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PDB ID	:	8H37
EMDB ID	:	EMD-34453
Title	:	Cryo-EM Structure of the KBTBD2-CUL3-Rbx1-p85a tetrameric complex
Authors	:	Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on	:	2022-10-08
Resolution	:	7.52 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.52 Å.

Ramachandran outliers

Sidechain outliers

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.



154571

154315

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.

4023

3826

Mol	Chain	Length	Quality of chain		
1	С	768	59%	27%	7% • 6%
1	F	768	63%	26%	• 6%
1	М	768	62%	27%	5% 6%
1	Ο	768	61%	29%	• 6%
2	D	108	• 51% 20%	7% •	18%
2	Е	108	39% 32%	10% •	18%
2	Q	108	48% 27%	6% ·	18%
2	R	108	• 34% 37%	10% •	18%



Conti	nuea _I ron	i previous	page		
Mol	Chain	Length	Quality of chain		
3	А	623	58%	27%	6% 9%
3	В	623	65%	24%	• 9%
3	Ν	623	66%	23%	• 9%
3	Р	623	69%	19%	• 11%
4	G	724	14% 7% • 77%		
4	Н	724	17% 6% · 77%		
4	Ι	724	5% 16% 6% • 77%		
4	J	724	5% 16% 6% • 77%		



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 49321 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	Atoms					AltConf	Trace
1	С	720	Total	С	Ν	Ο	\mathbf{S}	0	0
1	U	120	5791	3633	1024	1095	39	0	0
1	Б	720	Total	С	Ν	Ο	S	0	0
1	Г	720	5677	3558	1010	1073	36	0	0
1	М	720	Total	С	Ν	Ο	S	0	0
1	111	120	5672	3553	1008	1074	37	0	0
1	0	720	Total	С	Ν	Ο	S	0	0
1	0	120	5767	3620	1017	1091	39	0	0

• Molecule 1 is a protein called Cullin-3.

• Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
0	F	80	Total	С	Ν	0	S	0	0
	Ľ	09	737	466	135	127	9	0	0
0	Л	80	Total	С	Ν	0	S	0	0
	D	69	737	466	135	127	9	0	0
0	D	. 89	Total	С	Ν	0	S	0	0
	2 R		737	466	135	127	9	0	0
0	0	80	Total	С	Ν	0	S	0	0
2	Q	Q 89	737	466	135	127	9	0	0

• Molecule 3 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Λ	567	Total	С	Ν	0	S	0	0
0	Л	507	4559	2918	750	853	38	0	0
3	В	564	Total	С	Ν	0	S	0	0
0	D	304	4510	2884	746	842	38	0	0
2	N	564	Total	С	Ν	0	S	0	0
0	3 N	304	4510	2880	746	846	38	0	0
9	D	557	Total	С	Ν	0	S	0	0
3	Г	557	4423	2833	725	831	34	0	0

There are 4 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	252	ASP	SER	engineered mutation	UNP Q8IY47
В	252	ASP	SER	engineered mutation	UNP Q8IY47
N	252	ASP	SER	engineered mutation	UNP Q8IY47
Р	252	ASP	SER	engineered mutation	UNP Q8IY47

• Molecule 4 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace						
4	С	169	Total	С	Ν	0	S	0	0						
4	G	100	1424	885	256	278	5	0	0						
4	Ц	169	Total	С	Ν	0	S	0	0						
4	11	108	1341	828	246	263	4	0	0						
4	Т	169	Total	С	Ν	0	S	0	0						
4	1	1	1	1	1			108	1360	840	250	266	4	0	0
4	т	168	Total	С	Ν	0	S	0	0						
4	J	100	1327	816	244	263	4	0	0						

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	Е	3	Total Zn 3 3	0
5	D	3	Total Zn 3 3	0
5	R	3	Total Zn 3 3	0
5	Q	3	Total Zn 3 3	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain C: 59% 27% 7% • 6% PHE GGLY GGLY VAL LYS GGLV GGLY VAL CGLY VAL GGLY VAL GGLY VAL GGLY VAL ASN ASN • Molecule 1: Cullin-3
- Molecule 1: Cullin-3















• Molecule 1: Cullin-3





• Molecule 2: E3 ubiquitin-protein ligase RBX1





• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain R:	34%	37%	10% •	18%
MET ALA ALA ALA ALA MET MET VAL	THAF THAF PRIO SER SER SER ALY ALA ALA ALA ALA CLY CLY FZO FZO FZO FZO FZO FZO FZO FZO FZO FZO	V24 V25 V27 V27 V27 V28 V27 V27 V27 V27 V23 V33 V35 V35 V35 V35 V35 V35 V35 V35 V3	L3/ V38 V38 V38 V38 V41 V41 C42 L44 L44 C45 C45 C45 R46 N47 H48	149 152 154 154 154 057 058 056 056 056 056
A63 T64 565 E66 A71 W72	N76 F79 134 134 W87 W87 W87 W87 W87 W87 W87 W93 W93 W93 W93 W93 W93 W93 W93 W93 W93	097 1097 1000 1001 1002 1003 1003 1004 1006		
• Molecule	e 2: E3 ubiquitin-prot	ein ligase RBX1		
Chain Q:	48%	2	7% 6% •	18%
MET ALA ALA ALA MET ASP VAL	THR PRO SER SER SER SER ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	W27 N28 A29 A35 D36 D36 D36 D40 D40 D41 C42	C45 R46 M47 M50 M50 D51 I54 N59	E66 W72 V74 134 W87 W87 W87 W87 W87 W87 W87 T90
R91 Q92 V93 C94 D95 L96 D97 N00	R90 E102 K105 K105 G107 H108			
• Molecule	e 3: Kelch repeat and	BTB domain-con	taining protein	2
Chain A:	58%		27%	6% 9%
MET SER THR GLN GLU R7 R7	190 110 117 117 129 129 129 129 129 129 129 129 129 129	853 864 865 865 866 867 867 875 875 877	A108 C109 Q112 V113 R119 Y123 K126	K127 1128 E131 N132 C133 C133 C133 C133 D176 D176 D176
L186 W201 R209	2226 2226 7229 7229 7241 8241 8243 8243 8243 8243 8243 7255 7255 7255 7255 7255 7255 7255 725	M263 M263 K265 F271 F271 F271 F271 F271 F271 F277 S275 S275 S275 S275 S275 S275 S275	C280 C280 C281 C282 C284 C284 C285 C287 C287 C287 C287 C287 C287	K297 L298 C299 S300 P301 P301 P305 H305 K305 V305
(309 (311 (311 (312 (312 (313 (314 (315) (315) (315) (315)	1311 1311 1318 1318 1320 1320 1320 1321 1328 1328 1328 1328 1328 148 148 148 148 148	EVER EVER SER SER SER LLYS CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	C349 7350 7351 7352 7355 7355 0356 0356 0356 7356 7356 7356 7356 7356 7356 7356 7	M366 L367 L367 1369 R370 R372 R372 P373 S374 L375 V376
C377 C378 Y381 T382 Y383 A384	Cast Cast Cast Cast Cast Cast Cast Cast	7404 7405 7405 7406 7406 7406 7410 7410 7411 7411 7412 7412	V425 V427 V427 V431 V432 V435 F443 F443 F443 F445	8446 0447 0447 0445 0452 0456 0456 0456 0456 0456 0456 0456 7457 5459 8459
A462 K470 1471 F472 Y473	6476 6476 1477 1115 1115 1115 ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	THR THR VAL ASP GAS GAS GAS CASP CASP CASP CASP CASP CASP CASP CA	V004 N505 N507 B508 N509 N511 A513 A513 A513 A513 A513 A513 A513 A	P516 A517 K519 K519 F520 S521 V525 V525 V528 V528 V528
C535 V536 M538 M538 R539 E540 T541	L543 L543 K548 K548 K548 L555 L556 L556 L556 R560 R560 R561 S551 L563 L563 L563	1567 1572 1572 1573 1575 1576 1576 1578 1578 1578 1578 1578	C581 1582 V583 K584 K586 L586 C586 C589 C589 C589 C592 F592	S594 5594 6597 7599 7599 7509 7603 7603 7603 7606 71605 717 7605 717 717 717 717 717 717 717 717 717 71
THR GLU GLU PHE GLU LEU ASP	GLU MET ALA ALA PRO VAL			







