY:H	1.84	0.75
1:A:38:PRO:HA	1:A:65:LEU:HA	1.67	0.75
1:B:45:VAL:HG22	1:D:171:LEU:HD12	1.68	0.75
1:A:62:ARG:NH2	1:C:287:ILE:CD1	2.18	0.75
1:A:62:ARG:HH21	1:C:287:ILE:HD11	0.61	0.75
1:B:257:CYS:SG	1:B:258:PRO:HD3	2.26	0.75
1:C:200:PHE:HB3	1:C:206:ARG:HG2	1.69	0.74
1:K:195:GLU:CG	1:L:112:PRO:CG	2.64	0.74
1:D:65:LEU:N	1:F:287:ILE:HD12	2.03	0.74
1:F:163:VAL:HG13	1:F:175:ILE:HG12	1.68	0.74
1:B:63:GLY:CA	1:C:267:ILE:HA	2.17	0.74
1:D:257:CYS:SG	1:D:258:PRO:HD3	2.28	0.74
1:H:257:CYS:SG	1:H:258:PRO:HD3	2.27	0.74
1:N:19:ALA:HB3	1:N:29:ALA:HB3	1.69	0.74
1:C:19:ALA:HB3	1:C:29:ALA:HB3	1.70	0.73
1:B:164:PRO:HG2	1:B:171:LEU:HB3	1.69	0.73
1:F:45:VAL:CA	1:H:167:GLU:HB2	2.12	0.73
1:G:267:ILE:CD1	1:H:169:TYR:OH	2.37	0.73
1:D:43:VAL:HA	1:F:166:TYR:CD1	2.23	0.73
1:K:195:GLU:CG	1:L:112:PRO:CB	2.67	0.73
1:K:195:GLU:CB	1:L:112:PRO:CG	2.66	0.73
1:K:195:GLU:CB	1:L:112:PRO:CB	2.67	0.73
1:A:62:ARG:CZ	1:C:287:ILE:HD11	2.17	0.73
1:F:195:GLU:HA	1:G:172:PRO:HB2	1.71	0.72
1:D:43:VAL:CA	1:F:166:TYR:HD1	2.02	0.72
1:F:36:GLY:HA3	1:F:65:LEU:HD13	1.71	0.72
1:B:160:THR:HB	1:B:178:LEU:HB3	1.71	0.72
1:H:357:ILE:HG13	1:H:370:VAL:HG22	1.71	0.72
1:D:64:ILE:HG13	1:F:287:ILE:CG1	2.20	0.72
1:L:357:ILE:HG13	1:L:370:VAL:HG22	1.72	0.72
1:C:257:CYS:SG	1:C:258:PRO:HD3	2.29	0.71
1:D:45:VAL:HB	1:F:150:GLY:H	1.55	0.71
1:D:61:LYS:HZ1	1:F:291:LYS:HB3	1.54	0.71



	Interatomic	Clash
Atom-1 Atom-2	distance (\AA)	α overlap (Å)
1.D.101.LVS.HE2 1.E.172.PBO.HC2	1 72	$\frac{0.71}{0.71}$
1.B.60.SEB.O 1.D.287.ILE.HG21	1.12	0.71
1.B.163.VAL.HG22 1.B.175.ILE.HG23	1.51	0.71
1.D.47.MET.O 1.F.167.GLU.HG2	1.12	0.71
1:M:102:PRO:HB3 1:M:131:ALA:HB3	1.51	0.71
$1 \cdot N \cdot 24 \cdot ASP \cdot HB2 = 1 \cdot N \cdot 340 \cdot TBP \cdot HH2$	1.10	0.71
1:B:38:PBO:HA 1:B:65:LEU:HA	1.04	0.71
$1 \cdot L \cdot 244 \cdot \Delta SP \cdot HB2 = 1 \cdot L \cdot 245 \cdot CLV \cdot H\Delta2$	1.73	0.71
1.E.244.RSF.IID2 1.E.246.GL1.III22	2 20	0.71
1.1.257 CVS SG 1.1.258 PBO HD3	2.20	0.71
$1 \cdot E \cdot 100 \cdot SEB \cdot HB2 = 1 \cdot E \cdot 170 \cdot \Delta SP \cdot HB2$	1 72	0.71
1.1.135.5EI(.1122 1.1.115.K51.11122 1.1.266.PHE:CG 1.K.173.HIS.HB3	2.26	0.70
1.D.61.LVS.HZ2 1.F.201.LVS.HD2	0.77	0.70
$1 \cdot D \cdot 65 \cdot L E U \cdot C D 2 \qquad 1 \cdot F \cdot 287 \cdot I L E \cdot H G 21$	2 21	0.70
1.E.183.ABC.HC3 1.F.270.CLU.HC2	1 73	0.70
$1 \cdot \Delta \cdot 174 \cdot \Delta I \cdot \Delta \cdot H \Delta = 1 \cdot \Delta \cdot 284 \cdot I \cdot VS \cdot HE2$	1.73	0.70
1.A.174.ALA.HA = 1.A.204.L15.HE2 $1.F.10.\Delta L\Delta \cdot HB3 = 1.F.20.\Delta L\Delta \cdot HB3$	1.75	0.70
1.F.29.ALA.IID9 1.K.101.IVS.HF2 1.I.110.I FU.HD22	1.74	0.70
1.R.191.D15.HB2 1.D.110.DE0.HD22	2 9 99	0.70
1.D.39.ARG.IID3 1.D.00.11Rt.CG2	2.22	0.70
1.D.61.III5.INZ 1.F.231.III5.IID3	2.00	0.03
1.1.2.04.112.0 1.1.2.01.112.0D1 1.1.201.41.4.4.4 1.N.287.11.E.0D1	1 75	0.09
1.E.204.ALA.IIA 1.N.201.ILE.IID12 1.E.257.CVS.SC 1.E.258.PBO.HD3	0.30	0.09
1.E.251.015.5G 1.E.256.110.11D5	1 73	0.03
1.I. 100.MET.HA 1.I. 200.VAL.HC11	1.75	0.09
1.D.130.MET.HA 1.E.203.VAL.HG11 1.D.44.MET.HF1 1.F.203.LEU.HD13	1.74	0.03
1.D.44.WILLIND1 1.1.235.LD0.HD15	2.06	0.09
1.N.265.SFR.HA 1.N.270.CI U.HA	1.74	0.09
$1 \cdot \Lambda \cdot 62 \cdot \Lambda BC \cdot HC3 = 1 \cdot C \cdot 286 \cdot \Lambda SP \cdot CB$	2.74	0.05
1.1.02.111(3.11(3) = 1.0.200.1151.0D 1.0.285.0VS:SC	2.22	0.09
1.D.202.HE.HR 1.L.75.ILE.HG12	1 75	0.09
1.N.160.THR.HB 1.N.178.LEU.HB2	1.75	0.09
1·D·197·GLV·HA2 1·E·112·PRO·HA	1.70	0.09
1:H·285:CVS·HB3 1:H·280·ILE·HD11	1.72	0.00
1.11.200.015.11D0 1.11.200.11D11 1.1.1.80.LEU.HD11 1.1.200.11D1	1.70	0.68
1.K.264.PRO.HR2 1.K.271.SER.HR3	1.75	0.00
1:D:58:ALA:O 1:D:62:ABC:HB3	1.10	0.00
$1 \cdot J \cdot 266 \cdot PHE \cdot CD2$ $1 \cdot K \cdot 173 \cdot HIS \cdot CD2$	2.82	0.68
1·F·213·LYS·HA 1·F·217·CVS·SC	2.02	0.68
1.D.45.VAL.HG13 1.F.165.ILE.CR	2.04	0.67
1:D:53:TYR:HB2 1:F:288:ASP:OD1	1.93	0.67



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:64:ILE:CA	1:F:287:ILE:CD1	2.70	0.67
1:F:163:VAL:HG22	1:F:175:ILE:HG23	1.76	0.67
1:D:65:LEU:HD23	1:F:287:ILE:CG1	2.14	0.67
1:F:45:VAL:HG11	1:H:166:TYR:HE1	1.54	0.67
1:J:160:THR:HB	1:J:178:LEU:HB2	1.76	0.67
1:D:49:GLN:N	1:F:166:TYR:CD2	2.62	0.67
1:D:44:MET:HB2	1:F:289:ILE:HG21	1.76	0.67
1:I:191:LYS:HE2	1:J:172:PRO:HB2	1.77	0.67
1:L:242:LEU:HB2	1:L:245:GLY:HA3	1.76	0.67
1:L:300:SER:HA	1:L:335:ARG:HB2	1.77	0.67
1:D:57:GLU:CD	1:F:291:LYS:CE	2.54	0.66
1:I:19:ALA:HB3	1:I:29:ALA:HB3	1.76	0.66
1:J:193:LEU:HA	1:J:196:ARG:HB3	1.77	0.66
1:L:36:GLY:HA3	1:L:65:LEU:HD13	1.77	0.66
1:L:257:CYS:SG	1:L:258:PRO:HD3	2.35	0.66
1:M:9:VAL:HG21	1:M:344:SER:HA	1.78	0.66
1:D:43:VAL:HA	1:F:166:TYR:HE1	1.57	0.66
1:E:210:ARG:HB2	1:F:269:MET:SD	2.36	0.66
1:G:286:ASP:HB3	1:G:289:ILE:HG12	1.77	0.66
1:N:266:PHE:HB3	1:N:269:MET:SD	2.35	0.66
1:D:45:VAL:HG13	1:F:165:ILE:CD1	2.24	0.66
1:I:180:LEU:HD11	1:I:264:PRO:HB3	1.76	0.66
1:D:201:VAL:HB	1:E:177:ARG:HB3	1.76	0.66
1:B:64:ILE:HD13	1:C:267:ILE:HD12	1.76	0.66
1:F:45:VAL:HG13	1:H:166:TYR:CZ	2.31	0.66
1:N:106:THR:HG22	1:N:140:LEU:HD12	1.78	0.66
1:F:160:THR:HB	1:F:178:LEU:HB3	1.77	0.65
1:I:189:LEU:HA	1:I:192:ILE:HG12	1.78	0.65
1:D:102:PRO:HB3	1:D:131:ALA:HB3	1.78	0.65
1:E:10:CYS:SG	1:E:89:THR:HG21	2.37	0.65
1:F:45:VAL:CG1	1:H:166:TYR:OH	2.39	0.65
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.79	0.65
1:E:116:ARG:NH2	1:E:374:CYS:SG	2.70	0.65
1:F:257:CYS:SG	1:F:258:PRO:HD3	2.37	0.65
1:G:7:ALA:HA	1:G:102:PRO:HG2	1.79	0.65
1:I:102:PRO:HB3	1:I:131:ALA:HB3	1.79	0.65
1:K:357:ILE:HG13	1:K:370:VAL:HG22	1.78	0.65
1:A:243:PRO:HB2	1:C:322:PRO:CB	2.27	0.65
1:F:46:GLY:H	1:H:167:GLU:HB3	1.62	0.64
1:F:45:VAL:CB	1:H:166:TYR:CE1	2.80	0.64
1:D:43:VAL:HG11	1:F:166:TYR:HB2	1.78	0.64



EMD-1088, 3	3B5U
-------------	------

	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:44:MET:HB2	1:F:289:ILE:HG22	1.79	0.64
1:D:213:LYS:HA	1:D:217:CYS:SG	2.37	0.64
1:K:244:ASP:HB3	1:M:287:ILE:O	1.98	0.64
1:L:111:ASN:C	1:L:112:PRO:CA	2.64	0.64
1:B:213:LYS:HA	1:B:217:CYS:SG	2.38	0.64
1:D:65:LEU:HD21	1:F:287:ILE:HG21	1.79	0.64
1:N:257:CYS:SG	1:N:258:PRO:HD3	2.38	0.64
1:B:45:VAL:HB	1:D:166:TYR:HB3	1.79	0.64
1:D:57:GLU:OE2	1:F:291:LYS:CE	2.46	0.64
1:F:45:VAL:CA	1:H:167:GLU:CB	2.68	0.64
1:I:164:PRO:HG3	1:I:174:ALA:HB3	1.79	0.64
1:N:155:SER:HA	1:N:160:THR:HA	1.80	0.64
1:G:213:LYS:HA	1:G:217:CYS:SG	2.38	0.63
1:M:10:CYS:SG	1:M:89:THR:HG21	2.37	0.63
1:A:137:GLN:HG2	1:A:339:VAL:HG11	1.80	0.63
1:C:245:GLY:H	1:E:325:MET:HB2	1.63	0.63
1:C:267:ILE:HG21	1:D:284:LYS:HG3	1.80	0.63
1:J:266:PHE:CE1	1:K:173:HIS:ND1	2.66	0.63
1:K:160:THR:HB	1:K:178:LEU:HB2	1.80	0.63
1:E:357:ILE:HG21	1:E:370:VAL:HG22	1.79	0.63
1:M:257:CYS:SG	1:M:258:PRO:HD3	2.38	0.63
1:N:162:ASN:OD1	1:N:277:THR:HG23	1.99	0.63
1:B:109:PRO:HA	1:B:136:ILE:HG23	1.80	0.63
1:D:43:VAL:HG11	1:F:169:TYR:CD1	2.23	0.63
1:D:44:MET:HG2	1:F:293:LEU:HD21	0.64	0.63
1:F:45:VAL:C	1:H:167:GLU:HG3	2.19	0.63
1:K:164:PRO:HG2	1:K:171:LEU:HB2	1.81	0.63
1:L:289:ILE:HA	1:L:291:LYS:HG2	1.81	0.62
1:N:66:THR:HG22	1:N:68:LYS:HG2	1.80	0.62
1:E:160:THR:HB	1:E:178:LEU:HB2	1.81	0.62
1:N:357:ILE:HG13	1:N:370:VAL:HG22	1.81	0.62
1:G:9:VAL:HG21	1:G:344:SER:HA	1.80	0.62
1:N:200:PHE:HA	1:N:205:GLU:HB3	1.82	0.62
1:B:60:SER:OG	1:D:287:ILE:HD13	1.99	0.62
1:D:197:GLY:HA2	1:E:113:LYS:H	1.64	0.62
1:E:62:ARG:HH21	1:E:62:ARG:HB2	1.65	0.62
1:D:45:VAL:CG1	1:F:165:ILE:CD1	2.78	0.62
1:D:160:THR:HB	1:D:178:LEU:HB3	1.82	0.62
1:1:242:LEU:HD11	1:1:248:1LE:HD13	1.80	0.62
1:K:205:GLU:HG2	1:M:287:ILE:HG13	1.82	0.62
1:D:36:GLY:HA3	1:D:65:LEU:HD22	1.81	0.62