• Molecule 4: Phosphatidylinositol 3-kinase regulatory subunit alpha



Chain	H:		17%	Ď	6	5%	,	-	-	-	-			-	77	%		-	-	-	-	-	-			
MET SER ALA GLU GLY	GLN	ARG	LEU TYR	ASP TYR I VS	LYS	ARG	GLU ASP	ILE ASP	LEU HIS	GLY	ASP ILE	THR	VAL ASN	LYS GLY	SER LEU	VAL ALA I FII	GLY	SER	GLY	GLU ALA ARG	PRO GLU	GLU	GLY TRP	LEU ASN GLY	TYR ASN	
GLU THR GLY GLU	ARG GLY	PHE	GLY	TYR VAL	TYR	GLY	LYS	ILE SER	PRO PRO	THR PRO	LYS PRO	ARG PRO	PRO ARG	PRO LEU	PRO VAL	ALA PRO GI V	SER	LYS THR	GLU	ASP VAL GLU	GLN	ALA LEU	THR LEU	PRO ASP LEU	ALA GLU	
GLN PHE ALA PRO PRO	ASP ILE	PRO PPO	LEU LEU	ILE LYS	VAL	ALA	dLU GLU	GLY GLY	GLU	CYS SER	THR	TYR ARG	GLN	SER SER	SER ASN	ALA	LEU ARG	GLN	ASP	CYS ASP THR	PRO	VAL ASP	GLU	MET ILE ASP	VAL	
VAL LEU ALA ASP ALA	PHE	TYR	LEU	LEU PRO ASM	PRO VAT	ILE	ALA	VAL TYR	SER GLU	MET ILE	SER	ALA PRO	GLU VAL	GLN SER	SER GLU	GLU TYR TIF	GLN	LYS	LYS	ILE ARG SER	PRO	ILE PRO	HIS GLN	TYR TRP LEU	THR	
GLN TYR LEU LEU	HIS PHE	PHE LYS	SER	THR SER GED	LYS	LEU	ASN	ARG VAL	LEU SER	GLU	PHE SER	PRO MET	LEU	ARG PHE	SER ALA	ALA SER SFR	ASP ASN	THR GLU	ASN LEU	ILE LYS VAL	ILE GLU	ILEU	ILE SER	THR GLU TRP	ASN GLU	
ARG GLN PRO ALA PRO	ALA LEU	PRO T VS	PRO PRO	LYS PRO TUB	THR	ALA	ASN	MET ASN	ASN ASN	MET SER	LEU GLN	ASP ALA	GLU TRP	TYR TRP	GLY ASP	ILE SER ABC	GLU	VAL ASN	GLU GLU	LEU ARG ASP	THR	ASP GLY	THR PHE	LEU VAL ARG	ASP ALA	
SER THR LYS MET HIS	GLY ASP	THR	THR	ARG LYS	GLY	ASN T VC	LEU	LYS ILE	PHE HIS	ARG ASP	GLY GLY	TYR GLY	PHE SER	ASP PRO	LEU THR	PHE SER SER	VAL VAL	GLU	ASN	HIS TYR ARG	ASN GLU	SER	ALA GLN	TYR ASN PRO	LEU	
																							•	••	••	•
ASP VAL LYS LEU LEU	TYR PRO	VAL SER 1 VC	TYR GLN	0433 N763	T454	Q457 E457	K459	E462	L466 Y467	E468 E469	R472	E476	1477	K480 R481	1484	E485 A486 F487	N488 E489	E496	<mark>0499</mark>	E502	S505 K506	E507	F512 K513	E515	G516 N517	E518
K519 E520 I521	M525 H526	D529	R534	1538 1538 1539	R542	R543 R544	L545 E546	E547 D548	K550 K550		R562 M563					NGOO	GLU ASN THE	GLU	GLN TYR	SER	VAL GLU	ASP	GLU ASP 1 EU	PRO HIS	HIS ASP GLU	
LYS THR TRP ASN VAL	GLY SER	ASN	ASN LYS	ALA GLU ASM	LEU LEU	ARG	LYS ARG	ASP GLY	THR PHE	LEU VAL	ARG GLU	SER	GLN	GLY CYS	TYR ALA	CYS SER VAT	VAL VAL	ASP GLY	GLU VAL	LYS HIS CYS	VAL	ASN LYS	THR ALA	THR GLY TYR	GLY	
ALA GLU PRO TYR ASN	LEU TYR	SER	CLU GLU	LEU VAL	HIS	GLN	THR	LEU VAL	GLN	ASN ASP	SER	ASN VAL	THR LEU	ALA TYR	PRO VAL	TYR ALA GI N	GLN ARG	ARG								
• Mole	ecul	e 4:	: Pl	ıosp	pha	atic	lyli	nos	ito	13	-kiı	nas	se 1	regi	ulat	tory	y su	bu	nit	alp	oha					
Chain	I:	0%	16%		6%	•	-	-	-	-	-	-	-	-	77%	_	-	-	-	-	-	-	_			
MET SER ALA GLU GLY	GLN	ARG ARG	LEU TYR	ASP TYR I VS	LYS	ARG	GLU ASP	ILE ASP	LEU HIS	CLY GLY	ASP ILE	THR	VAL ASN	CLY GLY	SER	VAL ALA I FII	GLY	SER	GLY	GLU ALA ARG	PRO GLU	GLU	GL Y TRP	LEU ASN GL_Y	TYR ASN	
GLU THR GLY GLU	ARG GLY	PHE	GLY THR	TYR VAL CT II	TYR	GLY	LYS	ILE SER	PRO PRO	THR PRO	LYS PRO	ARG PRO	PRO ARG	PRO LEU	PRO VAL	ALA PRO CI V	SER	LYS THR	GLU	ASP VAL GI,U	GLN GLN	ALA LEU	THR LEU	PRO ASP LEU	ALA GLU	
GLN PHE ALA PRO	ASP ILE	PRO PRO	LEU LEU	ILE LYS	VAL	ALA	GLU LYS	GLY GLY	LEU GLU	CYS SER	THR LEU	TYR ARG	THR GLN	SER SER	SER ASN	ALA	LEU ARG	GLN	ASP	CYS ASP THR	PRO	VAL ASP	GLU GLU	MET ILE ASP	VAL	
VAL LEU ALA ASP ALA	PHE	TYR 1 Ell	LEU ASP	LEU PRO ASN	PRO VAT	UAL TLE DDO	ALA ALA	VAL TYR	SER GLU	MET ILE	SER	ALA PRO	GLU VAL	GLN SER	SER GLU	GLU TYR TIF	GLN	LEU	LYS	ILE ARG SFR	PRO	ILE PRO	HIS	TYR TRP LEU	THR	
GLN TYR LEU LEU	HIS PHE	LYS	SER GLN	THR SER SER	LYS	LEU	ASN	ARG VAL	LEU SER	GLU ILE	PHE SER	PRO MET	LEU PHE	ARG PHE	SER ALA	ALA SER SFR	ASP ASN	THR GLU	ASN LEU	ILE LYS VAL	ILE GLU	ILE LEU	ILE SER	THR GLU TRP	ASN GLU	
ARG GLN PRO PRO	ALA LEU	PRO 1 VS	PRO PRO	LYS PRO TUB	THR VAT	ALA	ASN	MET ASN	ASN ASN	MET SER	GLN	ASP ALA	GLU TRP	TYR TRP	GLY ASP	ILE SER ARG	GLU	VAL ASN	GLU	LEU ARG ASP	THR	ASP GLY	THR PHE	LEU VAL ARG	ASP ALA	
		_			_	_			_	_	_	_	_	_				_	_			_				







PRO VAL TYR ALA GLN GLN ARG ARG



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	239068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.603	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	511.488, 511.488, 511.488	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.664, 2.664, 2.664	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	С	0.45	0/5879	0.52	0/7905	
1	F	0.42	0/5760	0.50	0/7752	
1	М	0.53	0/5753	0.53	0/7743	
1	0	0.42	0/5854	0.51	0/7873	
2	D	0.54	0/759	0.62	0/1029	
2	Ε	0.56	0/759	0.67	0/1029	
2	Q	0.58	0/759	0.61	0/1029	
2	R	0.54	0/759	0.65	0/1029	
3	А	0.52	0/4667	0.52	0/6335	
3	В	0.35	0/4616	0.43	0/6268	
3	Ν	0.33	0/4616	0.43	0/6266	
3	Р	0.35	0/4527	0.45	0/6151	
4	G	0.38	0/1443	0.46	0/1926	
4	Н	0.41	0/1356	0.48	0/1813	
4	Ι	0.42	0/1376	0.47	0/1839	
4	J	0.38	0/1342	0.46	0/1797	
All	All	0.44	0/50225	0.50	0/67784	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	5791	0	5773	203	0
1	F	5677	0	5575	135	0
1	М	5672	0	5583	146	0
1	0	5767	0	5730	142	0
2	D	737	0	686	23	0
2	Е	737	0	686	43	0
2	Q	737	0	686	16	0
2	R	737	0	686	54	0
3	А	4559	0	4441	107	0
3	В	4510	0	4385	113	0
3	N	4510	0	4373	126	0
3	Р	4423	0	4245	107	0
4	G	1424	0	1387	34	0
4	Н	1341	0	1243	22	0
4	Ι	1360	0	1276	28	0
4	J	1327	0	1203	25	0
5	D	3	0	0	0	0
5	Е	3	0	0	0	0
5	Q	3	0	0	0	0
5	R	3	0	0	0	0
All	All	49321	0	47958	1198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1198) 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 (\AA)	overlap (Å)
3:B:154:ARG:HD3	3:B:357:GLN:NE2	1.43	1.33
3:N:154:ARG:HD3	3:N:357:GLN:NE2	1.43	1.30
1:M:531:ALA:HB3	2:R:27:TRP:CZ3	1.76	1.20
3:N:298:LEU:HD23	3:N:591:LEU:HD21	1.26	1.18
3:N:14:ALA:HB2	3:P:18:LEU:HD22	1.21	1.15
3:P:298:LEU:CD2	3:P:591:LEU:HD21	1.76	1.13
3:B:298:LEU:HD23	3:B:591:LEU:HD21	1.26	1.11
3:P:298:LEU:HD23	3:P:591:LEU:HD21	1.14	1.10
3:N:185:ASN:CG	3:N:356:GLN:HE22	1.59	1.05
2:D:39:VAL:O	2:D:40:ASP:HB3	1.56	1.04
3:B:185:ASN:CG	3:B:356:GLN:HE22	1.59	1.03
1:F:68:LYS:HE3	3:B:142:LEU:HD12	1.40	1.03
3:N:154:ARG:HD3	3:N:357:GLN:HE21	0.94	1.03
3:P:154:ARG:HD3	3:P:357:GLN:NE2	1.74	1.03



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:Q:39:VAL:O	2:Q:40:ASP:HB3	1.56	1.02
3:B:154:ARG:CD	3:B:357:GLN:NE2	2.22	1.02
3:N:154:ARG:CD	3:N:357:GLN:NE2	2.22	1.02
2:E:37:ILE:HD11	2:E:39:VAL:HG22	1.44	0.99
3:B:154:ARG:HD3	3:B:357:GLN:HE21	0.94	0.99
1:C:480:SER:HB2	1:C:506:ARG:HB3	1.40	0.97
1:C:440:LEU:HB3	1:C:477:MET:SD	2.04	0.97
1:C:85:LEU:HA	1:C:88:LYS:HB3	1.46	0.96
1:C:440:LEU:HD13	1:C:477:MET:HG3	1.47	0.96
1:C:54:PHE:HB2	3:A:59:MET:CE	1.95	0.96
2:R:37:ILE:HD11	2:R:39:VAL:HG22	1.44	0.95
1:F:768:ALA:HB1	2:D:89:LYS:HB3	1.47	0.95
1:M:531:ALA:HB3	2:R:27:TRP:HZ3	1.14	0.95
3:P:154:ARG:HH11	3:P:357:GLN:HE22	1.13	0.95
1:F:68:LYS:NZ	3:B:142:LEU:HA	1.81	0.95
3:N:57:ARG:CZ	3:P:24:PHE:HZ	1.79	0.94
1:C:349:LYS:NZ	1:C:417:VAL:HG12	1.82	0.94
3:N:298:LEU:CD2	3:N:591:LEU:HD21	1.98	0.94
3:N:14:ALA:CB	3:P:18:LEU:HD22	1.97	0.93
1:C:484:MET:SD	1:C:504:THR:HG22	2.09	0.93
3:P:297:LYS:HB3	3:P:592:GLU:OE1	1.70	0.91
3:B:298:LEU:CD2	3:B:591:LEU:HD21	1.99	0.91
2:R:79:PHE:CD2	2:R:84:ILE:HG21	2.06	0.91
3:N:30:PHE:HE1	3:P:60:PHE:CB	1.84	0.90
1:O:59:ARG:CZ	3:N:75:ARG:HD2	2.01	0.90
3:N:30:PHE:CE1	3:P:60:PHE:CB	2.55	0.90
1:O:96:SER:HB3	1:O:104:THR:HG21	1.54	0.89
3:A:308:VAL:HB	3:A:320:ILE:HG13	1.53	0.89
1:F:96:SER:HB3	1:F:104:THR:HG21	1.54	0.88
3:A:497:VAL:HG23	3:A:514:ASN:ND2	1.87	0.87
1:M:531:ALA:CB	2:R:27:TRP:CZ3	2.56	0.87
2:R:71:ALA:CB	2:R:84:ILE:HD11	2.05	0.86
2:E:71:ALA:CB	2:E:84:ILE:HD11	2.04	0.86
1:C:484:MET:CE	1:C:504:THR:HG22	2.05	0.86
1:C:54:PHE:HB2	3:A:59:MET:HE1	1.58	0.85
1:C:349:LYS:HZ3	1:C:417:VAL:HG12	1.39	0.85
1:M:531:ALA:CB	2:R:27:TRP:HZ3	1.87	0.85
3:P:154:ARG:HD3	3:P:357:GLN:HE21	1.39	0.84
3:P:185:ASN:CG	3:P:356:GLN:HE22	1.82	0.84
1:F:531:ALA:CB	2:D:27:TRP:CZ3	2.62	0.82
1:0:53:SER:HA	3:N:66:GLU:OE2	1.79	0.82



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:O:440:LEU:HD13	1:O:477:MET:HG3	1.61	0.82		
1:F:440:LEU:HD13	1:F:477:MET:HG3	1.61	0.81		
2:R:39:VAL:HG12	2:R:39:VAL:O	1.82	0.80		
3:P:154:ARG:NH1	3:P:357:GLN:NE2	2.29	0.80		
3:N:14:ALA:HB2	3:P:18:LEU:CD2	2.07	0.80		
1:O:55:GLU:OE2	3:N:72:VAL:HG13	1.81	0.80		
2:E:71:ALA:HB3	2:E:84:ILE:HD11	1.63	0.79		
3:N:61:MET:SD	3:P:29:LEU:HD22	2.22	0.79		
3:P:154:ARG:NH1	3:P:357:GLN:HE22	1.79	0.79		
2:R:71:ALA:HB3	2:R:84:ILE:HD11	1.63	0.79		
1:C:484:MET:SD	1:C:504:THR:HA	2.22	0.78		
1:F:68:LYS:HZ1	3:B:142:LEU:HA	1.43	0.78		
1:F:89:VAL:HG11	1:F:151:VAL:HG22	1.65	0.78		
1:M:525:PRO:HB2	1:M:528:PRO:HD2	1.64	0.78		
3:N:154:ARG:HH11	3:N:357:GLN:NE2	1.82	0.78		
1:O:89:VAL:HG11	1:O:151:VAL:HG22	1.65	0.78		
2:E:39:VAL:HG12	2:E:39:VAL:O	1.82	0.78		
1:O:59:ARG:HD2	3:N:75:ARG:HB2	1.67	0.77		
3:B:185:ASN:CG	3:B:356:GLN:NE2	2.37	0.77		
1:M:277:VAL:HG21	1:M:312:THR:HB	1.65	0.77		
3:B:154:ARG:HH11	3:B:357:GLN:NE2	1.82	0.76		
1:F:531:ALA:HB1	2:D:27:TRP:CZ3	2.22	0.75		
1:O:54:PHE:HB2	3:N:59:MET:HE3	1.67	0.75		
3:N:265:LYS:HD3	3:N:587:TYR:CE1	2.22	0.75		
1:C:91:GLU:HA	1:C:94:LEU:HB2	1.67	0.75		
1:O:49:ASN:ND2	3:N:64:LEU:HD21	2.02	0.75		
3:N:24:PHE:HZ	3:P:57:ARG:NE	1.83	0.75		
3:B:265:LYS:HD3	3:B:587:TYR:CE1	2.22	0.75		
3:A:253:MET:HB3	3:A:258:LYS:HG3	1.69	0.74		
1:C:125:TYR:HD1	3:A:112:GLN:HE21	1.35	0.74		
3:N:185:ASN:CG	3:N:356:GLN:NE2	2.37	0.74		
1:M:531:ALA:HB3	2:R:27:TRP:CE3	2.22	0.74		
1:O:54:PHE:HB2	3:N:59:MET:CE	2.16	0.74		
3:B:297:LYS:HB3	3:B:592:GLU:OE1	1.87	0.74		
3:A:308:VAL:HB	3:A:320:ILE:CG1	2.17	0.74		
1:F:37:LEU:HD13	1:F:57:LEU:HD12	1.68	0.74		
3:N:358:ASN:ND2	3:N:591:LEU:O	2.21	0.74		
3:A:427:VAL:HG23	3:A:432:TYR:HB2	1.70	0.74		
3:P:253:MET:HB3	3:P:258:LYS:HG3	1.69	0.74		
1:F:93:VAL:HG11	1:F:156:CYS:SG	2.28	0.73		
1:F:531:ALA:HB1	2:D:27:TRP:CE3	2.24	0.73		



Atom 1	Atom 2	Interatomic	Clash
	Atom-2	distance (\AA)	overlap (Å)
3:B:358:ASN:ND2	3:B:591:LEU:O	2.21	0.73
1:F:531:ALA:HB3	2:D:27:TRP:CZ3	2.24	0.73
1:F:68:LYS:CE	3:B:142:LEU:HD12	2.19	0.72
1:M:480:SER:HB2	1:M:506:ARG:HB3	1.69	0.72
1:O:93:VAL:HG11	1:0:156:CYS:SG	2.29	0.72
3:P:298:LEU:HD23	3:P:591:LEU:CD2	2.08	0.71
3:B:261:LEU:HG	3:B:587:TYR:CE1	2.25	0.71
3:B:266:GLU:HG3	3:B:588:PRO:HG3	1.73	0.71
3:N:261:LEU:HG	3:N:587:TYR:CE1	2.25	0.71
3:P:154:ARG:CD	3:P:357:GLN:NE2	2.53	0.71
1:C:274:LYS:HA	1:C:277:VAL:HG22	1.72	0.71
1:O:59:ARG:NH2	3:N:75:ARG:HD2	2.06	0.71
2:R:34:ALA:HA	2:R:76:ASN:ND2	2.05	0.70
1:C:58:TYR:HH	3:A:112:GLN:CD	1.94	0.70
1:M:262:LYS:HB3	1:M:266:ARG:NH1	2.07	0.70
2:R:71:ALA:HB3	2:R:84:ILE:CD1	2.22	0.70
2:R:79:PHE:CD2	2:R:84:ILE:CG2	2.74	0.70
1:F:378:LEU:HD23	1:F:421:PHE:O	1.92	0.70
2:E:71:ALA:HB3	2:E:84:ILE:CD1	2.22	0.69
3:P:459:ARG:HB3	3:P:476:GLY:HA2	1.74	0.69
4:G:466:LEU:HD13	4:G:563:MET:HG2	1.75	0.69
3:N:266:GLU:HG3	3:N:588:PRO:HG3	1.73	0.69
1:C:58:TYR:OH	3:A:112:GLN:CD	2.31	0.69
3:B:397:ARG:HB3	3:B:415:LEU:HB2	1.74	0.69
3:P:372:LYS:HD3	3:P:580:ARG:HH21	1.58	0.69
3:N:397:ARG:HB3	3:N:415:LEU:HB2	1.74	0.68
1:M:89:VAL:HA	1:M:92:ASP:HB2	1.75	0.68
1:M:622:ILE:HG12	1:M:627:LEU:HD13	1.75	0.68
4:J:466:LEU:HD13	4:J:563:MET:HG2	1.75	0.68
1:C:259:PRO:HA	1:C:262:LYS:HG2	1.75	0.68
4:H:466:LEU:HD13	4:H:563:MET:HG2	1.75	0.68
3:N:185:ASN:ND2	3:N:356:GLN:HE22	1.92	0.68
3:N:436:LEU:O	3:N:455:ARG:NH2	2.26	0.68
3:P:185:ASN:CG	3:P:356:GLN:NE2	2.47	0.68
1:C:506:ARG:HB2	2:E:30:VAL:HG22	1.76	0.68
1:M:68:LYS:HE3	3:P:141:ASP:O	1.93	0.68
1:O:54:PHE:CZ	3:N:64:LEU:CD1	2.76	0.68
3:A:302:PRO:HD2	3:A:305:LEU:HB2	1.74	0.67
3:B:185:ASN:ND2	3:B:356:GLN:HE22	1.92	0.67
1:F:622:ILE:HG12	1:F:627:LEU:HD13	1.77	0.67
3:B:436:LEU:O	3:B:455:ARG:NH2	2.26	0.67