EMD-1088, 3	3B5U
-------------	------

	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:160:THR:HB	1:H:178:LEU:HB2	1.81	0.62
1:D:298:VAL:HG22	1:D:330:ILE:HB	1.82	0.62
1:B:63:GLY:HA3	1:C:268:GLY:N	2.15	0.62
1:A:10:CYS:HB3	1:A:105:LEU:HD23	1.80	0.61
1:A:153:LEU:HD21	1:A:274:ILE:HG23	1.81	0.61
1:C:178:LEU:HD11	1:C:277:THR:HG21	1.81	0.61
1:N:103:THR:O	1:N:132:MET:HA	2.00	0.61
1:C:328:LYS:HZ1	1:C:330:ILE:HG12	1.63	0.61
1:D:47:MET:C	1:F:167:GLU:HG2	2.21	0.61
1:A:36:GLY:HA2	1:A:66:THR:O	2.00	0.61
1:D:61:LYS:HZ1	1:F:291:LYS:HD3	1.58	0.61
1:E:287:ILE:HD12	1:E:287:ILE:H	1.65	0.61
1:J:153:LEU:HA	1:J:161:HIS:O	2.00	0.61
1:N:189:LEU:HD13	1:N:257:CYS:SG	2.40	0.61
1:F:45:VAL:HA	1:H:167:GLU:HB3	1.78	0.61
1:D:44:MET:HE2	1:F:293:LEU:HD22	1.82	0.61
1:F:45:VAL:CG2	1:H:166:TYR:HE1	1.83	0.61
1:F:46:GLY:N	1:H:167:GLU:HG3	2.15	0.61
1:I:63:GLY:HA3	1:J:268:GLY:H	1.66	0.61
1:J:105:LEU:HB2	1:J:134:VAL:HG12	1.82	0.61
1:D:65:LEU:CD2	1:F:287:ILE:HG13	2.14	0.61
1:F:248:ILE:HG23	1:F:250:ILE:HD11	1.81	0.61
1:D:43:VAL:CG1	1:F:169:TYR:HD1	2.08	0.61
1:J:266:PHE:CZ	1:K:173:HIS:ND1	2.68	0.61
1:E:265:SER:HB3	1:F:285:CYS:HA	1.81	0.61
1:F:45:VAL:HG13	1:H:166:TYR:CE1	2.33	0.60
1:L:189:LEU:HA	1:L:192:ILE:HG12	1.83	0.60
1:D:170:ALA:HB1	1:D:175:ILE:HD11	1.83	0.60
1:J:205:GLU:HA	1:L:288:ASP:HB2	1.82	0.60
1:M:34:ILE:HG21	1:M:67:LEU:HB3	1.83	0.60
1:C:203:THR:HG21	1:D:267:ILE:HG23	1.84	0.60
1:D:57:GLU:OE2	1:F:291:LYS:HD2	2.02	0.60
1:K:63:GLY:HA3	1:L:267:ILE:HA	1.83	0.60
1:C:9:VAL:HG21	1:C:344:SER:HA	1.83	0.60
1:J:266:PHE:HE1	1:K:171:LEU:HB3	1.66	0.60
1:L:305:MET:SD	1:L:336:LYS:HB3	2.42	0.60
1:E:189:LEU:HD13	1:E:257:CYS:SG	2.42	0.60
1:K:164:PRO:HG3	1:K:174:ALA:HB3	1.84	0.60
1:A:32:PRO:HB2	1:A:34:ILE:HG12	1.84	0.60
1:A:189:LEU:HD13	1:A:257:CYS:SG	2.42	0.60
1:D:120:THR:HG21	1:D:370:VAL:HG21	1.82	0.60


Continued from pretious page		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:205:GLU:HB3	1:L:289:ILE:H	1.66	0.60
1:L:164:PRO:HG2	1:L:171:LEU:HB2	1.83	0.60
1:C:11:ASP:HB3	1:C:18:LYS:HB2	1.84	0.60
1:B:63:GLY:CA	1:C:268:GLY:H	2.14	0.60
1:G:170:ALA:O	1:G:172:PRO:HD3	2.01	0.60
1:I:9:VAL:HG21	1:I:344:SER:HA	1.84	0.60
1:K:32:PRO:HB2	1:K:34:ILE:HG12	1.83	0.60
1:M:282:ILE:HG12	1:M:293:LEU:HD23	1.83	0.60
1:A:160:THR:HB	1:A:178:LEU:HB3	1.84	0.60
1:K:10:CYS:HA	1:K:18:LYS:O	2.02	0.60
1:J:266:PHE:CE2	1:K:173:HIS:HB2	2.37	0.59
1:C:357:ILE:HG21	1:C:370:VAL:HG22	1.84	0.59
1:E:213:LYS:HA	1:E:217:CYS:SG	2.42	0.59
1:J:266:PHE:CG	1:K:173:HIS:CD2	2.90	0.59
1:L:155:SER:HA	1:L:160:THR:HA	1.84	0.59
1:H:190:MET:SD	1:H:209:VAL:HG21	2.42	0.59
1:J:266:PHE:CE1	1:K:171:LEU:HB3	2.37	0.59
1:D:44:MET:SD	1:F:293:LEU:CG	2.87	0.59
1:C:86:TRP:HH2	1:C:119:MET:HG2	1.68	0.59
1:B:63:GLY:HA3	1:C:267:ILE:CA	2.31	0.59
1:C:328:LYS:NZ	1:C:330:ILE:HG12	2.18	0.59
1:E:207:GLU:HB3	1:F:269:MET:H	1.68	0.59
1:L:219:VAL:HG22	1:L:258:PRO:HB3	1.84	0.59
1:A:103:THR:O	1:A:132:MET:HA	2.03	0.59
1:A:203:THR:OG1	1:C:287:ILE:HG23	2.03	0.58
1:E:250:ILE:HG23	1:E:253:GLU:HB2	1.85	0.58
1:F:70:PRO:HG3	1:F:85:ILE:HD12	1.85	0.58
1:J:203:THR:HB	1:K:268:GLY:HA3	1.85	0.58
1:K:195:GLU:HG2	1:L:112:PRO:CG	2.33	0.58
1:D:47:MET:HA	1:F:167:GLU:OE2	2.03	0.58
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.84	0.58
1:K:153:LEU:HD21	1:K:274:ILE:HG23	1.85	0.58
1:A:53:TYR:CZ	1:A:61:LYS:CD	2.86	0.58
1:E:164:PRO:HG2	1:E:171:LEU:HB2	1.85	0.58
1:G:189:LEU:HD12	1:G:192:ILE:HD11	1.85	0.58
1:D:64:ILE:HG13	1:F:287:ILE:CD1	2.34	0.58
1:A:19:ALA:HB3	1:A:29:ALA:HB3	1.84	0.58
1:J:7:ALA:HA	1:J:102:PRO:HG2	1.86	0.58
1:E:10:CYS:HB3	1:E:105:LEU:HD23	1.85	0.58
1:I:153:LEU:HA	1:I:161:HIS:O	2.03	0.58
1:J:120:THR:HG21	1:J:370:VAL:HG21	1.86	0.58



EMD-1088,	3B5U
-----------	------

Continued from precious page			Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:J:219:VAL:HG21	1:J:309:ILE:HB	1.86	0.58
1:D:38:PRO:HB3	1:D:64:ILE:HD12	1.86	0.58
1:A:53:TYR:CZ	1:A:61:LYS:HD2	2.39	0.58
1:I:240:TYR:HB3	1:I:248:ILE:HG22	1.85	0.58
1:C:205:GLU:N	1:E:287:ILE:HD13	2.19	0.57
1:D:44:MET:O	1:F:165:ILE:C	2.42	0.57
1:D:48:GLY:C	1:F:166:TYR:CE2	2.78	0.57
1:I:286:ASP:O	1:I:290:ARG:HG3	2.04	0.57
1:C:207:GLU:O	1:C:210:ARG:HB2	2.04	0.57
1:G:109:PRO:HA	1:G:136:ILE:HG23	1.85	0.57
1:A:153:LEU:HA	1:A:161:HIS:O	2.05	0.57
1:J:213:LYS:HA	1:J:217:CYS:SG	2.45	0.57
1:L:213:LYS:HA	1:L:217:CYS:SG	2.43	0.57
1:B:194:THR:HG22	1:B:198:TYR:O	2.04	0.57
1:D:33:SER:O	1:D:70:PRO:HD2	2.04	0.57
1:D:61:LYS:HZ1	1:F:291:LYS:CB	2.16	0.57
1:I:164:PRO:HG2	1:I:171:LEU:HB2	1.85	0.57
1:I:98:PRO:HB2	1:I:129:VAL:HG12	1.87	0.57
1:E:19:ALA:HB3	1:E:29:ALA:HB3	1.85	0.57
1:G:160:THR:HB	1:G:178:LEU:HB3	1.86	0.57
1:M:151:ILE:HB	1:M:293:LEU:HG	1.86	0.57
1:A:165:ILE:HG12	1:A:170:ALA:HA	1.87	0.57
1:D:194:THR:HG22	1:D:198:TYR:H	1.70	0.57
1:F:9:VAL:HG21	1:F:344:SER:HA	1.85	0.57
1:K:62:ARG:HG3	1:K:67:LEU:HD11	1.87	0.57
1:K:195:GLU:HB3	1:L:112:PRO:N	2.19	0.57
1:B:165:ILE:HA	1:B:170:ALA:HA	1.86	0.57
1:C:163:VAL:HG22	1:C:175:ILE:HG23	1.87	0.57
1:E:268:GLY:H	1:F:290:ARG:HE	1.51	0.57
1:K:195:GLU:HG3	1:L:112:PRO:CA	2.35	0.57
1:B:63:GLY:HA3	1:C:268:GLY:H	1.70	0.56
1:G:10:CYS:HA	1:G:18:LYS:O	2.04	0.56
1:A:9:VAL:HG21	1:A:344:SER:HA	1.86	0.56
1:A:37:ARG:O	1:A:66:THR:N	2.37	0.56
1:D:359:LYS:HD2	1:D:360:GLN:HB2	1.87	0.56
1:J:9:VAL:HG21	1:J:344:SER:HA	1.87	0.56
1:L:330:ILE:O	1:L:332:PRO:HD3	2.05	0.56
1:N:213:LYS:HA	1:N:217:CYS:SG	2.45	0.56
1:D:44:MET:CG	1:F:293:LEU:CG	2.77	0.56
1:K:153:LEU:HA	1:K:161:HIS:O	2.05	0.56
1:E:153:LEU:HA	1:E:161:HIS:O	2.06	0.56



EMD-1088, 3	3B5U
-------------	------

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:142:LEU:HG	1:G:147:ARG:HB2	1.87	0.56
1:B:286:ASP:HB3	1:B:289:ILE:HD11	1.88	0.56
1:K:188:TYR:HE2	1:K:257:CYS:HA	1.71	0.56
1:L:75:ILE:HD11	1:L:177:ARG:HH22	1.70	0.56
1:N:135:ALA:HB3	1:N:140:LEU:HD11	1.88	0.56
1:A:98:PRO:HB2	1:A:127:PHE:O	2.06	0.56
1:A:152:VAL:O	1:A:162:ASN:HA	2.06	0.55
1:A:262:PHE:O	1:A:275:HIS:HE1	1.88	0.55
1:B:104:LEU:HG	1:B:133:TYR:HB3	1.89	0.55
1:J:359:LYS:HD2	1:J:360:GLN:HB2	1.87	0.55
1:K:286:ASP:O	1:K:290:ARG:HG3	2.07	0.55
1:A:252:ASN:H	1:A:252:ASN:ND2	2.04	0.55
1:E:190:MET:SD	1:F:272:ALA:HB3	2.47	0.55
1:G:148:THR:HB	1:G:167:GLU:HA	1.88	0.55
1:I:103:THR:O	1:I:132:MET:HA	2.06	0.55
1:K:213:LYS:HD3	1:K:214:GLU:HG3	1.89	0.55
1:L:369:ILE:HA	1:L:372:ARG:HB2	1.89	0.55
1:E:198:TYR:CZ	1:E:248:ILE:HA	2.41	0.55
1:G:242:LEU:HG	1:G:243:PRO:HD2	1.87	0.55
1:I:10:CYS:HB3	1:I:105:LEU:HD23	1.89	0.55
1:J:164:PRO:HG2	1:J:171:LEU:HB2	1.87	0.55
1:B:63:GLY:HA3	1:C:266:PHE:O	2.07	0.55
1:J:303:THR:HG23	1:J:306:TYR:HE2	1.72	0.55
1:G:44:MET:HB2	1:G:47:MET:HB2	1.89	0.55
1:H:359:LYS:HD2	1:H:360:GLN:HB2	1.86	0.55
1:L:280:ASN:HA	1:L:283:MET:HB3	1.87	0.55
1:B:300:SER:HA	1:B:335:ARG:HB2	1.88	0.55
1:C:244:ASP:HB3	1:E:287:ILE:HG23	1.88	0.55
1:F:7:ALA:HA	1:F:102:PRO:HG2	1.89	0.55
1:B:238:LYS:HE3	1:B:238:LYS:HA	1.88	0.55
1:H:162:ASN:OD1	1:H:277:THR:HG23	2.07	0.55
1:I:32:PRO:HB2	1:I:34:ILE:HG12	1.89	0.55
1:D:7:ALA:HA	1:D:102:PRO:HG2	1.89	0.55
1:D:46:GLY:HA2	1:F:149:THR:HG23	1.89	0.55
1:C:7:ALA:HA	1:C:102:PRO:HG2	1.88	0.54
1:D:45:VAL:HG11	1:F:142:LEU:CD1	2.34	0.54
1:F:188:TYR:HA	1:F:191:LYS:HD3	1.88	0.54
1:L:32:PRO:HB2	1:L:34:ILE:HG12	1.88	0.54
1:D:44:MET:CE	1:F:293:LEU:HD22	2.38	0.54
1:K:106:THR:HG22	1:K:140:LEU:HD12	1.89	0.54
1:L:64:ILE:HG13	1:L:65:LEU:HG	1.89	0.54



Interstomic Clash			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:148:THR:HB	1:A:167:GLU:HA	1.90	0.54
1:D:357:ILE:HG21	1:D:370:VAL:HG22	1.88	0.54
1:E:153:LEU:HD21	1:E:274:ILE:HD12	1.89	0.54
1:I:190:MET:SD	1:I:209:VAL:HG21	2.48	0.54
1:J:98:PRO:HB2	1:J:129:VAL:HG12	1.88	0.54
1:M:103:THR:O	1:M:132:MET:HA	2.07	0.54
1:N:330:ILE:O	1:N:332:PRO:HD3	2.08	0.54
1:F:140:LEU:HD22	1:F:343:GLY:HA2	1.89	0.54
1:D:43:VAL:HG21	1:F:169:TYR:O	2.07	0.54
1:G:10:CYS:HB3	1:G:105:LEU:HD23	1.90	0.54
1:C:189:LEU:HD13	1:C:257:CYS:SG	2.48	0.54
1:D:61:LYS:HA	1:E:268:GLY:HA2	1.89	0.54
1:E:190:MET:HA	1:E:209:VAL:HG11	1.90	0.54
1:F:161:HIS:HA	1:F:176:MET:O	2.08	0.54
1:J:162:ASN:O	1:J:175:ILE:HA	2.07	0.54
1:K:162:ASN:OD1	1:K:277:THR:HG23	2.06	0.54
1:B:103:THR:O	1:B:132:MET:HA	2.07	0.54
1:D:62:ARG:O	1:E:270:GLU:HA	2.08	0.54
1:A:203:THR:OG1	1:C:287:ILE:CG2	2.56	0.54
1:A:304:THR:O	1:A:309:ILE:HG21	2.07	0.54
1:F:304:THR:O	1:F:309:ILE:HG21	2.07	0.54
1:K:330:ILE:O	1:K:332:PRO:HD3	2.08	0.54
1:N:98:PRO:HB2	1:N:127:PHE:O	2.08	0.54
1:N:190:MET:O	1:N:194:THR:HG23	2.08	0.54
1:D:44:MET:HG2	1:F:293:LEU:CG	2.32	0.54
1:D:203:THR:HG21	1:E:269:MET:HA	1.90	0.54
1:E:304:THR:HA	1:E:309:ILE:HD13	1.90	0.54
1:H:162:ASN:O	1:H:175:ILE:HA	2.08	0.54
1:B:162:ASN:O	1:B:175:ILE:HA	2.08	0.54
1:D:57:GLU:OE2	1:F:291:LYS:HE3	2.04	0.54
1:M:109:PRO:HA	1:M:136:ILE:HG23	1.90	0.54
1:A:114:ALA:HA	1:A:117:GLU:HB2	1.88	0.53
1:C:305:MET:SD	1:C:336:LYS:HD3	2.49	0.53
1:G:359:LYS:HD2	1:G:360:GLN:HB2	1.89	0.53
1:A:299:MET:SD	1:A:313:MET:HG3	2.48	0.53
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.90	0.53
1:B:330:ILE:O	1:B:332:PRO:HD3	2.08	0.53
1:H:163:VAL:HG22	1:H:175:ILE:HG23	1.91	0.53
1:K:197:GLY:O	1:L:77:THR:HA	2.08	0.53
1:D:239:SER:HA	1:D:248:ILE:O	2.07	0.53
1:E:180:LEU:HD21	1:F:283:MET:HG2	1.90	0.53