Atom-1	Atom-2	Interatomic	Clash
110111-1	1100111-2	distance (Å)	overlap (Å)
4:I:466:LEU:HD13	4:I:563:MET:HG2	1.75	0.67
1:C:622:ILE:HG12	1:C:627:LEU:HD13	1.76	0.67
1:F:425:LYS:HZ2	1:F:462:CYS:HB2	1.58	0.67
3:N:57:ARG:CZ	3:P:24:PHE:CZ	2.71	0.67
3:P:297:LYS:HB3	3:P:592:GLU:CD	2.14	0.67
1:C:58:TYR:OH	3:A:112:GLN:NE2	2.27	0.67
1:O:425:LYS:HZ2	1:O:462:CYS:HB2	1.58	0.67
3:B:372:LYS:HD3	3:B:580:ARG:HH21	1.60	0.67
1:O:532:PHE:HB2	2:Q:27:TRP:HH2	1.59	0.66
3:N:154:ARG:CD	3:N:357:GLN:HE22	2.07	0.66
1:M:66:LEU:HD21	3:P:143:PHE:CE1	2.31	0.66
1:C:277:VAL:HG21	1:C:312:THR:HB	1.77	0.66
3:A:427:VAL:CG2	3:A:432:TYR:HB2	2.25	0.66
1:O:54:PHE:CZ	3:N:64:LEU:HD11	2.30	0.66
3:N:372:LYS:HD3	3:N:580:ARG:HH21	1.60	0.66
1:O:525:PRO:HD2	1:O:528:PRO:HB2	1.78	0.66
1:C:488:ARG:HD3	1:C:503:LEU:O	1.96	0.66
1:C:75:THR:HA	1:C:78:ARG:HD2	1.77	0.65
1:M:81:VAL:O	1:M:84:HIS:HB3	1.96	0.65
1:C:697:ASP:HA	1:C:700:LYS:HD2	1.77	0.65
1:F:531:ALA:CB	2:D:27:TRP:CE3	2.78	0.65
3:B:154:ARG:CD	3:B:357:GLN:HE22	2.07	0.65
3:B:301:PRO:HD2	3:B:360:TRP:HD1	1.61	0.65
3:A:517:ALA:HB1	3:A:521:SER:CB	2.27	0.65
3:N:301:PRO:HD2	3:N:360:TRP:HD1	1.61	0.65
1:C:59:ARG:NH2	3:A:75:ARG:HD2	2.12	0.65
4:J:459:LYS:HB3	4:J:570:LEU:HD13	1.79	0.65
3:P:300:SER:HA	3:P:360:TRP:HE1	1.62	0.65
1:O:622:ILE:HG12	1:O:627:LEU:HD13	1.77	0.65
3:A:17:LEU:CD1	3:B:51:THR:HB	2.27	0.65
4:G:453:ASN:HA	4:G:577:ARG:HH12	1.61	0.65
1:F:459:LYS:HZ2	1:F:467:THR:HB	1.62	0.65
4:G:459:LYS:HB3	4:G:570:LEU:HD13	1.79	0.65
1:C:54:PHE:CB	3:A:59:MET:CE	2.75	0.64
1:F:54:PHE:HA	1:F:57:LEU:HD23	1.79	0.64
1:O:525:PRO:HB2	1:O:528:PRO:HD2	1.78	0.64
1:M:504:THR:O	2:R:28:ASN:HA	1.98	0.64
3:A:325:VAL:HG12	3:A:345:ARG:HB3	1.78	0.64
3:N:459:ARG:NH1	3:N:498:THR:OG1	2.30	0.64
1:C:504:THR:O	2:E:28:ASN:HA	1.98	0.64
3:B:459:ARG:NH1	3:B:498:THR:OG1	2.30	0.64



	bus page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:37:ILE:HD11	2:E:39:VAL:CG2	2.25	0.64
4:G:449:LEU:HD21	4:G:594:LEU:CD2	2.27	0.64
2:R:37:ILE:HD11	2:R:39:VAL:CG2	2.25	0.64
3:A:109:CYS:O	3:A:112:GLN:NE2	2.31	0.64
4:H:459:LYS:HB3	4:H:570:LEU:HD13	1.79	0.64
3:N:57:ARG:NH2	3:P:24:PHE:HZ	1.95	0.64
1:C:556:SER:HA	1:C:595:SER:HA	1.80	0.63
1:M:531:ALA:CB	2:R:27:TRP:CE3	2.81	0.63
1:M:248:VAL:HG11	1:M:257:GLU:HB2	1.81	0.63
4:I:459:LYS:HB3	4:I:570:LEU:HD13	1.79	0.63
3:P:109:CYS:O	3:P:112:GLN:NE2	2.31	0.63
2:E:94:CYS:HB2	2:E:101:TRP:HB2	1.79	0.63
1:C:437:ALA:HA	1:C:513:TRP:HZ3	1.63	0.63
1:O:266:ARG:HG2	1:O:307:PRO:HD3	1.80	0.63
1:C:54:PHE:CB	3:A:59:MET:HE1	2.28	0.63
1:F:102:LEU:O	1:F:106:ASN:ND2	2.32	0.63
3:N:301:PRO:HD2	3:N:360:TRP:CD1	2.34	0.63
1:C:102:LEU:O	1:C:106:ASN:ND2	2.32	0.63
1:F:556:SER:HA	1:F:595:SER:HA	1.80	0.63
1:O:556:SER:HA	1:O:595:SER:HA	1.80	0.63
1:C:74:TYR:HA	1:C:77:LEU:HD12	1.81	0.62
1:M:503:LEU:HD11	1:M:531:ALA:HB1	1.79	0.62
2:E:44:ILE:CD1	2:E:84:ILE:HG22	2.28	0.62
1:C:525:PRO:HB2	1:C:528:PRO:HD2	1.82	0.62
1:0:102:LEU:O	1:O:106:ASN:ND2	2.32	0.62
2:R:44:ILE:CD1	2:R:84:ILE:HG22	2.28	0.62
1:C:703:ILE:HB	1:C:741:ILE:HD13	1.80	0.62
3:P:436:LEU:O	3:P:455:ARG:NH2	2.31	0.62
1:C:221:SER:HB3	1:C:268:LEU:HD22	1.81	0.62
3:B:301:PRO:HD2	3:B:360:TRP:CD1	2.34	0.62
3:B:352:TRP:HB3	3:B:363:LYS:HE3	1.82	0.62
3:A:243:SER:HB2	3:A:292:ALA:HB2	1.80	0.62
1:F:66:LEU:C	1:F:68:LYS:H	2.02	0.62
3:N:154:ARG:HH11	3:N:357:GLN:HE22	1.48	0.61
1:C:54:PHE:HB2	3:A:59:MET:HE3	1.82	0.61
1:M:556:SER:HA	1:M:595:SER:HA	1.80	0.61
1:M:83:GLU:HA	1:M:86:ILE:HG22	1.82	0.61
3:P:154:ARG:HH11	3:P:357:GLN:NE2	1.85	0.61
1:O:66:LEU:C	1:O:68:LYS:H	2.02	0.61
3:N:154:ARG:NH1	3:N:357:GLN:NE2	2.49	0.61
1:F:86:ILE:HA	1:F:150:GLN:HE22	1.66	0.61