EMD-1088,	3B5U
-----------	------

	Interatomic		Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:F:359:LYS:HD2	1:F:360:GLN:HB2	1.90	0.53	
1:N:300:SER:HA	1:N:335:ARG:HB2	1.90	0.53	
1:A:186:THR:HG21	1:A:210:ARG:HB3	1.91	0.53	
1:D:43:VAL:HG22	1:F:171:LEU:HG	1.89	0.53	
1:D:45:VAL:CA	1:F:165:ILE:O	2.49	0.53	
1:K:19:ALA:HB3	1:K:29:ALA:HB3	1.91	0.53	
1:D:188:TYR:HE2	1:D:257:CYS:HA	1.73	0.53	
1:E:148:THR:HB	1:E:167:GLU:HA	1.89	0.53	
1:G:163:VAL:HA	1:G:175:ILE:HG12	1.90	0.53	
1:K:272:ALA:HB1	1:K:276:GLU:HB2	1.91	0.53	
1:E:238:LYS:HE3	1:E:238:LYS:HA	1.90	0.53	
1:E:266:PHE:CZ	1:F:282:ILE:HA	2.44	0.53	
1:K:100:GLU:HG3	1:K:101:HIS:CD2	2.44	0.53	
1:D:43:VAL:CG1	1:F:166:TYR:HB2	2.38	0.53	
1:K:359:LYS:HD2	1:K:360:GLN:N	2.24	0.53	
1:L:39:ARG:HE	1:M:263:GLN:HG2	1.73	0.53	
1:I:216:LEU:HB3	1:I:254:ARG:HG3	1.91	0.53	
1:A:7:ALA:HA	1:A:102:PRO:HG2	1.91	0.53	
1:F:193:LEU:HB3	1:F:200:PHE:HE1	1.73	0.53	
1:F:290:ARG:HD2	1:F:294:TYR:HE2	1.73	0.53	
1:I:100:GLU:HG2	1:I:101:HIS:CD2	2.44	0.53	
1:I:185:LEU:HD21	1:I:261:LEU:HB2	1.91	0.53	
1:A:22:ALA:HB1	1:A:348:SER:HB2	1.91	0.52	
1:B:359:LYS:HD2	1:B:360:GLN:N	2.24	0.52	
1:D:359:LYS:HD2	1:D:360:GLN:N	2.24	0.52	
1:A:243:PRO:O	1:C:322:PRO:C	2.47	0.52	
1:D:45:VAL:CG1	1:F:142:LEU:HD13	2.35	0.52	
1:J:15:GLY:O	1:J:32:PRO:HA	2.10	0.52	
1:J:240:TYR:HB3	1:J:248:ILE:HG22	1.91	0.52	
1:A:312:ARG:O	1:A:316:GLU:HB2	2.09	0.52	
1:D:45:VAL:CG2	1:F:164:PRO:HA	2.32	0.52	
1:K:305:MET:SD	1:K:336:LYS:HB3	2.49	0.52	
1:L:9:VAL:HG21	1:L:344:SER:HA	1.92	0.52	
1:M:7:ALA:HB3	1:M:22:ALA:HB2	1.92	0.52	
1:D:45:VAL:HG22	1:F:165:ILE:H	1.73	0.52	
1:D:57:GLU:OE1	1:F:291:LYS:HE2	2.02	0.52	
1:D:153:LEU:HD21	1:D:274:ILE:HG23	1.91	0.52	
1:I:200:PHE:HA	1:I:205:GLU:HB3	1.91	0.52	
1:N:58:ALA:HB1	1:N:65:LEU:HD11	1.91	0.52	
1:N:70:PRO:HG2	1:N:71:ILE:HG13	1.91	0.52	
1:N:159:VAL:HA	1:N:178:LEU:O	2.10	0.52	



EMD-1088,	3B5U
-----------	------

Interatomic Clash			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:164:PRO:HG3	1:E:174:ALA:HB3	1.90	0.52
1:H:39:ARG:HD3	1:H:66:THR:HG23	1.91	0.52
1:C:44:MET:HB2	1:C:47:MET:HB2	1.91	0.52
1:D:42:GLY:HA3	1:F:285:CYS:CB	2.40	0.52
1:F:359:LYS:HD2	1:F:360:GLN:N	2.24	0.52
1:G:162:ASN:O	1:G:175:ILE:HA	2.10	0.52
1:I:61:LYS:HE3	1:K:166:TYR:HE1	1.75	0.52
1:L:296:ASN:HA	1:L:330:ILE:HD11	1.91	0.52
1:C:296:ASN:HA	1:C:330:ILE:HD11	1.91	0.52
1:D:45:VAL:CG1	1:F:165:ILE:HD13	2.39	0.52
1:I:210:ARG:HB3	1:I:210:ARG:CZ	2.39	0.52
1:J:284:LYS:HB2	1:J:284:LYS:HZ3	1.74	0.52
1:A:53:TYR:CE2	1:A:61:LYS:HD2	2.44	0.52
1:B:64:ILE:HG23	1:C:267:ILE:CG1	2.38	0.52
1:A:9:VAL:O	1:A:19:ALA:HA	2.10	0.52
1:F:238:LYS:HE3	1:F:238:LYS:HA	1.92	0.52
1:G:8:LEU:HG	1:G:101:HIS:HB3	1.92	0.52
1:G:106:THR:HG21	1:G:339:VAL:HG12	1.92	0.52
1:L:40:HIS:HE1	1:M:263:GLN:O	1.93	0.52
1:A:53:TYR:HD2	1:A:57:GLU:HB3	1.75	0.52
1:A:65:LEU:HB2	1:B:267:ILE:HD12	1.92	0.52
1:A:261:LEU:HG	1:A:274:ILE:HG13	1.92	0.52
1:C:213:LYS:HA	1:C:217:CYS:SG	2.50	0.52
1:C:265:SER:OG	1:C:270:GLU:HA	2.10	0.52
1:B:105:LEU:O	1:B:134:VAL:HA	2.10	0.51
1:D:19:ALA:HB3	1:D:29:ALA:HB3	1.91	0.51
1:I:162:ASN:O	1:I:175:ILE:HA	2.10	0.51
1:K:359:LYS:HD2	1:K:360:GLN:HB2	1.91	0.51
1:N:355:MET:HA	1:N:373:LYS:HD3	1.92	0.51
1:A:53:TYR:CD2	1:A:57:GLU:HB3	2.45	0.51
1:A:104:LEU:HA	1:A:133:TYR:O	2.10	0.51
1:D:286:ASP:HB3	1:D:289:ILE:HG23	1.91	0.51
1:E:201:VAL:HG12	1:E:202:THR:HG23	1.93	0.51
1:K:15:GLY:O	1:K:32:PRO:HA	2.09	0.51
1:N:359:LYS:HD2	1:N:360:GLN:N	2.25	0.51
1:A:153:LEU:HD11	1:A:274:ILE:HD13	1.91	0.51
1:D:197:GLY:CA	1:E:112:PRO:HA	2.40	0.51
1:J:204:ALA:HA	1:J:207:GLU:HB2	1.92	0.51
1:D:45:VAL:HG22	1:F:165:ILE:N	2.26	0.51
1:I:194:THR:HB	1:J:110:LEU:HB3	1.93	0.51
1:A:136:ILE:HD12	1:A:136:ILE:H	1.75	0.51



EMD-1088,	3B5U
-----------	------

Interatomic Clash			Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
$1 \cdot C \cdot 162 \cdot ASN \cdot OD1$	1·C·277·THB·HG23	2.11	0.51
1:D:68:LYS:O	1:D:70:PRO:HD3	2.10	0.51
1.H.182.GLY.HA2	1·H·303·THB·OG1	2.10	0.51
1:H:359:LYS:HD2	1:H:360:GLN:N	2.26	0.51
1:K:192:ILE:HA	1:L:112:PRO:CG	2.34	0.51
1:B:349:LEU:HB3	1:B:352:PHE:HB2	1.91	0.51
1:D:238:LYS:HE3	1:D:238:LYS:HA	1.92	0.51
1:J:174:ALA:HA	1:J:284:LYS:HZ3	1.76	0.51
1:N:137:GLN:HG2	1:N:339:VAL:HG11	1.93	0.51
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.92	0.51
1:E:206:ARG:NH1	1:F:271:SER:O	2.43	0.51
1:N:294:TYR:HE1	1:N:321:ALA:HB1	1.75	0.51
1:D:45:VAL:HG13	1:F:165:ILE:HD12	1.92	0.51
1:D:48:GLY:C	1:F:166:TYR:CD2	2.84	0.51
1:F:191:LYS:HB3	1:G:173:HIS:HB2	1.93	0.51
1:H:11:ASP:O	1:H:17:VAL:HA	2.11	0.51
1:I:153:LEU:HD23	1:I:299:MET:HG2	1.92	0.51
1:I:160:THR:HB	1:I:178:LEU:HB3	1.93	0.51
1:A:359:LYS:HD2	1:A:360:GLN:HB2	1.92	0.51
1:D:45:VAL:CG1	1:F:165:ILE:HD12	2.40	0.51
1:D:49:GLN:HA	1:F:166:TYR:CZ	2.46	0.51
1:E:160:THR:O	1:E:177:ARG:HA	2.11	0.51
1:G:34:ILE:O	1:G:54:VAL:HA	2.11	0.51
1:I:163:VAL:HG22	1:I:175:ILE:HG23	1.93	0.51
1:L:359:LYS:HD2	1:L:360:GLN:HB2	1.93	0.51
1:B:357:ILE:HG13	1:B:370:VAL:HG22	1.93	0.51
1:E:359:LYS:HD2	1:E:360:GLN:HB2	1.93	0.51
1:A:238:LYS:HE3	1:A:238:LYS:HA	1.92	0.50
1:J:163:VAL:HG22	1:J:175:ILE:HG23	1.92	0.50
1:K:244:ASP:HB2	1:M:290:ARG:HB2	1.92	0.50
1:M:19:ALA:HB3	1:M:29:ALA:HB3	1.93	0.50
1:E:99:GLU:HB3	1:E:128:ASN:ND2	2.26	0.50
1:M:359:LYS:HD2	1:M:360:GLN:N	2.26	0.50
1:B:174:ALA:HB2	1:B:285:CYS:SG	2.51	0.50
1:L:322:PRO:O	1:L:325:MET:HG2	2.10	0.50
1:D:61:LYS:NZ	1:F:291:LYS:CG	2.72	0.50
1:D:182:GLY:HA2	1:D:303:THR:OG1	2.11	0.50
1:D:210:ARG:O	1:D:213:LYS:HB3	2.11	0.50
1:F:212:ILE:HG23	1:F:216:LEU:HD12	1.93	0.50
1:H:328:LYS:HZ1	1:H:330:ILE:HG13	1.76	0.50
1:E:106:THR:HG22	$1:\overline{\text{E:140:LEU:HD12}}$	1.93	0.50



EMD-1088,	3B5U
-----------	------

Continuea from pretious page		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:359:LYS:HD2	1:E:360:GLN:N	2.27	0.50
1:H:210:ARG:HH11	1:H:210:ARG:HB2	1.77	0.50
1:I:139:VAL:HA	1:I:165:ILE:HD13	1.93	0.50
1:D:64:ILE:HG12	1:F:285:CYS:O	2.11	0.50
1:F:45:VAL:HG22	1:H:166:TYR:CE1	2.27	0.50
1:D:305:MET:SD	1:D:336:LYS:HB3	2.51	0.50
1:F:193:LEU:HG	1:F:250:ILE:HD12	1.93	0.50
1:I:305:MET:SD	1:I:336:LYS:HB3	2.51	0.50
1:J:10:CYS:HA	1:J:18:LYS:O	2.12	0.50
1:J:100:GLU:HG2	1:J:101:HIS:CD2	2.46	0.50
1:J:332:PRO:HB2	1:J:335:ARG:HB3	1.92	0.50
1:K:162:ASN:HB2	1:K:176:MET:HB2	1.93	0.50
1:A:153:LEU:HD13	1:A:162:ASN:ND2	2.27	0.50
1:E:120:THR:HG21	1:E:370:VAL:HG21	1.94	0.50
1:F:174:ALA:HB2	1:F:284:LYS:HG2	1.93	0.50
1:G:267:ILE:HD13	1:H:169:TYR:OH	2.11	0.50
1:N:102:PRO:HD3	1:N:130:PRO:HG2	1.93	0.50
1:E:34:ILE:O	1:E:54:VAL:HA	2.12	0.50
1:G:166:TYR:HB2	1:G:289:ILE:HD13	1.94	0.50
1:M:37:ARG:HB3	1:M:38:PRO:CD	2.42	0.50
1:C:203:THR:HG22	1:C:206:ARG:NH2	2.27	0.49
1:G:151:ILE:HB	1:G:293:LEU:HG	1.94	0.49
1:L:292:ASP:HB3	1:L:296:ASN:HD22	1.76	0.49
1:L:312:ARG:HD2	1:L:315:LYS:HE3	1.94	0.49
1:E:213:LYS:HG3	1:E:306:TYR:OH	2.12	0.49
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.94	0.49
1:N:109:PRO:HA	1:N:136:ILE:HG23	1.93	0.49
1:B:11:ASP:HB3	1:B:18:LYS:HB2	1.95	0.49
1:C:359:LYS:HD2	1:C:360:GLN:HB2	1.93	0.49
1:D:64:ILE:H	1:F:287:ILE:HD13	1.75	0.49
1:H:36:GLY:HA3	1:H:65:LEU:HD13	1.93	0.49
1:J:263:GLN:HE21	1:J:263:GLN:HA	1.76	0.49
1:K:193:LEU:HB3	1:K:198:TYR:HB2	1.93	0.49
1:L:10:CYS:HA	1:L:18:LYS:O	2.12	0.49
1:M:283:MET:SD	1:M:290:ARG:NH2	2.85	0.49
1:I:104:LEU:HA	1:I:133:TYR:O	2.12	0.49
1:J:243:PRO:HD2	1:L:291:LYS:HD3	1.95	0.49
1:B:8:LEU:HA	1:B:21:PHE:HA	1.94	0.49
1:G:242:LEU:HD13	1:G:248:ILE:HD11	1.93	0.49
1:I:239:SER:HA	1:I:248:ILE:O	2.13	0.49
1:J:153:LEU:HD21	1:J:274:ILE:HD12	1.95	0.49



EMD-1088,	3B5U
-----------	------

Interstomic Clash			Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:L:193:LEU:HG	1:L:250:ILE:HD11	1.94	0.49
1:L:212:ILE:HG23	1:L:216:LEU:HD12	1.95	0.49
1:L:242:LEU:HD11	1:L:248:ILE:HD13	1.93	0.49
1:N:7:ALA:HA	1:N:102:PRO:HG2	1.94	0.49
1:N:282:ILE:HG22	1:N:290:ARG:HD2	1.94	0.49
1:B:19:ALA:HB3	1:B:29:ALA:HB3	1.95	0.49
1:D:43:VAL:CG1	1:F:169:TYR:CD1	2.91	0.49
1:D:44:MET:CG	1:F:293:LEU:HD11	2.39	0.49
1:L:210:ARG:O	1:L:213:LYS:HB3	2.12	0.49
1:A:10:CYS:HA	1:A:18:LYS:O	2.12	0.49
1:A:117:GLU:HB3	1:A:367:PRO:HB3	1.94	0.49
1:B:15:GLY:O	1:B:32:PRO:HA	2.12	0.49
1:E:200:PHE:H	1:F:180:LEU:HD22	1.77	0.49
1:K:195:GLU:HB2	1:L:112:PRO:CB	2.42	0.49
1:E:109:PRO:HA	1:E:136:ILE:HG23	1.93	0.49
1:F:46:GLY:N	1:H:167:GLU:CG	2.76	0.49
1:G:278:THR:HG21	1:G:297:ASN:OD1	2.12	0.49
1:I:252:ASN:HA	1:I:255:PHE:HE2	1.76	0.49
1:L:106:THR:HG22	1:L:140:LEU:HD12	1.95	0.49
1:L:204:ALA:HB1	1:N:287:ILE:HG23	1.94	0.49
1:N:299:MET:O	1:N:332:PRO:HD2	2.13	0.49
1:A:86:TRP:HH2	1:A:119:MET:HG2	1.78	0.49
1:B:205:GLU:O	1:B:208:ILE:HG12	2.13	0.49
1:D:61:LYS:HZ3	1:F:291:LYS:CD	2.06	0.49
1:D:240:TYR:HB3	1:D:248:ILE:HB	1.94	0.49
1:J:102:PRO:HA	1:J:131:ALA:O	2.12	0.49
1:K:203:THR:O	1:K:207:GLU:HB2	2.12	0.49
1:A:264:PRO:HD3	1:A:273:GLY:HA3	1.95	0.49
1:E:22:ALA:HB1	1:E:348:SER:HB2	1.95	0.49
1:F:290:ARG:HD2	1:F:294:TYR:CE2	2.48	0.49
1:I:155:SER:HA	1:I:160:THR:HA	1.94	0.49
1:K:217:CYS:HA	1:K:254:ARG:O	2.13	0.49
1:C:8:LEU:HG	1:C:101:HIS:HB3	1.94	0.48
1:F:74:GLY:O	1:F:108:ALA:HB2	2.12	0.48
1:G:186:THR:HG21	1:G:210:ARG:HG2	1.94	0.48
1:M:238:LYS:HE3	1:M:238:LYS:HA	1.95	0.48
1:N:59:GLN:OE1	1:N:62:ARG:NH1	2.46	0.48
1:N:242:LEU:HD22	1:N:246:GLN:HB3	1.94	0.48
1:B:64:ILE:HG23	1:C:267:ILE:HB	0.69	0.48
1:C:153:LEU:HD21	1:C:274:ILE:HG23	1.96	0.48
1:F:10:CYS:HA	1:F:18:LYS:O	2.13	0.48



EMD-1088,	3B5U
-----------	------

Continueu from prettous page		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:153:LEU:HA	1:L:161:HIS:O	2.13	0.48
1:M:114:ALA:HA	1:M:117:GLU:HB2	1.96	0.48
1:N:104:LEU:HG	1:N:133:TYR:HB3	1.94	0.48
1:N:140:LEU:O	1:N:342:GLY:HA3	2.13	0.48
1:B:60:SER:OG	1:D:287:ILE:CD1	2.61	0.48
1:B:137:GLN:HA	1:B:339:VAL:HG13	1.95	0.48
1:E:191:LYS:HA	1:E:194:THR:OG1	2.13	0.48
1:I:106:THR:HG22	1:I:140:LEU:HD12	1.95	0.48
1:I:189:LEU:HD13	1:I:257:CYS:SG	2.53	0.48
1:L:162:ASN:O	1:L:175:ILE:HA	2.13	0.48
1:L:299:MET:O	1:L:332:PRO:HD2	2.12	0.48
1:A:239:SER:HA	1:A:248:ILE:O	2.13	0.48
1:E:195:GLU:HA	1:F:177:ARG:HB3	1.96	0.48
1:B:43:VAL:HB	1:D:169:TYR:OH	2.13	0.48
1:D:106:THR:HG21	1:D:339:VAL:HG12	1.96	0.48
1:D:162:ASN:O	1:D:175:ILE:HA	2.14	0.48
1:G:32:PRO:HB2	1:G:34:ILE:HG12	1.94	0.48
1:K:162:ASN:O	1:K:175:ILE:HA	2.13	0.48
1:A:359:LYS:HD2	1:A:360:GLN:N	2.28	0.48
1:J:262:PHE:O	1:J:275:HIS:HE1	1.97	0.48
1:A:53:TYR:CZ	1:A:61:LYS:HD3	2.47	0.48
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.96	0.48
1:F:61:LYS:O	1:F:65:LEU:HG	2.14	0.48
1:F:119:MET:O	1:F:123:MET:HG2	2.13	0.48
1:G:12:ASN:HA	1:G:17:VAL:HG22	1.95	0.48
1:J:102:PRO:HB3	1:J:131:ALA:HB3	1.96	0.48
1:M:155:SER:HA	1:M:160:THR:HA	1.95	0.48
1:B:286:ASP:O	1:B:289:ILE:HG13	2.14	0.48
1:I:359:LYS:HD2	1:I:360:GLN:HB2	1.95	0.48
1:J:182:GLY:O	1:J:213:LYS:NZ	2.44	0.48
1:A:330:ILE:O	1:A:332:PRO:HD3	2.13	0.48
1:B:62:ARG:HG2	1:C:268:GLY:HA2	1.96	0.48
1:B:64:ILE:N	1:C:267:ILE:HA	2.29	0.48
1:D:45:VAL:HG11	1:F:165:ILE:HD13	1.95	0.48
1:E:191:LYS:O	1:F:176:MET:SD	2.72	0.48
1:I:238:LYS:O	1:I:249:THR:HA	2.14	0.48
1:J:10:CYS:HB3	1:J:105:LEU:HD23	1.96	0.48
1:J:205:GLU:HB2	1:L:286:ASP:HB3	1.96	0.48
1:L:39:ARG:NH2	1:M:264:PRO:HD2	2.29	0.48
1:M:164:PRO:HG3	1:M:174:ALA:HB3	1.96	0.48
1:G:267:ILE:HD11	1:H:169:TYR:OH	2.13	0.48



EMD-1088,	3B5U
-----------	------

Unterstomia Clash			
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:J:151:ILE:HD11	1:J:162:ASN:HB3	1.95	0.48
1:K:252:ASN:O	1:K:256:ARG:NH2	2.47	0.48
1:L:253:GLU:HA	1:L:256:ARG:HE	1.78	0.48
1:B:155:SER:HA	1:B:160:THR:HA	1.96	0.47
1:D:57:GLU:OE2	1:F:291:LYS:CD	2.61	0.47
1:D:164:PRO:HG3	1:D:285:CYS:SG	2.54	0.47
1:E:152:VAL:HA	1:E:298:VAL:HB	1.96	0.47
1:G:332:PRO:HB2	1:G:335:ARG:HB3	1.96	0.47
1:H:10:CYS:SG	1:H:89:THR:HG21	2.53	0.47
1:J:292:ASP:O	1:J:296:ASN:HB2	2.14	0.47
1:M:162:ASN:O	1:M:175:ILE:HA	2.14	0.47
1:N:152:VAL:O	1:N:162:ASN:HA	2.14	0.47
1:A:15:GLY:O	1:A:32:PRO:HA	2.14	0.47
1:B:11:ASP:O	1:B:17:VAL:HA	2.14	0.47
1:B:39:ARG:CD	1:B:66:THR:HG23	2.37	0.47
1:D:11:ASP:O	1:D:17:VAL:HA	2.14	0.47
1:D:45:VAL:CG1	1:F:142:LEU:CD1	2.92	0.47
1:D:197:GLY:HA3	1:D:198:TYR:HA	1.67	0.47
1:G:103:THR:O	1:G:132:MET:HA	2.13	0.47
1:J:44:MET:HB2	1:J:47:MET:HB2	1.97	0.47
1:K:152:VAL:O	1:K:162:ASN:HA	2.14	0.47
1:K:188:TYR:HA	1:K:191:LYS:HD3	1.95	0.47
1:L:39:ARG:HH21	1:M:264:PRO:HD2	1.79	0.47
1:A:135:ALA:HB3	1:A:140:LEU:HD11	1.97	0.47
1:B:250:ILE:HG23	1:B:253:GLU:HB2	1.96	0.47
1:D:298:VAL:HA	1:D:330:ILE:O	2.14	0.47
1:I:105:LEU:O	1:I:134:VAL:HA	2.14	0.47
1:N:9:VAL:HG21	1:N:344:SER:HA	1.97	0.47
1:D:15:GLY:O	1:D:32:PRO:HA	2.14	0.47
1:F:9:VAL:HG13	1:F:104:LEU:HD22	1.96	0.47
1:G:86:TRP:HH2	1:G:119:MET:HG3	1.79	0.47
1:K:11:ASP:HA	1:K:106:THR:OG1	2.15	0.47
1:K:198:TYR:CZ	1:K:248:ILE:HG13	2.48	0.47
1:L:359:LYS:HD2	1:L:360:GLN:N	2.28	0.47
1:E:62:ARG:HE	1:E:67:LEU:HD11	1.78	0.47
1:H:36:GLY:HA2	1:H:66:THR:O	2.15	0.47
1:H:99:GLU:HA	1:H:130:PRO:HD3	1.96	0.47
1:I:10:CYS:HA	1:I:18:LYS:O	2.15	0.47
1:I:118:LYS:NZ	1:I:121:GLN:OE1	2.47	0.47
1:J:8:LEU:HG	1:J:101:HIS:HB3	1.95	0.47
1:K:58:ALA:O	1:K:62:ARG:HB2	2.14	0.47



EMD-1088,	3B5U
-----------	------

Interstomic Clash			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:8:LEU:HG	1:L:101:HIS:HB3	1.96	0.47
1:M:152:VAL:O	1:M:162:ASN:HA	2.14	0.47
1:D:251:GLY:O	1:D:254:ARG:HG3	2.15	0.47
1:L:9:VAL:O	1:L:19:ALA:HA	2.15	0.47
1:A:286:ASP:O	1:A:290:ARG:HG3	2.15	0.47
1:D:64:ILE:CG1	1:F:286:ASP:HA	2.44	0.47
1:D:200:PHE:HZ	1:D:248:ILE:HG12	1.79	0.47
1:E:86:TRP:CH2	1:E:119:MET:HG3	2.50	0.47
1:E:287:ILE:HA	1:E:290:ARG:HB2	1.95	0.47
1:F:201:VAL:HG21	1:G:177:ARG:HD3	1.95	0.47
1:G:45:VAL:HG23	1:I:167:GLU:HB3	1.96	0.47
1:H:186:THR:OG1	1:H:213:LYS:HD2	2.14	0.47
1:I:109:PRO:HA	1:I:136:ILE:HG23	1.97	0.47
1:I:186:THR:HG23	1:I:213:LYS:HB2	1.94	0.47
1:L:63:GLY:O	1:M:270:GLU:HB2	2.15	0.47
1:L:304:THR:HA	1:L:309:ILE:HD13	1.95	0.47
1:N:71:ILE:HA	1:N:76:ILE:HA	1.96	0.47
1:N:105:LEU:O	1:N:134:VAL:HA	2.15	0.47
1:D:62:ARG:HG3	1:D:67:LEU:HD21	1.95	0.47
1:C:32:PRO:HG2	1:C:55:GLY:HA2	1.97	0.47
1:D:39:ARG:NH2	1:E:264:PRO:O	2.48	0.47
1:I:252:ASN:OD1	1:J:113:LYS:NZ	2.47	0.47
1:K:147:ARG:NH1	1:K:296:ASN:OD1	2.46	0.47
1:K:213:LYS:HA	1:K:217:CYS:SG	2.54	0.47
1:A:62:ARG:CD	1:C:287:ILE:HD11	2.34	0.47
1:F:136:ILE:HD12	1:F:136:ILE:H	1.80	0.47
1:F:369:ILE:O	1:F:373:LYS:HB2	2.14	0.47
1:G:19:ALA:HB3	1:G:29:ALA:HB3	1.96	0.47
1:G:32:PRO:HG2	1:G:55:GLY:HA2	1.97	0.47
1:G:45:VAL:HG21	1:I:167:GLU:OE1	2.14	0.47
1:G:263:GLN:HE21	1:G:263:GLN:HA	1.79	0.47
1:J:359:LYS:HD2	1:J:360:GLN:N	2.29	0.47
1:K:153:LEU:HD23	1:K:299:MET:HG2	1.96	0.47
1:K:239:SER:HA	1:K:248:ILE:O	2.15	0.47
1:L:192:ILE:HA	1:L:195:GLU:HB2	1.96	0.47
1:M:86:TRP:CH2	1:M:119:MET:HG3	2.49	0.47
1:A:162:ASN:OD1	1:A:277:THR:HG23	2.16	0.46
1:F:142:LEU:HD22	1:F:165:ILE:HD13	1.97	0.46
1:F:153:LEU:HA	1:F:161:HIS:O	2.15	0.46
1:H:36:GLY:O	1:H:52:SER:HA	2.15	0.46
1:K:188:TYR:CE2	1:K:257:CYS:HA	2.50	0.46