	ous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:84:HIS:O	1:M:88:LYS:HB2	2.01	0.60
1:O:526:PRO:HD2	1:O:603:MET:SD	2.41	0.60
3:N:24:PHE:HZ	3:P:57:ARG:CD	2.13	0.60
1:F:459:LYS:NZ	1:F:467:THR:HB	2.16	0.60
3:N:352:TRP:HB3	3:N:363:LYS:HE3	1.82	0.60
1:O:459:LYS:NZ	1:O:467:THR:HB	2.16	0.60
2:R:79:PHE:HB2	2:R:84:ILE:HG23	1.82	0.60
3:B:154:ARG:HH11	3:B:357:GLN:HE22	1.48	0.60
3:B:154:ARG:NH1	3:B:357:GLN:NE2	2.49	0.60
1:F:527:ALA:HB3	1:F:528:PRO:HD3	1.82	0.60
1:O:86:ILE:HA	1:O:150:GLN:HE22	1.66	0.60
3:N:370:ARG:NH1	3:N:386:GLY:O	2.34	0.60
2:R:34:ALA:HA	2:R:76:ASN:HD21	1.65	0.60
3:A:517:ALA:CB	3:A:521:SER:CB	2.80	0.60
1:C:524:ILE:HG22	1:C:529:ARG:HG3	1.84	0.60
1:O:273:MET:HB2	1:O:303:PHE:CZ	2.36	0.60
3:B:370:ARG:NH1	3:B:386:GLY:O	2.34	0.60
4:J:453:ASN:HA	4:J:577:ARG:HH12	1.65	0.60
3:P:267:GLU:HG2	3:P:585:LYS:HG2	1.84	0.60
3:P:459:ARG:NH1	3:P:498:THR:OG1	2.35	0.59
1:M:86:ILE:HA	1:M:150:GLN:HE22	1.66	0.59
2:D:72:TRP:HE1	2:D:108:HIS:HA	1.68	0.59
1:F:106:ASN:O	1:F:110:ASN:ND2	2.36	0.59
2:E:44:ILE:HD12	2:E:84:ILE:CG2	2.33	0.59
4:I:547:GLU:HA	4:I:550:LYS:HG2	1.84	0.59
3:N:44:CYS:SG	3:N:45:HIS:N	2.75	0.59
1:C:106:ASN:O	1:C:110:ASN:ND2	2.36	0.59
1:C:349:LYS:NZ	1:C:417:VAL:CG1	2.62	0.59
1:F:703:ILE:HD11	1:F:744:ARG:HD3	1.84	0.59
3:P:397:ARG:NH1	3:P:415:LEU:O	2.36	0.59
3:A:350:PHE:CD1	3:A:352:TRP:CH2	2.91	0.59
1:C:748:LEU:HA	1:C:751:ARG:HG3	1.84	0.59
1:M:106:ASN:O	1:M:110:ASN:ND2	2.36	0.59
2:Q:72:TRP:HE1	2:Q:108:HIS:HA	1.68	0.59
3:B:535:CYS:SG	3:B:564:ARG:NH1	2.75	0.58
3:N:30:PHE:CZ	3:P:60:PHE:CB	2.85	0.58
3:P:396:ARG:HD2	3:P:397:ARG:H	1.68	0.58
1:F:458:LEU:HB3	$1:\overline{F:467:THR:HG22}$	1.86	0.58
2:R:44:ILE:HD12	2:R:84:ILE:CG2	2.33	0.58
3:A:573:TRP:HD1	3:A:597:LYS:HG2	1.67	0.58
3:B:44:CYS:SG	3:B:45:HIS:N	2.75	0.58



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
3:P:185:ASN:ND2	3:P:356:GLN:HE22	2.01	0.58		
1:M:68:LYS:NZ	3:P:142:LEU:O	2.31	0.58		
1:O:106:ASN:O	1:O:110:ASN:ND2	2.36	0.58		
3:N:535:CYS:SG	3:N:564:ARG:NH1	2.75	0.58		
1:C:92:ASP:O	1:C:96:SER:HB2	2.03	0.58		
3:P:154:ARG:HD3	3:P:357:GLN:HE22	1.63	0.58		
3:P:535:CYS:SG	3:P:564:ARG:NH1	2.77	0.58		
1:C:85:LEU:CA	1:C:88:LYS:HB3	2.27	0.58		
1:F:525:PRO:HD2	1:F:528:PRO:HB2	1.85	0.58		
1:O:703:ILE:HD11	1:O:744:ARG:HD3	1.85	0.58		
3:A:373:PRO:HA	3:A:387:GLY:HA3	1.84	0.58		
3:N:22:LYS:HE2	3:N:90:TYR:HB3	1.85	0.58		
1:O:54:PHE:CB	3:N:59:MET:CE	2.82	0.58		
4:H:547:GLU:HA	4:H:550:LYS:HG2	1.84	0.58		
2:R:94:CYS:HB2	2:R:101:TRP:HB2	1.85	0.58		
4:G:547:GLU:HA	4:G:550:LYS:HG2	1.85	0.58		
1:C:274:LYS:CA	1:C:277:VAL:HG22	2.34	0.58		
3:B:355:ALA:O	3:B:587:TYR:HD2	1.87	0.57		
4:J:547:GLU:HA	4:J:550:LYS:HG2	1.85	0.57		
1:C:267:GLU:O	1:C:268:LEU:C	2.42	0.57		
1:F:525:PRO:HA	1:F:603:MET:HE2	1.87	0.57		
1:O:458:LEU:HB3	1:O:467:THR:HG22	1.86	0.57		
1:O:503:LEU:HD11	1:O:531:ALA:HB1	1.86	0.57		
2:R:79:PHE:HD2	2:R:84:ILE:HG21	1.61	0.57		
1:C:265:GLU:HA	1:C:269:ILE:HG13	1.87	0.57		
1:C:202:GLU:HA	1:C:206:GLU:HB3	1.87	0.57		
1:O:93:VAL:HA	1:O:97:LEU:HG	1.87	0.57		
3:N:355:ALA:O	3:N:587:TYR:HD2	1.87	0.57		
1:C:703:ILE:HD11	1:C:744:ARG:HD3	1.87	0.56		
1:M:202:GLU:HA	1:M:206:GLU:HB3	1.87	0.56		
1:O:202:GLU:HA	1:O:206:GLU:HB3	1.87	0.56		
3:B:201:TRP:O	3:B:209:ARG:NH1	2.36	0.56		
1:C:121:ASP:HB3	3:A:58:ALA:HB1	1.86	0.56		
1:F:220:GLU:HA	1:F:223:LYS:HG2	1.87	0.56		
3:A:497:VAL:HG23	3:A:514:ASN:HD22	1.69	0.56		
1:C:125:TYR:CD1	3:A:112:GLN:NE2	2.71	0.56		
1:C:274:LYS:HA	1:C:277:VAL:CG2	2.36	0.56		
1:F:612:THR:OG1	1:F:655:ASN:O	2.24	0.56		
1:O:612:THR:OG1	1:O:655:ASN:O	2.24	0.56		
3:A:201:TRP:O	3:A:209:ARG:NH1	2.38	0.56		
1:F:557:ALA:HB3	1:F:594:VAL:HG23	1.88	0.56		



Atom 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:O:54:PHE:CB	3:N:59:MET:HE1	2.36	0.56
3:A:285:SER:HB3	3:A:300:SER:HB3	1.87	0.56
3:B:353:PHE:HB2	3:B:360:TRP:CZ2	2.41	0.56
3:N:201:TRP:O	3:N:209:ARG:NH1	2.36	0.56
3:N:274:ALA:N	3:N:284:SER:O	2.32	0.56
1:O:220:GLU:HA	1:O:223:LYS:HG2	1.87	0.56
3:B:392:GLY:HA2	3:B:396:ARG:HG2	1.88	0.56
3:P:297:LYS:O	3:P:592:GLU:HB3	2.06	0.56
1:M:87:ASN:O	1:M:88:LYS:C	2.43	0.56
2:Q:27:TRP:CZ2	2:Q:29:ALA:HB2	2.41	0.56
1:C:63:THR:HA	1:C:66:LEU:HD22	1.87	0.56
1:M:220:GLU:HA	1:M:223:LYS:HG2	1.87	0.56
1:O:532:PHE:HB2	2:Q:27:TRP:CH2	2.39	0.56
2:R:27:TRP:CZ2	2:R:29:ALA:HB2	2.40	0.56
3:A:603:PHE:HB3	4:G:467:TYR:HE2	1.71	0.56
3:A:350:PHE:HE2	3:A:366:MET:HB2	1.70	0.56
3:N:353:PHE:HB2	3:N:360:TRP:CZ2	2.41	0.56
1:F:93:VAL:HA	1:F:97:LEU:HG	1.87	0.55
1:M:557:ALA:HB3	1:M:594:VAL:HG23	1.88	0.55
1:O:557:ALA:HB3	1:O:594:VAL:HG23	1.88	0.55
1:C:612:THR:OG1	1:C:655:ASN:O	2.24	0.55
1:F:525:PRO:HA	1:F:603:MET:CE	2.36	0.55
4:I:453:ASN:HA	4:I:577:ARG:HH12	1.70	0.55
3:N:267:GLU:HG2	3:N:585:LYS:HG2	1.89	0.55
1:F:202:GLU:HA	1:F:206:GLU:HB3	1.87	0.55
1:O:49:ASN:HA	1:O:52:LEU:HD13	1.88	0.55
1:O:100:ASN:HB3	1:O:103:GLN:HB2	1.89	0.55
2:E:27:TRP:CZ2	2:E:29:ALA:HB2	2.40	0.55
1:C:480:SER:HA	1:C:507:VAL:H	1.72	0.55
1:M:129:VAL:O	1:M:132:GLN:NE2	2.40	0.55
1:C:409:GLU:OE2	1:C:453:ASN:ND2	2.40	0.55
1:F:100:ASN:HB3	1:F:103:GLN:HB2	1.89	0.55
1:M:478:SER:HA	1:M:481:ASN:HD21	1.72	0.55
2:D:27:TRP:CZ2	2:D:29:ALA:HB2	2.41	0.55
3:A:528:VAL:HG23	3:A:535:CYS:SG	2.46	0.55
1:M:506:ARG:HB2	2:R:30:VAL:HG22	1.88	0.55
4:G:449:LEU:HD21	4:G:594:LEU:HD22	1.89	0.55
4:G:496:GLU:HG2	4:G:499:GLN:HE21	1.72	0.55
3:N:185:ASN:OD1	3:N:356:GLN:NE2	2.40	0.55
3:N:392:GLY:HA2	3:N:396:ARG:HG2	1.87	0.55
1:0:717:MET:HB3	1:0:722:LEU:HG	1.89	0.55