EMD-1088,	3B5U
-----------	------

Interstomic Clash			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:242:LEU:HD22	1:K:242:LEU:H	1.80	0.46
1:K:242:LEU:O	1:K:244:ASP:N	2.48	0.46
1:A:147:ARG:NH1	1:A:296:ASN:OD1	2.48	0.46
1:A:198:TYB:OH	1:A:248:ILE:HA	2.14	0.46
1:B:148:THR:HB	1:B:167:GLU:HA	1.98	0.46
1:E:9:VAL:HA	1:E:104:LEU:O	2.15	0.46
1:I:36:GLY:HA3	1:I:65:LEU:HD13	1.96	0.46
1:J:190:MET:HG3	1:J:200:PHE:CD1	2.50	0.46
1:E:206:ARG:HB2	1:F:265:SER:HA	1.98	0.46
1:F:152:VAL:O	1:F:162:ASN:HA	2.16	0.46
1:L:109:PRO:HA	1:L:136:ILE:HG23	1.96	0.46
1:L:353:GLN:HA	1:L:356:TRP:CD1	2.50	0.46
1:M:37:ARG:HB3	1:M:38:PRO:HD2	1.97	0.46
1:D:32:PRO:O	1:D:55:GLY:HA2	2.15	0.46
1:D:193:LEU:HB3	1:D:198:TYR:HB2	1.97	0.46
1:F:102:PRO:HB3	1:F:131:ALA:HB3	1.97	0.46
1:G:155:SER:HA	1:G:160:THR:HA	1.96	0.46
1:H:153:LEU:HD12	1:H:161:HIS:O	2.14	0.46
1:I:359:LYS:HD2	1:I:360:GLN:N	2.30	0.46
1:L:11:ASP:HA	1:L:106:THR:OG1	2.15	0.46
1:C:119:MET:O	1:C:123:MET:HG2	2.15	0.46
1:E:266:PHE:CE1	1:F:282:ILE:HA	2.51	0.46
1:F:182:GLY:O	1:F:213:LYS:NZ	2.48	0.46
1:M:104:LEU:HA	1:M:133:TYR:O	2.16	0.46
1:D:65:LEU:HG	1:F:287:ILE:HG21	1.98	0.46
1:D:104:LEU:HG	1:D:133:TYR:HB3	1.97	0.46
1:H:139:VAL:HG22	1:H:170:ALA:HB2	1.97	0.46
1:J:219:VAL:HG22	1:J:258:PRO:HB3	1.97	0.46
1:B:283:MET:SD	1:B:290:ARG:NH2	2.89	0.46
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.98	0.46
1:D:49:GLN:N	1:F:166:TYR:CE2	2.84	0.46
1:D:58:ALA:HB1	1:D:65:LEU:HD11	1.97	0.46
1:D:212:ILE:HG23	1:D:216:LEU:HD12	1.98	0.46
1:E:207:GLU:HB3	1:F:269:MET:N	2.31	0.46
1:F:11:ASP:HA	1:F:106:THR:OG1	2.16	0.46
1:G:330:ILE:O	1:G:332:PRO:HD3	2.15	0.46
1:L:186:THR:HG21	1:L:210:ARG:HG2	1.98	0.46
1:M:174:ALA:HB1	1:M:281:SER:O	2.15	0.46
1:B:209:VAL:HA	1:B:212:ILE:HD12	1.97	0.46
1:D:61:LYS:NZ	1:F:291:LYS:CB	2.76	0.46
1:G:196:ARG:NH2	1:G:249:THR:OG1	2.49	0.46



EMD-1088,	3B5U
-----------	------

	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:286:ASP:O	1:J:290:ARG:HG3	2.16	0.46
1:J:305:MET:SD	1:J:336:LYS:HB3	2.56	0.46
1:K:195:GLU:H	1:L:112:PRO:HD2	1.81	0.46
1:C:106:THR:HG22	1:C:140:LEU:HD12	1.98	0.46
1:E:267:ILE:HB	1:F:287:ILE:O	2.16	0.46
1:H:155:SER:HA	1:H:160:THR:HA	1.96	0.46
1:I:192:ILE:HB	1:I:253:GLU:HG3	1.97	0.46
1:B:124:PHE:HE1	1:B:359:LYS:HA	1.80	0.46
1:B:286:ASP:O	1:B:290:ARG:HG2	2.15	0.46
1:C:162:ASN:O	1:C:175:ILE:HA	2.16	0.46
1:D:61:LYS:CE	1:F:291:LYS:HB3	2.46	0.46
1:E:268:GLY:H	1:F:290:ARG:NE	2.13	0.46
1:J:119:MET:O	1:J:123:MET:HG2	2.16	0.46
1:B:359:LYS:HD2	1:B:360:GLN:HB2	1.98	0.45
1:D:197:GLY:HA2	1:E:113:LYS:N	2.31	0.45
1:G:359:LYS:HD2	1:G:360:GLN:N	2.31	0.45
1:I:220:ALA:O	1:I:312:ARG:HD3	2.15	0.45
1:K:9:VAL:HA	1:K:104:LEU:O	2.16	0.45
1:N:9:VAL:O	1:N:19:ALA:HA	2.16	0.45
1:N:210:ARG:CZ	1:N:210:ARG:HB3	2.46	0.45
1:A:100:GLU:HG3	1:A:101:HIS:CD2	2.51	0.45
1:B:36:GLY:HA2	1:B:66:THR:O	2.16	0.45
1:D:8:LEU:HG	1:D:101:HIS:HB3	1.98	0.45
1:D:186:THR:HG21	1:D:210:ARG:HG2	1.98	0.45
1:F:17:VAL:O	1:F:30:VAL:HA	2.16	0.45
1:F:189:LEU:HD13	1:F:257:CYS:SG	2.55	0.45
1:J:73:HIS:HB3	1:J:177:ARG:NH1	2.32	0.45
1:N:162:ASN:O	1:N:175:ILE:HA	2.16	0.45
1:J:303:THR:HG23	1:J:306:TYR:CE2	2.51	0.45
1:K:9:VAL:HG21	1:K:344:SER:HA	1.98	0.45
1:K:71:ILE:HA	1:K:76:ILE:HA	1.99	0.45
1:K:238:LYS:HE3	1:K:238:LYS:HA	1.98	0.45
1:M:7:ALA:HA	1:M:102:PRO:HG2	1.99	0.45
1:M:37:ARG:HG3	1:M:51:ASP:O	2.17	0.45
1:M:153:LEU:HA	1:M:161:HIS:O	2.17	0.45
1:N:62:ARG:HA	1:N:65:LEU:HB3	1.98	0.45
1:N:133:TYR:CE1	1:N:135:ALA:HB2	2.51	0.45
1:B:108:ALA:HB3	1:B:111:ASN:HD22	1.81	0.45
1:H:238:LYS:HE3	1:H:238:LYS:HA	1.99	0.45
1:H:263:GLN:HE21	1:H:263:GLN:HA	1.81	0.45
1:J:11:ASP:HA	1:J:106:'THR:OG1	2.16	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1.M.11.ASP.O	1·M·17·VAL·HA	2.16	0.45
1:M:65:LEU:HG	1:N:269:MET:HA	1.98	0.45
1:N:324:THR:HB	1:N:325:MET:SD	2.57	0.45
1:B:102:PRO:HD3	1:B:130:PRO:HG2	1.98	0.45
1:B:111:ASN:OD1	1:B:115:ASN:HB3	2.16	0.45
1:B:163:VAL:HG13	1:B:175:ILE:HG12	1.98	0.45
1:D:263:GLN:HA	1:D:263:GLN:HE21	1.81	0.45
1:E:62:ARG:HB2	1:E:62:ARG:NH2	2.30	0.45
1:F:227:MET:HB2	1:F:255:PHE:HE1	1.82	0.45
1:C:118:LYS:NZ	1:C:121:GLN:OE1	2.48	0.45
1:D:65:LEU:CG	1:F:287:ILE:HG21	2.47	0.45
1:D:210:ARG:HB3	1:D:210:ARG:CZ	2.46	0.45
1:I:64:ILE:HG13	1:I:65:LEU:HG	1.98	0.45
1:M:135:ALA:HB3	1:M:140:LEU:HD11	1.99	0.45
1:A:105:LEU:O	1:A:134:VAL:HA	2.17	0.45
1:B:154:ASP:O	1:B:160:THR:HA	2.16	0.45
1:L:118:LYS:NZ	1:L:121:GLN:OE1	2.48	0.45
1:N:38:PRO:HB2	1:N:40:HIS:O	2.17	0.45
1:A:11:ASP:O	1:A:17:VAL:HA	2.17	0.45
1:A:305:MET:SD	1:A:336:LYS:HB3	2.57	0.45
1:B:136:ILE:HB	1:B:139:VAL:HG23	1.99	0.45
1:B:200:PHE:O	1:B:206:ARG:HG3	2.16	0.45
1:C:165:ILE:HA	1:C:170:ALA:HA	1.99	0.45
1:D:42:GLY:HA3	1:F:285:CYS:HB2	1.98	0.45
1:F:219:VAL:HG21	1:F:309:ILE:HB	1.98	0.45
1:I:7:ALA:HA	1:I:102:PRO:HG2	1.98	0.45
1:K:105:LEU:O	1:K:134:VAL:HA	2.17	0.45
1:K:240:TYR:O	1:K:248:ILE:HG22	2.16	0.45
1:C:100:GLU:HG2	1:C:101:HIS:CD2	2.52	0.45
1:C:291:LYS:HZ3	1:C:292:ASP:CG	2.19	0.45
1:E:7:ALA:HA	1:E:102:PRO:HG2	1.98	0.45
1:L:180:LEU:HD21	1:L:264:PRO:HB3	1.99	0.45
1:L:198:TYR:OH	1:L:248:ILE:HA	2.17	0.45
1:M:39:ARG:HB2	1:N:265:SER:C	2.36	0.45
1:N:162:ASN:OD1	1:N:176:MET:HB3	2.16	0.45
1:E:9:VAL:O	1:E:19:ALA:HA	2.17	0.45
1:I:294:TYR:O	1:I:327:ILE:HA	2.15	0.45
1:K:243:PRO:HB3	1:M:291:LYS:HE3	1.98	0.45
1:L:262:PHE:O	1:L:275:HIS:HE1	1.99	0.45
1:A:113:LYS:O	1:A:116:ARG:HB3	2.17	0.44
1:A:220:ALA:O	1:A:312:ARG:NH2	2.49	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:101:HIS:HA	1:B:102:PRO:HD2	1.85	0.44
1:D:17:VAL:HG23	1:D:33:SER:OG	2.18	0.44
1:F:153:LEU:HD21	1:F:274:ILE:HG23	1.99	0.44
1:I:8:LEU:HG	1:I:101:HIS:HB3	1.98	0.44
1:L:193:LEU:O	1:L:196:ARG:HB3	2.17	0.44
1:M:118:LYS:NZ	1:M:121:GLN:OE1	2.48	0.44
1:B:104:LEU:HA	1:B:133:TYR:O	2.17	0.44
1:C:10:CYS:HB3	1:C:105:LEU:HD23	1.99	0.44
1:D:182:GLY:O	1:D:213:LYS:NZ	2.50	0.44
1:D:188:TYR:CE2	1:D:257:CYS:HA	2.51	0.44
1:F:59:GLN:O	1:F:62:ARG:HD2	2.17	0.44
1:K:243:PRO:O	1:M:291:LYS:HG2	2.16	0.44
1:M:163:VAL:HG22	1:M:175:ILE:HG23	2.00	0.44
1:M:171:LEU:HA	1:M:172:PRO:HD3	1.71	0.44
1:N:230:ALA:HB1	1:N:252:ASN:HD22	1.82	0.44
1:B:17:VAL:C	1:B:18:LYS:HE3	2.38	0.44
1:J:104:LEU:HG	1:J:133:TYR:HB3	1.99	0.44
1:K:243:PRO:HB2	1:M:288:ASP:O	2.17	0.44
1:L:10:CYS:HB3	1:L:105:LEU:HD23	2.00	0.44
1:D:10:CYS:HB3	1:D:105:LEU:HD23	1.99	0.44
1:D:44:MET:O	1:F:165:ILE:O	2.35	0.44
1:D:328:LYS:HZ1	1:D:330:ILE:HG13	1.81	0.44
1:M:147:ARG:NH1	1:M:296:ASN:OD1	2.51	0.44
1:N:321:ALA:HA	1:N:322:PRO:HD2	1.67	0.44
1:C:196:ARG:NH2	1:C:249:THR:OG1	2.51	0.44
1:D:35:VAL:HG22	1:D:54:VAL:HG22	1.98	0.44
1:D:194:THR:HA	1:D:197:GLY:C	2.38	0.44
1:E:312:ARG:HD2	1:E:315:LYS:HE3	1.99	0.44
1:F:45:VAL:CG1	1:H:167:GLU:HG3	2.47	0.44
1:F:282:ILE:HG22	1:F:283:MET:N	2.33	0.44
1:M:162:ASN:HB2	1:M:176:MET:HB3	1.97	0.44
1:A:193:LEU:HB3	1:A:200:PHE:HE1	1.82	0.44
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.80	0.44
1:D:63:GLY:H	1:E:267:ILE:HA	1.82	0.44
1:E:38:PRO:HD2	1:E:51:ASP:O	2.17	0.44
1:H:212:ILE:HG23	1:H:216:LEU:HD12	1.99	0.44
1:K:186:THR:HG21	1:K:210:ARG:HG2	2.00	0.44
1:L:111:ASN:OD1	1:L:115:ASN:HB3	2.18	0.44
1:A:244:ASP:HA	1:C:323:SER:HB2	1.99	0.44
1:D:44:MET:SD	1:D:45:VAL:HG23	2.58	0.44
1:F:219:VAL:HG22	1:F:258:PRO:CB	2.47	0.44



EMD-1088,	3B5U
-----------	------

	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:194:THR:HG22	1:I:198:TYR:O	2.18	0.44
1:J:219:VAL:HG22	1:J:258:PRO:CB	2.48	0.44
1:A:154:ASP:O	1:A:160:THR:HA	2.18	0.44
1:B:135:ALA:HB3	1:B:140:LEU:HD11	1.98	0.44
1:C:163:VAL:HG13	1:C:175:ILE:HG12	2.00	0.44
1:C:366:GLY:O	1:C:369:ILE:HG22	2.18	0.44
1:E:287:ILE:HD12	1:E:287:ILE:N	2.30	0.44
1:F:103:THR:O	1:F:132:MET:HA	2.18	0.44
1:H:53:TYR:CD1	1:H:65:LEU:HD21	2.53	0.44
1:J:112:PRO:HG2	1:J:116:ARG:HB2	2.00	0.44
1:L:217:CYS:O	1:L:307:PRO:HD2	2.18	0.44
1:B:10:CYS:HA	1:B:18:LYS:O	2.18	0.44
1:D:49:GLN:HA	1:F:166:TYR:CE2	2.53	0.44
1:D:147:ARG:CZ	1:D:330:ILE:HG12	2.48	0.44
1:D:202:THR:H	1:D:205:GLU:HB2	1.82	0.44
1:D:230:ALA:HB1	1:D:252:ASN:HB3	1.99	0.44
1:E:219:VAL:HG22	1:E:258:PRO:HB2	1.99	0.44
1:F:45:VAL:CB	1:H:166:TYR:HE1	2.26	0.44
1:F:50:LYS:NZ	1:F:52:SER:O	2.49	0.44
1:H:155:SER:HB3	1:H:304:THR:HG23	1.99	0.44
1:K:193:LEU:O	1:K:196:ARG:HB3	2.17	0.44
1:A:133:TYR:HE2	1:A:374:CYS:HG	1.62	0.43
1:C:359:LYS:HD2	1:C:360:GLN:N	2.33	0.43
1:D:171:LEU:HA	1:D:172:PRO:HD2	1.83	0.43
1:H:262:PHE:HE2	1:H:309:ILE:HG13	1.82	0.43
1:I:45:VAL:HB	1:K:168:GLY:HA3	2.00	0.43
1:K:256:ARG:HD3	1:L:113:LYS:NZ	2.33	0.43
1:N:86:TRP:CH2	1:N:119:MET:HG3	2.53	0.43
1:N:124:PHE:HE1	1:N:359:LYS:HA	1.83	0.43
1:H:7:ALA:HA	1:H:102:PRO:HG2	2.00	0.43
1:H:9:VAL:HG13	1:H:104:LEU:HD22	2.00	0.43
1:H:53:TYR:HD1	1:H:65:LEU:HD21	1.83	0.43
1:H:118:LYS:NZ	1:H:121:GLN:OE1	2.49	0.43
1:K:189:LEU:HD12	1:K:192:ILE:HG13	2.00	0.43
1:K:220:ALA:O	1:K:312:ARG:HD3	2.18	0.43
1:L:105:LEU:O	1:L:134:VAL:HA	2.17	0.43
1:M:359:LYS:HD2	1:M:360:GLN:H	1.83	0.43
1:B:9:VAL:HG21	1:B:344:SER:HA	2.00	0.43
1:B:86:TRP:HH2	1:B:119:MET:HG2	1.82	0.43
1:D:163:VAL:HA	1:D:175:ILE:HG12	2.00	0.43
1:F:73:HIS:HB3	1:F:177:ARG:NH1	2.33	0.43



EMD-1088,	3B5U
-----------	------

	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:22:ALA:HB2	1:J:347:ALA:HB3	1.99	0.43
1:B:119:MET:O	1:B:123:MET:HG2	2.17	0.43
1:D:318:THR:HA	1:D:327:ILE:HD13	1.99	0.43
1:E:41:GLN:HA	1:E:49:GLN:OE1	2.19	0.43
1:H:282:ILE:HG22	1:H:290:ARG:HG2	2.00	0.43
1:K:306:TYR:HA	1:K:307:PRO:HD3	1.86	0.43
1:L:74:GLY:O	1:L:108:ALA:HB2	2.18	0.43
1:N:290:ARG:HH11	1:N:290:ARG:HD3	1.67	0.43
1:D:194:THR:HA	1:D:197:GLY:O	2.18	0.43
1:G:164:PRO:HG3	1:G:174:ALA:HB3	2.01	0.43
1:I:11:ASP:HA	1:I:106:THR:OG1	2.18	0.43
1:K:62:ARG:HG2	1:L:270:GLU:HB2	2.00	0.43
1:L:39:ARG:CZ	1:M:272:ALA:HA	2.48	0.43
1:L:248:ILE:HG23	1:L:250:ILE:HG12	1.99	0.43
1:N:101:HIS:HA	1:N:102:PRO:HD2	1.81	0.43
1:C:238:LYS:HE3	1:C:238:LYS:HA	1.99	0.43
1:I:104:LEU:HG	1:I:133:TYR:HB3	2.00	0.43
1:N:299:MET:HG3	1:N:329:ILE:HG21	2.00	0.43
1:C:170:ALA:O	1:C:172:PRO:HD3	2.19	0.43
1:C:210:ARG:CZ	1:C:210:ARG:HB3	2.48	0.43
1:F:116:ARG:HE	1:F:371:HIS:HA	1.83	0.43
1:G:198:TYR:CZ	1:G:248:ILE:HA	2.54	0.43
1:J:165:ILE:HA	1:J:169:TYR:O	2.19	0.43
1:L:44:MET:HB2	1:L:47:MET:HB2	2.01	0.43
1:B:111:ASN:HA	1:B:112:PRO:HD3	1.83	0.43
1:B:186:THR:HG21	1:B:210:ARG:HG2	2.01	0.43
1:B:210:ARG:O	1:B:213:LYS:HB3	2.19	0.43
1:D:57:GLU:HB3	1:F:288:ASP:OD1	2.18	0.43
1:F:239:SER:HA	1:F:248:ILE:O	2.18	0.43
1:F:306:TYR:HA	1:F:307:PRO:HD3	1.90	0.43
1:G:13:GLY:O	1:G:15:GLY:N	2.50	0.43
1:G:111:ASN:HA	1:G:112:PRO:HD3	1.86	0.43
1:G:193:LEU:O	1:G:198:TYR:HB2	2.18	0.43
1:G:357:ILE:HG21	1:G:370:VAL:HG22	2.00	0.43
1:M:265:SER:HA	1:M:270:GLU:CD	2.39	0.43
1:M:357:ILE:CD1	1:M:373:LYS:HD2	2.48	0.43
1:D:42:GLY:HA2	1:F:171:LEU:HD11	2.01	0.43
1:D:199:SER:HB3	1:E:75:ILE:HG12	2.00	0.43
1:E:17:VAL:O	1:E:30:VAL:HA	2.18	0.43
1:E:196:ARG:O	1:F:177:ARG:NH2	2.52	0.43
1:G:172:PRO:HA	1:G:175:ILE:HD12	1.99	0.43



EMD-1088,	3B5U
-----------	------

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:203:THR:C	1:J:205:GLU:H	2.23	0.43
1:M:100:GLU:HG3	1:M:101:HIS:HD2	1.82	0.43
1:M:212:ILE:HG23	1:M:216:LEU:HD12	2.01	0.43
1:N:147:ARG:CZ	1:N:330:ILE:HG12	2.48	0.43
1:B:108:ALA:HA	1:B:109:PRO:HD3	1.91	0.43
1:B:290:ARG:HA	1:B:293:LEU:HB2	2.00	0.43
1:D:202:THR:HA	1:E:179:ASP:OD1	2.19	0.43
1:M:58:ALA:HB1	1:M:65:LEU:HD11	2.01	0.43
1:N:151:ILE:O	1:N:297:ASN:HA	2.19	0.43
1:A:53:TYR:CD1	1:A:65:LEU:HD21	2.54	0.42
1:A:61:LYS:O	1:A:63:GLY:HA3	2.19	0.42
1:B:262:PHE:O	1:B:275:HIS:HE1	2.02	0.42
1:C:194:THR:HG22	1:C:198:TYR:O	2.19	0.42
1:D:71:ILE:HA	1:D:76:ILE:HA	2.01	0.42
1:D:189:LEU:HD13	1:D:257:CYS:SG	2.59	0.42
1:F:220:ALA:HB1	1:F:222:ASP:O	2.19	0.42
1:G:104:LEU:HA	1:G:133:TYR:O	2.19	0.42
1:I:99:GLU:HA	1:I:129:VAL:HA	2.01	0.42
1:J:113:LYS:HB3	1:J:113:LYS:HZ2	1.85	0.42
1:K:118:LYS:NZ	1:K:121:GLN:OE1	2.49	0.42
1:K:285:CYS:HB3	1:K:289:ILE:HD11	2.00	0.42
1:M:252:ASN:ND2	1:M:252:ASN:H	2.17	0.42
1:N:269:MET:SD	1:N:269:MET:N	2.92	0.42
1:A:278:THR:HG21	1:A:297:ASN:OD1	2.18	0.42
1:B:136:ILE:H	1:B:136:ILE:HD12	1.83	0.42
1:B:357:ILE:HD13	1:B:373:LYS:HD3	2.01	0.42
1:E:305:MET:HA	1:E:335:ARG:NH1	2.34	0.42
1:G:262:PHE:O	1:G:275:HIS:HE1	2.02	0.42
1:K:195:GLU:HG2	1:L:112:PRO:HG3	2.00	0.42
1:N:113:LYS:O	1:N:116:ARG:HB3	2.19	0.42
1:A:190:MET:HB2	1:A:209:VAL:HG11	2.01	0.42
1:A:217:CYS:SG	1:A:257:CYS:SG	3.15	0.42
1:C:149:THR:HA	1:C:165:ILE:O	2.19	0.42
1:E:10:CYS:HA	1:E:18:LYS:O	2.19	0.42
1:F:45:VAL:CG1	1:H:167:GLU:CG	2.93	0.42
1:K:262:PHE:O	1:K:275:HIS:HE1	2.01	0.42
1:L:163:VAL:HG22	1:L:175:ILE:HG23	2.01	0.42
1:L:283:MET:SD	1:L:290:ARG:NH2	2.92	0.42
1:M:189:LEU:HD13	1:M:257:CYS:SG	2.59	0.42
1:A:36:GLY:CA	1:A:66:THR:O	2.67	0.42
1:B:31:PHE:HA	1:B:32:PRO:HD2	1.87	0.42



EMD-1088,	3B5U
-----------	------

Interatomic Clash			Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:G:11:ASP:HA	1:G:106:THR:OG1	2.19	0.42
1:J:147:ARG:NH1	1:J:296:ASN:OD1	2.53	0.42
1:A:50:LYS:HD3	1:A:53:TYR:CZ	2.54	0.42
1:G:294:TYR:O	1:G:327:ILE:HA	2.19	0.42
1:J:32:PRO:HB2	1:J:34:ILE:HG12	2.01	0.42
1:J:61:LYS:O	1:J:65:LEU:HG	2.20	0.42
1:M:290:ARG:HA	1:M:293:LEU:HB2	2.01	0.42
1:B:111:ASN:HD21	1:B:115:ASN:ND2	2.18	0.42
1:D:59:GLN:O	1:D:62:ARG:HD2	2.19	0.42
1:D:236:LEU:O	1:D:251:GLY:HA2	2.20	0.42
1:E:147:ARG:NH1	1:E:296:ASN:OD1	2.52	0.42
1:E:180:LEU:HG	1:E:264:PRO:HB3	2.02	0.42
1:I:186:THR:O	1:I:189:LEU:HB3	2.20	0.42
1:K:36:GLY:HA3	1:K:65:LEU:HD13	2.02	0.42
1:L:286:ASP:O	1:L:290:ARG:NH1	2.53	0.42
1:B:60:SER:C	1:D:287:ILE:HG21	2.40	0.42
1:C:154:ASP:O	1:C:160:THR:HA	2.20	0.42
1:E:313:MET:O	1:E:317:ILE:HG12	2.20	0.42
1:J:217:CYS:HA	1:J:254:ARG:O	2.20	0.42
1:L:103:THR:H	1:L:132:MET:HA	1.84	0.42
1:M:10:CYS:HA	1:M:18:LYS:O	2.20	0.42
1:N:163:VAL:HG22	1:N:175:ILE:HG23	2.02	0.42
1:A:11:ASP:HA	1:A:106:THR:OG1	2.19	0.42
1:A:161:HIS:HA	1:A:176:MET:O	2.19	0.42
1:B:11:ASP:HA	1:B:106:THR:OG1	2.19	0.42
1:D:46:GLY:O	1:F:167:GLU:OE2	2.38	0.42
1:D:164:PRO:HG2	1:D:171:LEU:HB3	2.02	0.42
1:E:197:GLY:HA2	1:F:177:ARG:NH1	2.34	0.42
1:E:306:TYR:HA	1:E:307:PRO:HD3	1.92	0.42
1:F:45:VAL:CG2	1:H:166:TYR:HD1	2.16	0.42
1:F:219:VAL:HG22	1:F:258:PRO:HB3	2.02	0.42
1:G:11:ASP:HB3	1:G:18:LYS:HD2	2.01	0.42
1:H:204:ALA:HB3	1:J:287:ILE:HB	2.01	0.42
1:I:142:LEU:HD22	1:I:165:ILE:HB	2.02	0.42
1:J:9:VAL:HA	1:J:104:LEU:O	2.20	0.42
1:J:328:LYS:HB3	1:J:328:LYS:HE3	1.83	0.42
1:N:304:THR:O	1:N:309:ILE:HG21	2.19	0.42
1:A:102:PRO:HA	1:A:131:ALA:O	2.19	0.42
1:A:305:MET:HA	1:A:335:ARG:NH1	2.35	0.42
1:B:134:VAL:O	1:B:374:CYS:SG	2.78	0.42
1:B:162:ASN:OD1	1:B:277:THR:HG22	2.20	0.42



EMD-1088,	3B5U
-----------	------

	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:101:HIS:O	1:C:130:PRO:HD2	2.20	0.42
1:D:44:MET:SD	1:F:293:LEU:HD22	2.52	0.42
1:F:102:PRO:HA	1:F:131:ALA:O	2.20	0.42
1:F:289:ILE:O	1:F:291:LYS:HD3	2.20	0.42
1:H:135:ALA:HB3	1:H:140:LEU:HD11	2.02	0.42
1:L:138:ALA:HB2	1:L:163:VAL:HG21	2.02	0.42
1:A:39:ARG:NH1	1:B:267:ILE:HG22	2.34	0.42
1:D:43:VAL:HG22	1:F:171:LEU:CB	2.50	0.42
1:I:187:ASP:O	1:I:190:MET:HB3	2.20	0.42
1:I:213:LYS:HA	1:I:217:CYS:SG	2.59	0.42
1:K:299:MET:HB3	1:K:304:THR:HG21	2.00	0.42
1:L:86:TRP:CH2	1:L:119:MET:HG3	2.55	0.42
1:N:11:ASP:HA	1:N:106:THR:OG1	2.19	0.42
1:A:162:ASN:O	1:A:175:ILE:HA	2.19	0.41
1:B:290:ARG:HA	1:B:293:LEU:HD12	2.02	0.41
1:C:70:PRO:HB3	1:C:81:ASP:HB2	2.02	0.41
1:D:61:LYS:HZ1	1:F:291:LYS:CG	2.32	0.41
1:F:318:THR:HA	1:F:327:ILE:HD13	2.02	0.41
1:J:304:THR:O	1:J:309:ILE:HG21	2.19	0.41
1:K:230:ALA:HB1	1:K:252:ASN:HD22	1.84	0.41
1:N:328:LYS:HZ1	1:N:330:ILE:HG13	1.85	0.41
1:A:36:GLY:O	1:A:52:SER:HA	2.20	0.41
1:A:98:PRO:HG2	1:A:128:ASN:HD21	1.85	0.41
1:C:213:LYS:O	1:C:217:CYS:HB2	2.20	0.41
1:F:8:LEU:HG	1:F:101:HIS:HB3	2.02	0.41
1:F:99:GLU:H	1:F:99:GLU:CD	2.23	0.41
1:G:153:LEU:HD21	1:G:274:ILE:HD12	2.02	0.41
1:I:285:CYS:HB3	1:I:289:ILE:HD11	2.01	0.41
1:J:107:GLU:OE1	1:J:112:PRO:HG3	2.21	0.41
1:K:264:PRO:HD2	1:K:271:SER:O	2.20	0.41
1:N:153:LEU:HD21	1:N:274:ILE:HG23	2.02	0.41
1:D:189:LEU:HD12	1:D:192:ILE:HD11	2.02	0.41
1:D:196:ARG:HA	1:E:113:LYS:HD2	2.02	0.41
1:G:4:GLU:HG2	1:G:5:THR:HG23	2.02	0.41
1:I:11:ASP:OD1	1:I:18:LYS:NZ	2.51	0.41
1:I:171:LEU:HA	1:I:172:PRO:HD2	1.93	0.41
1:M:186:THR:OG1	1:M:213:LYS:HD2	2.19	0.41
1:N:322:PRO:O	1:N:327:ILE:HD11	2.20	0.41
1:D:17:VAL:O	1:D:30:VAL:HA	2.21	0.41
1:D:45:VAL:HG11	1:F:165:ILE:CD1	2.47	0.41
$1:E:174:\overline{ALA:HA}$	1:E:284:LYS:HZ3	1.85	0.41