A 1 -1	A 1 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:N:524:CYS:SG	3:N:526:ARG:NH1	2.80	0.55
1:C:129:VAL:O	1:C:132:GLN:NE2	2.40	0.55
1:C:557:ALA:HB3	1:C:594:VAL:HG23	1.88	0.55
1:C:704:GLU:O	1:C:707:ILE:HG22	2.06	0.55
1:M:717:MET:HB3	1:M:722:LEU:HG	1.89	0.55
1:O:409:GLU:OE2	1:O:453:ASN:ND2	2.40	0.55
3:P:397:ARG:HB3	3:P:415:LEU:HB2	1.89	0.55
1:C:49:ASN:HA	1:C:52:LEU:HD13	1.88	0.55
1:M:520:PRO:HG2	1:M:552:HIS:H	1.72	0.55
3:A:397:ARG:HG2	3:A:418:ALA:HA	1.89	0.55
3:B:185:ASN:OD1	3:B:356:GLN:NE2	2.40	0.55
4:H:496:GLU:HG2	4:H:499:GLN:HE21	1.72	0.55
1:F:129:VAL:O	1:F:132:GLN:NE2	2.40	0.55
1:C:99:ASN:O	1:C:100:ASN:C	2.44	0.54
1:M:261:VAL:HA	1:M:264:VAL:HB	1.89	0.54
1:M:365:LEU:HD12	1:M:368:GLN:HE21	1.72	0.54
4:H:453:ASN:HA	4:H:577:ARG:HH12	1.72	0.54
4:I:496:GLU:HG2	4:I:499:GLN:HE21	1.72	0.54
1:C:220:GLU:HA	1:C:223:LYS:HG2	1.87	0.54
1:M:612:THR:OG1	1:M:655:ASN:O	2.24	0.54
2:R:52:LEU:HD21	2:R:59:ASN:HA	1.89	0.54
1:C:478:SER:HA	1:C:481:ASN:HD21	1.72	0.54
1:F:409:GLU:OE2	1:F:453:ASN:ND2	2.40	0.54
2:R:79:PHE:CB	2:R:84:ILE:HG23	2.38	0.54
1:F:525:PRO:HB2	1:F:528:PRO:HD2	1.88	0.54
1:0:129:VAL:O	1:O:132:GLN:NE2	2.40	0.54
2:E:44:ILE:HD11	2:E:84:ILE:HG22	1.89	0.54
3:B:267:GLU:HG2	3:B:585:LYS:HG2	1.89	0.54
3:P:298:LEU:HD21	3:P:591:LEU:HD21	1.84	0.54
2:E:34:ALA:HA	2:E:76:ASN:ND2	2.23	0.54
4:G:484:ILE:HD11	4:G:542:ARG:HG3	1.89	0.54
1:C:87:ASN:O	1:C:88:LYS:C	2.46	0.54
1:M:276:ILE:C	1:M:278:GLU:H	2.10	0.54
1:M:409:GLU:OE2	1:M:453:ASN:ND2	2.40	0.54
1:O:365:LEU:HD12	1:O:368:GLN:HE21	1.73	0.54
3:B:297:LYS:HB3	3:B:592:GLU:CD	2.28	0.54
3:P:201:TRP:O	3:P:209:ARG:NH1	2.38	0.54
2:D:39:VAL:O	2:D:40:ASP:CB	2.42	0.54
1:F:365:LEU:HD12	1:F:368:GLN:HE21	1.72	0.54
4:J:496:GLU:HG2	4:J:499:GLN:HE21	1.72	0.54
1:F:248:VAL:HA	1:F:252:LEU:HB2	1.89	0.54



	ous puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:378:LEU:CD2	1:F:421:PHE:O	2.56	0.54
1:O:273:MET:HB2	1:O:303:PHE:HZ	1.72	0.54
1:O:614:GLU:OE1	1:O:617:GLN:NE2	2.41	0.53
3:P:414:PRO:O	3:P:449:TRP:NE1	2.41	0.53
1:C:437:ALA:HA	1:C:513:TRP:CZ3	2.43	0.53
1:C:717:MET:HB3	1:C:722:LEU:HG	1.89	0.53
1:F:717:MET:HB3	1:F:722:LEU:HG	1.89	0.53
1:M:614:GLU:OE1	1:M:617:GLN:NE2	2.41	0.53
1:O:459:LYS:HZ2	1:O:467:THR:HB	1.71	0.53
2:Q:39:VAL:O	2:Q:40:ASP:CB	2.42	0.53
1:F:68:LYS:HZ3	3:B:142:LEU:HA	1.70	0.53
1:F:614:GLU:OE1	1:F:617:GLN:NE2	2.42	0.53
1:C:77:LEU:O	1:C:78:ARG:C	2.46	0.53
1:C:488:ARG:NH2	1:C:502:ASP:HA	2.23	0.53
3:A:462:ALA:HB1	3:A:473:TYR:HB3	1.89	0.53
4:J:484:ILE:HD11	4:J:542:ARG:HG3	1.89	0.53
3:A:17:LEU:CD1	3:B:51:THR:CB	2.87	0.53
3:A:555:ASP:HB2	3:A:560:ARG:H	1.73	0.53
4:H:484:ILE:HD11	4:H:542:ARG:HG3	1.90	0.53
1:C:58:TYR:OH	1:C:125:TYR:HB2	2.08	0.53
1:C:217:PHE:HB3	1:C:268:LEU:HD23	1.91	0.53
1:O:525:PRO:HA	1:O:603:MET:HE2	1.90	0.53
2:R:39:VAL:O	2:R:39:VAL:CG1	2.53	0.53
1:C:59:ARG:CZ	3:A:75:ARG:HD2	2.39	0.53
1:O:525:PRO:HA	1:O:603:MET:CE	2.39	0.53
1:C:425:LYS:HD2	1:C:462:CYS:HB2	1.91	0.53
3:P:370:ARG:NH1	3:P:386:GLY:O	2.39	0.53
1:F:390:LEU:HG	1:F:681:GLN:HG2	1.91	0.53
1:0:723:VAL:HG11	1:0:742:LYS:HZ3	1.74	0.53
3:A:270:ILE:HD13	3:A:318:ILE:HG12	1.90	0.53
3:A:375:LEU:HD23	3:A:384:ALA:HA	1.90	0.53
4:G:469:GLU:HA	4:G:472:ARG:HG2	1.91	0.53
4:G:487:PHE:HE2	4:G:545:LEU:HG	1.74	0.53
3:B:524:CYS:SG	3:B:526:ARG:NH1	2.80	0.53
3:N:350:PHE:HD1	3:N:363:LYS:HB2	1.74	0.53
1:C:365:LEU:HD12	1:C:368:GLN:HE21	1.72	0.53
1:C:614:GLU:OE1	1:C:617:GLN:NE2	2.41	0.53
1:M:71:GLU:O	1:M:72:LYS:C	2.44	0.53
4:H:469:GLU:HA	4:H:472:ARG:HG2	1.91	0.53
1:C:166:LEU:HD22	1:C:212:MET:HG2	1.91	0.52
1:F:166:LEU:HD22	1:F:212:MET:HG2	1.92	0.52



A 1 -	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:350:PHE:HD1	3:A:352:TRP:CH2	2.27	0.52
3:P:435:THR:OG1	3:P:436:LEU:N	2.41	0.52
1:O:102:LEU:HD13	1:O:182:ALA:HB1	1.91	0.52
1:O:404:THR:OG1	1:O:407:GLU:OE2	2.20	0.52
4:H:487:PHE:HE2	4:H:545:LEU:HG	1.74	0.52
3:P:297:LYS:HB2	3:P:594:SER:OG	2.09	0.52
1:C:467:THR:HA	1:C:470:LEU:HB2	1.90	0.52
1:O:508:LEU:HD13	1:O:513:TRP:CE2	2.45	0.52
4:I:484:ILE:HD11	4:I:542:ARG:HG3	1.89	0.52
2:R:63:ALA:HB1	2:R:66:GLU:HA	1.92	0.52
3:B:346:THR:HG22	3:B:369:VAL:HB	1.92	0.52
1:C:274:LYS:O	1:C:277:VAL:HG22	2.09	0.52
3:B:274:ALA:HB1	3:B:575:LEU:HD22	1.92	0.52
3:B:296:TYR:HB3	3:B:591:LEU:HD22	1.92	0.52
3:N:94:LEU:HD11	3:N:104:LEU:HD21	1.91	0.52
1:0:426:ASP:OD2	1:O:699:ARG:NH2	2.42	0.52
2:R:44:ILE:HD11	2:R:84:ILE:HG22	1.89	0.52
3:A:393:GLU:HA	3:A:397:ARG:HD2	1.92	0.52
3:B:350:PHE:HD1	3:B:363:LYS:HB2	1.74	0.52
1:C:77:LEU:O	1:C:81:VAL:HG22	2.09	0.52
1:F:102:LEU:HD13	1:F:182:ALA:HB1	1.91	0.52
1:F:149:ASP:HA	1:F:153:ARG:HB2	1.92	0.52
1:M:548:LEU:HD21	2:R:31:ALA:HB1	1.92	0.52
3:A:108:ALA:O	3:A:112:GLN:N	2.43	0.52
4:G:502:GLU:O	4:G:505:SER:OG	2.24	0.52
3:B:53:SER:OG	3:B:111:LEU:O	2.28	0.52
1:O:240:ARG:NH1	1:O:243:GLU:OE2	2.43	0.52
3:N:346:THR:HG22	3:N:369:VAL:HB	1.92	0.52
3:N:467:PHE:HB3	3:N:472:PHE:HE2	1.75	0.52
1:C:248:VAL:HA	1:C:252:LEU:HB2	1.92	0.52
1:C:606:ASN:HD21	2:E:22:PHE:HD2	1.57	0.52
1:M:149:ASP:HA	1:M:153:ARG:HB2	1.92	0.52
1:M:166:LEU:HD22	1:M:212:MET:HG2	1.92	0.52
1:O:166:LEU:HD22	1:O:212:MET:HG2	1.91	0.52
3:A:285:SER:HB2	3:A:298:LEU:HB3	1.92	0.52
3:B:22:LYS:HE2	3:B:90:TYR:HB3	1.91	0.51
3:B:186:LEU:HB2	3:B:260:ARG:HD3	1.92	0.51
3:N:53:SER:OG	3:N:111:LEU:O	2.28	0.51
3:P:108:ALA:O	3:P:112:GLN:N	2.43	0.51
1:M:240:ARG:NH1	1:M:243:GLU:OE2	2.43	0.51
1:0:149:ASP:HA	1:0:153:ARG:HB2	1.92	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:O:472:GLY:HA3	1:O:512:TYR:CZ	2.45	0.51
3:B:549:TYR:OH	3:B:575:LEU:N	2.40	0.51
3:N:186:LEU:HB2	3:N:260:ARG:HD3	1.92	0.51
4:J:469:GLU:HA	4:J:472:ARG:HG2	1.91	0.51
3:P:154:ARG:CD	3:P:357:GLN:HE22	2.21	0.51
1:C:246:GLU:HA	1:C:249:MET:HE2	1.93	0.51
1:C:274:LYS:O	1:C:275:THR:C	2.49	0.51
1:F:240:ARG:NH1	1:F:243:GLU:OE2	2.43	0.51
4:J:487:PHE:HE2	4:J:545:LEU:HG	1.74	0.51
1:C:64:MET:O	1:C:69:HIS:HB2	2.11	0.51
1:C:125:TYR:HD1	3:A:112:GLN:NE2	2.06	0.51
4:I:469:GLU:HA	4:I:472:ARG:HG2	1.91	0.51
3:N:435:THR:OG1	3:N:436:LEU:N	2.42	0.51
3:N:459:ARG:NH2	3:N:473:TYR:O	2.44	0.51
1:C:59:ARG:HD2	3:A:76:ASN:OD1	2.10	0.51
1:O:441:LEU:HD21	1:O:508:LEU:HD11	1.91	0.51
3:P:305:LEU:HB3	3:P:325:VAL:HG12	1.93	0.51
1:O:55:GLU:OE2	3:N:72:VAL:CG1	2.56	0.51
3:B:371:ILE:HB	3:B:388:ASP:HB2	1.92	0.51
3:B:573:TRP:HB3	3:B:597:LYS:HD3	1.92	0.51
1:C:102:LEU:HD13	1:C:182:ALA:HB1	1.91	0.51
3:B:435:THR:OG1	3:B:436:LEU:N	2.42	0.51
1:C:240:ARG:NH1	1:C:243:GLU:OE2	2.43	0.51
1:F:472:GLY:HA3	1:F:512:TYR:CZ	2.46	0.51
1:F:531:ALA:CB	2:D:27:TRP:HZ3	2.17	0.51
1:M:246:GLU:HA	1:M:249:MET:HE2	1.92	0.51
3:B:226:SER:HB3	3:B:259:PRO:HB3	1.93	0.51
4:H:543:ARG:HH21	4:H:546:GLU:HG3	1.76	0.51
1:C:149:ASP:HA	1:C:153:ARG:HB2	1.92	0.51
1:M:83:GLU:O	1:M:84:HIS:C	2.45	0.51
1:O:440:LEU:HB3	1:0:477:MET:SD	2.51	0.51
3:B:274:ALA:N	3:B:284:SER:O	2.38	0.51
1:O:606:ASN:HD21	2:Q:22:PHE:HD2	1.57	0.50
3:A:10:ASN:HD21	3:B:119:ARG:HH22	1.59	0.50
3:A:44:CYS:SG	3:A:45:HIS:N	2.84	0.50
3:B:467:PHE:HB3	3:B:472:PHE:HE2	1.75	0.50
4:I:487:PHE:HE2	4:I:545:LEU:HG	1.74	0.50
3:N:188:VAL:H	3:N:262:GLY:HA3	1.76	0.50
1:F:348:LEU:HA	1:F:351:ARG:HG2	1.93	0.50
1:F:404:THR:OG1	1:F:407:GLU:OE2	2.20	0.50
2:R:71:ALA:HB1	2:R:84:ILE:HD11	1.93	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:45:GLN:HB3	1:C:84:HIS:CD2	2.47	0.50
1:F:528:PRO:HA	1:F:531:ALA:HB3	1.94	0.50
2:Q:20:LYS:HE3	2:Q:23:GLU:HG2	1.93	0.50
3:A:61:MET:HE2	3:B:30:PHE:CZ	2.46	0.50
3:A:119:ARG:HH22	3:B:10:ASN:HD22	1.59	0.50
3:N:348:ASN:ND2	3:N:366:MET:O	2.32	0.50
3:P:44:CYS:SG	3:P:45:HIS:N	2.84	0.50
3:P:385:ILE:HG21	3:P:433:VAL:HG21	1.93	0.50
1:C:86:ILE:HG12	1:C:150:GLN:NE2	2.25	0.50
1:C:349:LYS:HE2	1:C:418:LEU:HB2	1.92	0.50
1:M:323:GLU:HG2	1:M:326:LYS:HZ3	1.77	0.50
1:M:404:THR:OG1	1:M:407:GLU:OE2	2.20	0.50
2:R:44:ILE:HD12	2:R:84:ILE:HG23	1.93	0.50
4:I:459:LYS:HA	4:I:462:GLU:HG3	1.93	0.50
1:C:451:GLU:HB3	1:C:474:PHE:CE1	2.47	0.50
1:M:606:ASN:HD21	2:R:22:PHE:HD2	1.57	0.50
4:I:543:ARG:HH21	4:I:546:GLU:HG3	1.76	0.50
1:M:632:GLN:HG3	1:M:633:SER:N	2.27	0.50
2:E:45:CYS:HB2	2:E:54:ILE:HG12	1.93	0.50
3:P:459:ARG:NH1	3:P:475:GLY:O	2.45	0.50
1:F:440:LEU:HB3	1:F:477:MET:SD	2.51	0.50
2:E:44:ILE:HD12	2:E:84:ILE:HG23	1.93	0.50
4:G:543:ARG:HH21	4:G:546:GLU:HG3	1.76	0.50
3:P:22:LYS:HE2	3:P:90:TYR:HB3	1.93	0.50
1:C:41:ILE:HD12	1:C:80:VAL:HG11	1.94	0.50
1:C:632:GLN:HG3	1:C:633:SER:N	2.27	0.50
3:B:459:ARG:NH2	3:B:473:TYR:O	2.44	0.50
3:N:301:PRO:N	3:N:302:PRO:HD2	2.27	0.50
1:F:526:PRO:HD2	1:F:603:MET:SD	2.52	0.50
1:F:606:ASN:HD21	2:D:22:PHE:HD2	1.57	0.50
1:M:270:SER:HA	1:M:273:MET:HB3	1.93	0.50
4:H:459:LYS:HA	4:H:462:GLU:HG3	1.93	0.50
1:C:476:ASP:HB3	1:C:508:LEU:HB3	1.94	0.49
1:C:524:ILE:CG2	1:C:529:ARG:HG3	2.41	0.49
3:N:301:PRO:HB2	3:N:360:TRP:HB2	1.94	0.49
1:C:524:ILE:HB	1:C:529:ARG:CG	2.42	0.49
1:M:66:LEU:HD21	3:P:143:PHE:CD1	2.46	0.49
1:M:527:ALA:HB3	1:M:528:PRO:HD3	1.94	0.49
1:M:559:LEU:O	1:M:592:LEU:N	2.39	0.49
1:O:473:MET:HG3	1:O:513:TRP:CZ2	2.46	0.49
1:C:274:LYS:O	1:C:278:GLU:HG2	2.12	0.49