EMD-1088,	3B5U
-----------	------

Unititated from precious page			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:274:ILE:HG22	1:F:313:MET:SD	2.60	0.41
1:G:39:ARG:HD3	1:G:66:THR:HG23	2.01	0.41
1:J:306:TYR:HA	1:J:307:PRO:HD3	1.96	0.41
1:L:242:LEU:H	1:L:245:GLY:HA3	1.84	0.41
1:F:160:THR:O	1:F:177:ARG:HA	2.21	0.41
1:H:180:LEU:HD11	1:H:264:PRO:HB3	2.03	0.41
1:I:264:PRO:HB2	1:I:271:SER:HB3	2.03	0.41
1:J:10:CYS:HA	1:J:19:ALA:HA	2.01	0.41
1:B:9:VAL:O	1:B:19:ALA:HA	2.20	0.41
1:B:116:ARG:HH12	1:B:375:PHE:HD2	1.68	0.41
1:C:34:ILE:O	1:C:54:VAL:HA	2.21	0.41
1:D:190:MET:HB2	1:D:209:VAL:HG11	2.03	0.41
1:F:11:ASP:OD1	1:F:18:LYS:NZ	2.51	0.41
1:F:269:MET:O	1:F:270:GLU:HB2	2.21	0.41
1:H:163:VAL:HA	1:H:175:ILE:HG12	2.02	0.41
1:H:239:SER:HA	1:H:248:ILE:O	2.21	0.41
1:K:98:PRO:O	1:K:129:VAL:HA	2.21	0.41
1:L:253:GLU:HG3	1:L:256:ARG:HH21	1.85	0.41
1:M:160:THR:OG1	1:M:181:ALA:HB2	2.20	0.41
1:N:71:ILE:HG23	1:N:76:ILE:HG12	2.01	0.41
1:N:274:ILE:HG22	1:N:313:MET:SD	2.61	0.41
1:N:362:TYR:OH	1:N:367:PRO:HG3	2.21	0.41
1:A:38:PRO:HB2	1:A:40:HIS:O	2.21	0.41
1:B:113:LYS:O	1:B:116:ARG:HB3	2.21	0.41
1:B:203:THR:HG21	1:C:268:GLY:O	2.20	0.41
1:D:10:CYS:HA	1:D:18:LYS:O	2.20	0.41
1:E:62:ARG:NH2	1:F:266:PHE:O	2.52	0.41
1:E:190:MET:CA	1:E:209:VAL:HG11	2.51	0.41
1:F:11:ASP:O	1:F:17:VAL:HA	2.21	0.41
1:H:101:HIS:O	1:H:130:PRO:HD2	2.20	0.41
1:J:152:VAL:O	1:J:162:ASN:HA	2.19	0.41
1:K:190:MET:HA	1:K:209:VAL:HG11	2.02	0.41
1:A:61:LYS:C	1:A:63:GLY:HA3	2.41	0.41
1:A:200:PHE:HA	1:A:205:GLU:HB3	2.03	0.41
1:B:8:LEU:HG	1:B:101:HIS:HB3	2.03	0.41
1:B:10:CYS:HB3	1:B:105:LEU:HD23	2.01	0.41
1:B:63:GLY:C	1:C:267:ILE:HA	2.40	0.41
1:E:101:HIS:HA	1:E:102:PRO:HD2	1.96	0.41
1:N:113:LYS:HB2	1:N:113:LYS:HE3	1.94	0.41
1:B:289:ILE:HA	1:B:292:ASP:OD2	2.21	0.41
1:E:162:ASN:OD1	1:E:277:THR:HG23	2.21	0.41



EMD-1088,	3B5U
-----------	------

Continuea from previous page			
Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:E:191:LYS:HD2	1:F:1/0:MET:HG2	2.02	0.41
1:F:213:LYS:HD3	1:F:214:GLU:HG3	2.02	0.41
I:G:17:VAL:O	1:G:30:VAL:HA	2.20	0.41
1:G:196:ARG:HE	1:G:249:THR:HG23	1.86	0.41
1:G:287:ILE:HA	1:G:290:ARG:HG3	2.03	0.41
1:H:149:THR:HA	1:H:165:ILE:O	2.21	0.41
1:H:189:LEU:HD12	1:H:192:ILE:HD11	2.03	0.41
1:I:201:VAL:HG21	1:J:179:ASP:OD2	2.21	0.41
1:J:202:THR:HG21	1:L:285:CYS:HA	2.03	0.41
1:M:359:LYS:HD2	1:M:360:GLN:HB2	2.02	0.41
1:N:304:THR:HA	1:N:309:ILE:HD13	2.02	0.41
1:A:186:THR:O	1:A:189:LEU:HB3	2.21	0.41
1:A:281:SER:HA	1:A:284:LYS:NZ	2.36	0.41
1:C:101:HIS:HA	1:C:102:PRO:HD2	1.86	0.41
1:C:305:MET:SD	1:C:336:LYS:HB3	2.61	0.41
1:D:39:ARG:NH2	1:E:271:SER:O	2.54	0.41
1:E:162:ASN:O	1:E:175:ILE:HA	2.20	0.41
1:E:218:TYR:O	1:E:255:PHE:HA	2.21	0.41
1:E:219:VAL:HG22	1:E:258:PRO:CB	2.51	0.41
1:F:46:GLY:N	1:H:167:GLU:HB3	2.32	0.41
1:G:159:VAL:HA	1:G:178:LEU:O	2.20	0.41
1:I:17:VAL:O	1:I:30:VAL:HA	2.21	0.41
1:N:118:LYS:NZ	1:N:121:GLN:OE1	2.48	0.41
1:A:188:TYR:CE2	1:A:257:CYS:HA	2.56	0.40
1:C:304:THR:HA	1:C:309:ILE:HD13	2.03	0.40
1:D:45:VAL:CA	1:F:165:ILE:H	2.34	0.40
1:D:359:LYS:NZ	1:D:360:GLN:OE1	2.54	0.40
1:F:108:ALA:O	1:F:111:ASN:HB2	2.21	0.40
1:G:38:PRO:HD2	1:G:51:ASP:O	2.21	0.40
1:I:9:VAL:O	1:I:19:ALA:HA	2.22	0.40
1:I:210:ARG:O	1:I:213:LYS:HB3	2.21	0.40
1:J:248:ILE:HD12	1:J:248:ILE:HA	1.97	0.40
1:K:155:SER:HA	1:K:160:THR:HA	2.03	0.40
1:L:34:ILE:O	1:L:54:VAL:HA	2.22	0.40
1:M:291:LYS:HG3	1:M:292:ASP:H	1.85	0.40
1:N:294:TYR:O	1:N:327:ILE:HA	2.21	0.40
1:A:112:PRO:O	1:A:115:ASN:HB3	2.21	0.40
1:A:137:GLN:HG2	1:A:339:VAL:CG1	2.48	0.40
1:B:32:PRO:HB2	1:B:34:ILE:HG12	2.03	0.40
1:D:9:VAL:O	1:D:19:ALA:HA	2.20	0.40
1:D:217:CYS:HA	1:D:254:ARG:O	2.21	0.40



EMD-1088, 3B	5U
--------------	----

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:108:ALA:O	1:J:111:ASN:HB2	2.22	0.40
1:M:53:TYR:HB2	1:N:268:GLY:HA2	2.03	0.40
1:N:14:SER:O	1:N:183:ARG:NH2	2.53	0.40
1:N:79:TRP:HA	1:N:82:MET:HB2	2.02	0.40
1:A:44:MET:SD	1:C:166:TYR:HD1	2.45	0.40
1:A:99:GLU:H	1:A:99:GLU:CD	2.25	0.40
1:B:190:MET:HA	1:B:209:VAL:HG11	2.04	0.40
1:C:8:LEU:HA	1:C:20:GLY:O	2.22	0.40
1:E:11:ASP:OD1	1:E:18:LYS:NZ	2.52	0.40
1:F:100:GLU:HG3	1:F:101:HIS:CD2	2.55	0.40
1:I:11:ASP:HB3	1:I:18:LYS:HB2	2.03	0.40
1:M:10:CYS:HB3	1:M:105:LEU:HD23	2.04	0.40
1:M:328:LYS:HZ1	1:M:330:ILE:HG12	1.86	0.40
1:E:161:HIS:HA	1:E:176:MET:O	2.20	0.40
1:I:155:SER:HB3	1:I:304:THR:HG23	2.03	0.40
1:L:50:LYS:NZ	1:L:52:SER:O	2.51	0.40
1:M:33:SER:O	1:M:34:ILE:HG23	2.22	0.40
1:C:243:PRO:O	1:E:291:LYS:HB3	2.21	0.40
1:D:46:GLY:HA2	1:F:149:THR:HA	2.04	0.40
1:D:198:TYR:CE2	1:D:248:ILE:HG23	2.57	0.40
1:D:202:THR:N	1:D:205:GLU:HB2	2.37	0.40
1:F:101:HIS:HA	1:F:102:PRO:HD2	1.85	0.40
1:H:10:CYS:HA	1:H:18:LYS:O	2.22	0.40
1:H:19:ALA:HB3	1:H:29:ALA:HB3	2.04	0.40
1:H:31:PHE:HA	1:H:32:PRO:HD2	1.92	0.40
1:I:132:MET:HG3	1:I:357:ILE:HB	2.03	0.40
1:K:151:ILE:O	1:K:297:ASN:HA	2.22	0.40
1:K:171:LEU:O	1:K:175:ILE:HG13	2.22	0.40
1:K:332:PRO:HB2	1:K:335:ARG:HB3	2.03	0.40
1:L:38:PRO:HD2	1:L:51:ASP:O	2.21	0.40
1:L:193:LEU:HD21	1:L:212:ILE:HD13	2.03	0.40
1:M:75:ILE:HG23	1:M:111:ASN:ND2	2.36	0.40
1:M:279:TYR:O	1:M:283:MET:HB2	2.21	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	Pe	erce	entiles
1	А	373/377~(99%)	297 (80%)	63 (17%)	13 (4%)		3	25
1	В	373/377~(99%)	298 (80%)	58 (16%)	17 (5%)		2	21
1	С	373/377~(99%)	310 (83%)	55 (15%)	8 (2%)		7	36
1	D	373/377~(99%)	310 (83%)	49 (13%)	14 (4%)		3	24
1	Е	373/377~(99%)	303 (81%)	56 (15%)	14 (4%)		3	24
1	F	373/377~(99%)	291 (78%)	62 (17%)	20 (5%)		2	19
1	G	373/377~(99%)	315 (84%)	46 (12%)	12 (3%)		4	26
1	Н	373/377~(99%)	308 (83%)	55 (15%)	10 (3%)		5	31
1	Ι	373/377~(99%)	318 (85%)	45 (12%)	10 (3%)		5	31
1	J	373/377~(99%)	308 (83%)	48 (13%)	17 (5%)		2	21
1	К	373/377~(99%)	323 (87%)	33 (9%)	17 (5%)		2	21
1	L	373/377~(99%)	311 (83%)	44 (12%)	18 (5%)		2	21
1	М	373/377~(99%)	300 (80%)	54 (14%)	19 (5%)		2	19
1	N	373/377~(99%)	307 (82%)	51 (14%)	15 (4%)		3	23
All	All	5222/5278~(99%)	4299 (82%)	719 (14%)	204 (4%)		5	23

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	4	GLU
1	А	236	LEU
1	А	252	ASN
1	А	272	ALA
1	В	113	LYS
1	В	323	SER
1	С	236	LEU
1	D	49	GLN
1	D	61	LYS



Mol	Chain	Res	Type
1	D	236	LEU
1	D	323	SER
1	Е	111	ASN
1	Е	128	ASN
1	Е	222	ASP
1	Е	263	GLN
1	Е	266	PHE
1	Е	359	LYS
1	F	14	SER
1	F	173	HIS
1	F	254	ARG
1	F	265	SER
1	F	270	GLU
1	F	282	ILE
1	F	289	ILE
1	G	14	SER
1	G	222	ASP
1	Н	62	ARG
1	Н	236	LEU
1	Ι	236	LEU
1	J	112	PRO
1	J	137	GLN
1	J	175	ILE
1	J	242	LEU
1	J	335	ARG
1	K	234	SER
1	К	267	ILE
1	K	270	GLU
1	K	350	SER
1	L	236	LEU
1	L	325	MET
1	М	2	GLU
1	М	37	ARG
1	М	173	HIS
1	М	236	LEU
1	М	263	GLN
1	Ν	47	MET
1	N	322	PRO
1	А	55	GLY
1	А	61	LYS
1	А	181	ALA
1	В	2	GLU



Mol	Chain	Res	Type
1	В	4	GLU
1	В	14	SER
1	В	45	VAL
1	В	199	SER
1	В	252	ASN
1	В	254	ARG
1	С	181	ALA
1	D	69	TYR
1	D	113	LYS
1	D	267	ILE
1	D	335	ARG
1	Е	14	SER
1	F	4	GLU
1	F	266	PHE
1	F	290	ARG
1	G	113	LYS
1	G	236	LEU
1	Н	2	GLU
1	Н	323	SER
1	Ι	253	GLU
1	J	14	SER
1	J	359	LYS
1	K	266	PHE
1	K	323	SER
1	K	335	ARG
1	L	62	ARG
1	L	204	ALA
1	L	291	LYS
1	L	359	LYS
1	М	41	GLN
1	М	67	LEU
1	М	68	LYS
1	М	323	SER
1	М	359	LYS
1	N	14	SER
1	Ν	128	ASN
1	Ν	267	ILE
1	А	2	GLU
1	А	335	ARG
1	А	374	CYS
1	В	181	ALA
1	С	204	ALA



Mol	Chain	Res	Type
1	D	15	GLY
1	D	60	SER
1	Е	73	HIS
1	Е	157	ASP
1	F	44	MET
1	F	222	ASP
1	F	234	SER
1	F	359	LYS
1	G	359	LYS
1	Н	181	ALA
1	Н	359	LYS
1	Ι	2	GLU
1	Ι	335	ARG
1	J	272	ALA
1	Κ	181	ALA
1	К	236	LEU
1	K	359	LYS
1	L	2	GLU
1	L	49	GLN
1	L	112	PRO
1	L	222	ASP
1	L	254	ARG
1	L	286	ASP
1	М	270	GLU
1	М	283	MET
1	М	335	ARG
1	Ν	2	GLU
1	Ν	62	ARG
1	N	175	ILE
1	В	359	LYS
1	D	359	LYS
1	E	335	ARG
1	F	283	MET
1	F	285	CYS
1	G	2	GLU
1	G	4	GLU
1	G	181	ALA
1	G	242	LEU
1	Н	14	SER
1	Н	335	ARG
1	H	374	CYS
1	Ι	222	ASP



Mol	Chain	Res	Type
1	J	234	SER
1	J	274	ILE
1	K	63	GLY
1	K	222	ASP
1	K	233	SER
1	K	243	PRO
1	L	15	GLY
1	L	181	ALA
1	L	246	GLN
1	М	242	LEU
1	Ν	181	ALA
1	Ν	222	ASP
1	N	251	GLY
1	N	270	GLU
1	А	222	ASP
1	В	234	SER
1	В	274	ILE
1	В	373	LYS
1	С	14	SER
1	С	274	ILE
1	С	335	ARG
1	D	253	GLU
1	Е	62	ARG
1	F	264	PRO
1	G	253	GLU
1	Н	274	ILE
1	Ι	14	SER
1	J	15	GLY
1	J	171	LEU
1	J	244	ASP
1	K	251	GLY
1	L	263	GLN
1	M	38	PRO
1	M	181	ALA
1	N	234	SER
1	A	372	ARG
1	В	222	ASP
1	С	62	ARG
1	D	181	ALA
1	Е	171	LEU
1	F	109	PRO
1	F	251	GLY



Mol	Chain	Res	Type
1	Ι	181	ALA
1	Ι	242	LEU
1	J	136	ILE
1	J	374	CYS
1	K	274	ILE
1	М	159	VAL
1	М	171	LEU
1	В	339	VAL
1	Е	15	GLY
1	К	175	ILE
1	L	251	GLY
1	А	242	LEU
1	D	175	ILE
1	F	274	ILE
1	Ι	159	VAL
1	L	243	PRO
1	М	175	ILE
1	G	251	GLY
1	Ι	251	GLY
1	J	111	ASN
1	В	159	VAL
1	С	175	ILE
1	G	274	ILE
1	J	71	ILE
1	Ν	43	VAL
1	N	159	VAL
1	Е	267	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	318/320~(99%)	284 (89%)	34 (11%)	6 23
1	В	318/320~(99%)	285~(90%)	33~(10%)	7 24
1	С	318/320~(99%)	281 (88%)	37 (12%)	5 21



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	D	318/320~(99%)	284~(89%)	34 (11%)	6	23
1	Ε	318/320~(99%)	282~(89%)	36 (11%)	6	21
1	F	318/320~(99%)	287~(90%)	31 (10%)	8	27
1	G	318/320~(99%)	294 (92%)	24 (8%)	13	38
1	Н	318/320~(99%)	291~(92%)	27~(8%)	10	33
1	Ι	318/320~(99%)	288 (91%)	30 (9%)	8	28
1	J	318/320~(99%)	277 (87%)	41 (13%)	4	18
1	Κ	318/320~(99%)	289 (91%)	29~(9%)	9	29
1	L	318/320~(99%)	286 (90%)	32 (10%)	7	25
1	М	318/320~(99%)	286~(90%)	32 (10%)	7	25
1	Ν	318/320~(99%)	271 (85%)	47 (15%)	3	15
All	All	4452/4480 (99%)	3985 (90%)	467 (10%)	10	24

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	2	GLU
1	А	18	LYS
1	А	61	LYS
1	А	66	THR
1	А	99	GLU
1	А	109	PRO
1	А	112	PRO
1	А	115	ASN
1	А	128	ASN
1	А	159	VAL
1	А	176	MET
1	А	195	GLU
1	А	207	GLU
1	А	210	ARG
1	А	215	LYS
1	А	218	TYR
1	А	221	LEU
1	А	238	LYS
1	А	244	ASP
1	А	249	THR
1	А	252	ASN
1	А	263	GLN



Mol	Chain	Res	Type
1	А	266	PHE
1	А	270	GLU
1	А	275	HIS
1	А	277	THR
1	А	287	ILE
1	А	288	ASP
1	А	292	ASP
1	А	297	ASN
1	А	303	THR
1	А	316	GLU
1	А	334	GLU
1	А	359	LYS
1	В	18	LYS
1	В	62	ARG
1	В	66	THR
1	В	100	GLU
1	В	107	GLU
1	В	115	ASN
1	В	128	ASN
1	В	155	SER
1	В	159	VAL
1	В	166	TYR
1	В	169	TYR
1	В	187	ASP
1	В	195	GLU
1	В	207	GLU
1	В	213	LYS
1	В	218	TYR
1	В	221	LEU
1	В	238	LYS
1	В	249	THR
1	В	252	ASN
1	В	263	GLN
1	B	284	LYS
1	В	285	CYS
1	В	288	ASP
1	В	293	LEU
1	В	297	ASN
1	B	303	THR
1	В	311	ASP
1	В	316	GLU
1	В	324	THR



Mol	Chain	Res	Type
1	В	334	GLU
1	В	356	TRP
1	В	359	LYS
1	С	2	GLU
1	С	18	LYS
1	С	51	ASP
1	С	77	THR
1	С	100	GLU
1	С	109	PRO
1	С	115	ASN
1	С	126	THR
1	С	128	ASN
1	С	155	SER
1	С	159	VAL
1	С	167	GLU
1	С	172	PRO
1	С	173	HIS
1	С	176	MET
1	С	180	LEU
1	С	207	GLU
1	С	213	LYS
1	С	218	TYR
1	С	221	LEU
1	С	238	LYS
1	С	244	ASP
1	С	249	THR
1	С	252	ASN
1	С	256	ARG
1	С	263	GLN
1	С	265	SER
1	C	277	THR
1	C	278	THR
1	C	284	LYS
1	C	287	ILE
1	C	291	LYS
1	C	292	ASP
1	C	297	ASN
1	C	334	GLU
1	C	348	SER
1	C	359	LYS
1	D	16	LEU
1	D	18	LYS



Mol	Chain	Res	Type
1	D	44	MET
1	D	45	VAL
1	D	53	TYR
1	D	59	GLN
1	D	62	ARG
1	D	66	THR
1	D	77	THR
1	D	99	GLU
1	D	103	THR
1	D	109	PRO
1	D	128	ASN
1	D	159	VAL
1	D	176	MET
1	D	201	VAL
1	D	207	GLU
1	D	221	LEU
1	D	224	GLU
1	D	226	GLU
1	D	238	LYS
1	D	252	ASN
1	D	263	GLN
1	D	266	PHE
1	D	277	THR
1	D	284	LYS
1	D	292	ASP
1	D	297	ASN
1	D	311	ASP
1	D	316	GLU
1	D	334	GLU
1	D	356	TRP
1	D	359	LYS
1	D	371	HIS
1	Е	14	SER
1	E	18	LYS
1	E	49	GLN
1	E	51	ASP
1	Е	56	ASP
1	E	57	GLU
1	E	67	LEU
1	E	80	ASP
1	E	109	PRO
1	Ε	115	ASN



Mol	Chain	Res	Type
1	Е	128	ASN
1	Е	157	ASP
1	Е	176	MET
1	Е	180	LEU
1	Е	187	ASP
1	Е	188	TYR
1	Е	190	MET
1	Е	195	GLU
1	Е	209	VAL
1	Е	213	LYS
1	Е	226	GLU
1	Е	238	LYS
1	Е	249	THR
1	Е	267	ILE
1	Ε	269	MET
1	Е	277	THR
1	Е	284	LYS
1	Е	286	ASP
1	Е	288	ASP
1	Е	292	ASP
1	Е	297	ASN
1	Е	316	GLU
1	Е	334	GLU
1	Е	352	PHE
1	Е	357	ILE
1	Е	359	LYS
1	F	18	LYS
1	F	99	GLU
1	F	115	ASN
1	F	121	GLN
1	F	128	ASN
1	F	149	THR
1	F	162	ASN
1	F	166	TYR
1	F	171	LEU
1	F	180	LEU
1	F	187	ASP
1	F	199	SER
1	F	203	THR
1	F	207	GLU
1	F	213	LYS
1	F	221	LEU



Mol	Chain	Res	Type
1	F	238	LYS
1	F	248	ILE
1	F	249	THR
1	F	263	GLN
1	F	270	GLU
1	F	277	THR
1	F	288	ASP
1	F	291	LYS
1	F	292	ASP
1	F	297	ASN
1	F	303	THR
1	F	311	ASP
1	F	334	GLU
1	F	352	PHE
1	F	359	LYS
1	G	18	LYS
1	G	51	ASP
1	G	62	ARG
1	G	66	THR
1	G	99	GLU
1	G	128	ASN
1	G	159	VAL
1	G	176	MET
1	G	203	THR
1	G	213	LYS
1	G	218	TYR
1	G	238	LYS
1	G	252	ASN
1	G	263	GLN
1	G	264	PRO
1	G	276	GLU
1	G	293	LEU
1	G	297	ASN
1	G	303	THR
1	G	311	ASP
1	G	334	GLU
1	G	359	LYS
1	G	368	SER
1	G	372	ARG
1	Н	2	GLU
1	H	18	LYS
1	Н	99	GLU


Mol	Chain	Res	Type
1	Н	109	PRO
1	Н	128	ASN
1	Н	159	VAL
1	Н	176	MET
1	Н	207	GLU
1	Н	210	ARG
1	Н	215	LYS
1	Н	218	TYR
1	Н	221	LEU
1	Н	238	LYS
1	Н	244	ASP
1	Н	248	ILE
1	Н	249	THR
1	Н	252	ASN
1	Н	260	THR
1	Н	263	GLN
1	Н	277	THR
1	Н	284	LYS
1	Н	297	ASN
1	Н	334	GLU
1	Н	356	TRP
1	Н	359	LYS
1	Н	368	SER
1	Н	371	HIS
1	Ι	2	GLU
1	Ι	18	LYS
1	Ι	49	GLN
1	Ι	57	GLU
1	Ι	59	GLN
1	Ι	62	ARG
1	Ι	100	GLU
1	Ι	109	PRO
1	Ι	128	ASN
1	Ι	159	VAL
1	Ι	176	MET
1	I	187	ASP
1	Ι	207	GLU
1	Ι	210	ARG
1	I	218	TYR
1	Ι	221	LEU
1	Ι	238	LYS
1	Ι	248	ILE



Mol	Chain	Res	Type
1	Ι	252	ASN
1	Ι	253	GLU
1	Ι	260	THR
1	Ι	263	GLN
1	Ι	284	LYS
1	Ι	297	ASN
1	Ι	303	THR
1	Ι	334	GLU
1	Ι	356	TRP
1	Ι	359	LYS
1	Ι	368	SER
1	Ι	371	HIS
1	J	2	GLU
1	J	18	LYS
1	J	62	ARG
1	J	75	ILE
1	J	80	ASP
1	J	100	GLU
1	J	111	ASN
1	J	112	PRO
1	J	115	ASN
1	J	128	ASN
1	J	134	VAL
1	J	159	VAL
1	J	179	ASP
1	J	194	THR
1	J	199	SER
1	J	201	VAL
1	J	202	THR
1	J	207	GLU
1	J	208	ILE
1	J	213	LYS
1	J	218	TYR
1	J	221	LEU
1	J	238	LYS
1	J	242	LEU
1	J	246	GLN
1	J	252	ASN
1	J	257	CYS
1	J	263	GLN
1	J	266	PHE
1	J	267	ILE



Mol	Chain	Res	Type	
1	J	277	THR	
1	J	284	LYS	
1	J	286	ASP	
1	J	292	ASP	
1	J	297	ASN	
1	J	311	ASP	
1	J	323	SER	
1	J	334	GLU	
1	J	348	SER	
1	J	359	LYS	
1	J	368	SER	
1	K	4	GLU	
1	К	18	LYS	
1	K	62	ARG	
1	Κ	99	GLU	
1	К	128	ASN	
1	K	159	VAL	
1	К	173	HIS	
1	K	176	MET	
1	K	187	ASP	
1	K	195	GLU	
1	K	203	THR	
1	K	207	GLU	
1	K	213	LYS	
1	K	215	LYS	
1	Κ	221	LEU	
1	Κ	238	LYS	
1	Κ	242	LEU	
1	K	244	ASP	
1	K	252	ASN	
1	Κ	257	CYS	
1	K	263	GLN	
1	K	277	THR	
1	K	286	ASP	
1	K	297	ASN	
1	K	311	ASP	
1	K	334	GLU	
1	K	357	ILE	
1	K	359	LYS	
1	K	371	HIS	
1	L	2	GLU	
1	L	3	ASP	



Mol	Chain	Res	Type	
1	L	4	GLU	
1	L	18	LYS	
1	L	51	ASP	
1	L	72	GLU	
1	L	75	ILE	
1	L	80	ASP	
1	L	99	GLU	
1	L	109	PRO	
1	L	128	ASN	
1	L	132	MET	
1	L	148	THR	
1	L	159	VAL	
1	L	199	SER	
1	L	207	GLU	
1	L	218	TYR	
1	L	221	LEU	
1	L	238	LYS	
1	L	244	ASP	
1	L	252	ASN	
1	L	260	THR	
1	L	263	GLN	
1	L	284	LYS	
1	L	289	ILE	
1	L	297	ASN	
1	L	316	GLU	
1	L	326	LYS	
1	L	334	GLU	
1	L	348	SER	
1	L	351	THR	
1	L	359	LYS	
1	М	2	GLU	
1	М	18	LYS	
1	М	34	ILE	
1	М	38	PRO	
1	М	45	VAL	
1	М	57	GLU	
1	М	62	ARG	
1	М	65	LEU	
1	М	72	GLU	
1	М	77	THR	
1	М	103	THR	
1	М	128	ASN	



Mol	Chain	Res	Type	
1	М	148	THR	
1	М	159	VAL	
1	М	215	LYS	
1	М	218	TYR	
1	М	238	LYS	
1	М	244	ASP	
1	М	248	ILE	
1	М	249	THR	
1	М	252	ASN	
1	М	276	GLU	
1	М	277	THR	
1	М	284	LYS	
1	М	292	ASP	
1	М	297	ASN	
1	М	303	THR	
1	М	324	THR	
1	М	334	GLU	
1	М	352	PHE	
1	М	359	LYS	
1	М	368	SER	
1	N	2	GLU	
1	N	4	GLU	
1	N	14	SER	
1	N	18	LYS	
1	Ν	24	ASP	
1	N	40	HIS	
1	Ν	43	VAL	
1	N	44	MET	
1	Ν	51	ASP	
1	Ν	59	GLN	
1	N	62	ARG	
1	N	100	GLU	
1	N	109	PRO	
1	Ν	128	ASN	
1	Ν	132	MET	
1	N	148	THR	
1	Ν	159	VAL	
1	Ν	176	MET	
1	Ν	180	LEU	
1	N	193	LEU	
1	N	199	SER	
1	N	210	ARG	



Mol	Chain	Res	Type
1	Ν	215	LYS
1	Ν	218	TYR
1	Ν	221	LEU
1	N	238	LYS
1	N	250	ILE
1	N	252	ASN
1	N	257	CYS
1	N	263	GLN
1	N	266	PHE
1	N	269	MET
1	N	271	SER
1	N	277	THR
1	N	278	THR
1	N	284	LYS
1	N	287	ILE
1	Ν	297	ASN
1	N	311	ASP
1	Ν	322	PRO
1	Ν	324	THR
1	N	325	MET
1	N	326	LYS
1	N	334	GLU
1	Ν	352	PHE
1	N	359	LYS
1	N	368	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type	
1	А	92	ASN	
1	А	111	ASN	
1	А	115	ASN	
1	А	128	ASN	
1	А	280	ASN	
1	В	41	GLN	
1	В	115	ASN	
1	В	162	ASN	
1	В	263	GLN	
1	В	275	HIS	
1	D	41	GLN	
1	D	111	ASN	
1	D	115	ASN	



Mol	Chain	Res	Type
1	D	263	GLN
1	D	275	HIS
1	Е	92	ASN
1	Е	128	ASN
1	Е	252	ASN
1	Е	371	HIS
1	F	111	ASN
1	F	115	ASN
1	F	252	ASN
1	F	263	GLN
1	F	280	ASN
1	G	111	ASN
1	G	115	ASN
1	G	162	ASN
1	G	263	GLN
1	G	275	HIS
1	Н	111	ASN
1	Н	115	ASN
1	Н	173	HIS
1	Н	263	GLN
1	Н	280	ASN
1	Ι	162	ASN
1	Ι	263	GLN
1	J	263	GLN
1	K	263	GLN
1	L	92	ASN
1	L	162	ASN
1	L	371	HIS
1	М	111	ASN
1	М	115	ASN
1	М	161	HIS
1	М	246	GLN
1	М	252	ASN
1	N	111	ASN
1	N	115	ASN
1	N	252	ASN

Continued from previous page...

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-1088. 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: 56



Z Index: 288



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

6.3 Largest variance slices (i)

6.3.1 Primary map





Z Index: 413

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 430.0. 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 687 nm^3 ; this corresponds to an approximate mass of 621 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-1088 and PDB model 3B5U. 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 430.0 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 (430.0).



9.4 Atom inclusion (i)



At the recommended contour level, 7% of all backbone atoms, 6% 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 (430.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.0648	0.0230	
А	0.0598	0.0150	1 0
В	0.0959	0.0190	
С	0.1130	0.0330	
D	0.0772	0.0110	
Е	0.0796	0.0250	
F	0.0855	0.0240	
G	0.0650	0.0290	
Н	0.0302	0.0040	
Ι	0.0209	0.0280	
J	0.0393	0.0190	0.0
K	0.0393	0.0280	<0.0
L	0.0521	0.0390	
М	0.0719	0.0240	
N	0.0768	0.0190	1