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:451:GLU:HB3	1:C:474:PHE:CZ	2.47	0.49
1:M:440:LEU:HD13	1:M:477:MET:HG3	1.93	0.49
1:M:723:VAL:HG11	1:M:742:LYS:HZ3	1.77	0.49
3:A:542:HIS:H	3:A:548:LYS:HG2	1.77	0.49
3:B:353:PHE:HB2	3:B:360:TRP:CH2	2.47	0.49
3:N:353:PHE:HB2	3:N:360:TRP:CH2	2.47	0.49
4:J:459:LYS:HD2	4:J:570:LEU:HD13	1.95	0.49
1:O:323:GLU:HG2	1:O:326:LYS:HZ1	1.77	0.49
3:B:301:PRO:N	3:B:302:PRO:HD2	2.27	0.49
4:I:453:ASN:HD21	4:I:598:LEU:HG	1.77	0.49
3:P:186:LEU:HB2	3:P:260:ARG:HD3	1.94	0.49
1:C:94:LEU:C	1:C:96:SER:H	2.16	0.49
1:M:264:VAL:O	1:M:268:LEU:HB3	2.13	0.49
1:O:598:GLN:HG2	1:O:634:LEU:HG	1.94	0.49
2:D:20:LYS:HE3	2:D:23:GLU:HG2	1.93	0.49
3:A:170:MET:O	3:A:209:ARG:NH2	2.37	0.49
3:N:371:ILE:HB	3:N:388:ASP:HB2	1.93	0.49
4:J:543:ARG:HH21	4:J:546:GLU:HG3	1.76	0.49
3:P:24:PHE:CD1	3:P:29:LEU:HD12	2.48	0.49
1:M:523:ASN:HD22	1:M:529:ARG:NH1	2.10	0.49
1:O:265:GLU:O	1:O:269:ILE:HG13	2.12	0.49
2:E:20:LYS:HE3	2:E:23:GLU:HG2	1.93	0.49
2:E:84:ILE:HD12	2:E:101:TRP:HZ2	1.77	0.49
3:A:24:PHE:CD1	3:A:29:LEU:HD12	2.48	0.49
3:N:226:SER:HB3	3:N:259:PRO:HB3	1.93	0.49
1:C:76:GLY:O	1:C:77:LEU:C	2.51	0.49
1:C:440:LEU:HD13	1:C:477:MET:CG	2.30	0.49
3:A:186:LEU:HB2	3:A:260:ARG:HD3	1.94	0.49
3:A:226:SER:HB3	3:A:259:PRO:HB3	1.95	0.49
3:B:188:VAL:H	3:B:262:GLY:HA3	1.77	0.49
3:P:370:ARG:NH2	3:P:398:THR:O	2.38	0.49
1:C:107:GLN:HA	1:C:110:ASN:HD21	1.78	0.48
1:C:217:PHE:HA	1:C:220:GLU:HG2	1.95	0.48
1:M:85:LEU:O	1:M:86:ILE:C	2.51	0.48
1:O:66:LEU:C	1:O:68:LYS:N	2.67	0.48
1:0:508:LEU:HD13	1:O:513:TRP:CD2	2.48	0.48
2:E:71:ALA:HB1	2:E:84:ILE:HD11	1.93	0.48
3:N:274:ALA:O	3:N:284:SER:N	2.38	0.48
3:P:366:MET:HG2	3:P:409:TRP:CZ2	2.48	0.48
1:F:68:LYS:HE3	3:B:142:LEU:CD1	2.28	0.48
1:F:198:ARG:HE	1:F:198:ARG:HB2	1.44	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:O:217:PHE:HA	1:O:220:GLU:HG2	1.95	0.48
4:G:459:LYS:HD2	4:G:570:LEU:HD13	1.95	0.48
4:I:566:ILE:HD12	4:I:566:ILE:HA	1.74	0.48
4:J:454:THR:O	4:J:458:GLU:HG2	2.13	0.48
1:M:107:GLN:HA	1:M:110:ASN:HD21	1.79	0.48
1:C:79:GLU:O	1:C:80:VAL:C	2.52	0.48
1:O:107:GLN:HA	1:O:110:ASN:HD21	1.78	0.48
3:B:261:LEU:HG	3:B:587:TYR:CZ	2.48	0.48
3:N:399:VAL:HG12	3:N:414:PRO:HA	1.96	0.48
1:C:503:LEU:O	1:C:504:THR:HG23	2.14	0.48
1:C:644:LEU:HD11	1:C:659:PHE:HB3	1.96	0.48
1:F:598:GLN:HG2	1:F:634:LEU:HG	1.94	0.48
1:O:644:LEU:HD11	1:O:659:PHE:HB3	1.96	0.48
2:R:20:LYS:HE3	2:R:23:GLU:HG2	1.93	0.48
3:B:301:PRO:HB2	3:B:360:TRP:HB2	1.94	0.48
1:C:94:LEU:C	1:C:96:SER:N	2.66	0.48
1:F:107:GLN:HA	1:F:110:ASN:HD21	1.78	0.48
1:M:559:LEU:HD11	2:R:22:PHE:HB3	1.95	0.48
2:E:44:ILE:HD12	2:E:84:ILE:HG22	1.96	0.48
3:A:265:LYS:HG2	3:A:585:LYS:HB3	1.96	0.48
1:C:54:PHE:HB3	3:A:59:MET:SD	2.54	0.48
1:C:491:LEU:HD11	1:C:500:GLY:HA3	1.95	0.48
1:F:279:MET:HE3	1:F:279:MET:HB3	1.82	0.48
1:F:644:LEU:HD11	1:F:659:PHE:HB3	1.96	0.48
2:D:45:CYS:HB2	2:D:54:ILE:HG12	1.96	0.48
2:Q:27:TRP:CE2	2:Q:29:ALA:HB2	2.49	0.48
4:I:527:ASN:HA	4:I:530:LYS:HE3	1.94	0.48
1:C:459:LYS:HG3	1:C:467:THR:HG21	1.95	0.48
1:F:524:ILE:H	1:F:524:ILE:HG12	1.50	0.48
1:M:83:GLU:O	1:M:86:ILE:HG22	2.13	0.48
1:M:390:LEU:HG	1:M:681:GLN:HG2	1.94	0.48
1:M:504:THR:OG1	2:R:27:TRP:O	2.31	0.48
1:O:559:LEU:HD11	2:Q:22:PHE:HB3	1.95	0.48
3:B:399:VAL:HG12	3:B:414:PRO:HA	1.96	0.48
3:N:235:GLN:HG3	3:N:242:LYS:HZ3	1.77	0.48
3:P:371:ILE:N	3:P:387:GLY:O	2.40	0.48
1:C:263:VAL:O	1:C:267:GLU:HG3	2.14	0.48
1:C:614:GLU:HA	1:C:617:GLN:HG2	1.96	0.48
1:F:328:LEU:HD22	1:F:348:LEU:HD21	1.95	0.48
2:E:27:TRP:CE2	2:E:29:ALA:HB2	2.49	0.48
3:P:572:LEU:HD22	3:P:572:LEU:HA	1.75	0.48



	hi o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:82:THR:O	1:C:83:GLU:C	2.51	0.48
1:C:267:GLU:HG3	1:C:267:GLU:H	1.49	0.48
1:C:504:THR:OG1	2:E:27:TRP:O	2.31	0.48
1:C:723:VAL:HG11	1:C:742:LYS:HZ3	1.79	0.48
1:M:76:GLY:O	1:M:77:LEU:C	2.51	0.48
1:O:614:GLU:HA	1:O:617:GLN:HG2	1.96	0.48
3:N:301:PRO:CG	3:N:360:TRP:HB2	2.44	0.48
3:N:549:TYR:OH	3:N:575:LEU:N	2.40	0.48
1:C:41:ILE:CD1	1:C:80:VAL:HG11	2.44	0.47
1:C:91:GLU:H	1:C:91:GLU:HG3	1.46	0.47
1:M:605:PHE:HE2	1:M:611:TYR:HB2	1.79	0.47
1:C:85:LEU:O	1:C:86:ILE:C	2.52	0.47
1:C:559:LEU:HD11	2:E:22:PHE:HB3	1.95	0.47
1:M:72:LYS:H	1:M:72:LYS:HG2	1.28	0.47
3:B:301:PRO:CG	3:B:360:TRP:HB2	2.44	0.47
1:M:265:GLU:HB2	1:M:306:VAL:HB	1.96	0.47
1:M:279:MET:HE3	1:M:279:MET:HB3	1.82	0.47
3:A:346:THR:HB	3:A:369:VAL:HG11	1.96	0.47
3:A:474:ILE:HG12	3:A:499:VAL:HG13	1.96	0.47
3:B:102:GLU:OE1	3:B:102:GLU:N	2.41	0.47
4:H:459:LYS:HD2	4:H:570:LEU:HD13	1.96	0.47
1:C:81:VAL:HG23	1:C:82:THR:H	1.79	0.47
1:C:386:GLU:OE1	1:C:386:GLU:N	2.44	0.47
1:C:696:ASP:HA	1:C:699:ARG:HD2	1.95	0.47
1:F:559:LEU:HD11	2:D:22:PHE:HB3	1.95	0.47
1:M:536:ARG:HA	1:M:548:LEU:HG	1.96	0.47
3:B:286:VAL:HG11	3:B:573:TRP:HH2	1.80	0.47
4:I:544:ARG:O	4:I:547:GLU:HG3	2.15	0.47
4:J:502:GLU:O	4:J:505:SER:OG	2.24	0.47
1:M:478:SER:HA	1:M:481:ASN:ND2	2.29	0.47
1:O:54:PHE:C	3:N:59:MET:HE1	2.35	0.47
2:D:27:TRP:CE2	2:D:29:ALA:HB2	2.49	0.47
4:H:539:ILE:HD12	4:H:542:ARG:HH21	1.80	0.47
1:M:614:GLU:HA	1:M:617:GLN:HG2	1.96	0.47
1:O:605:PHE:HE2	1:O:611:TYR:HB2	1.80	0.47
1:O:646:LYS:HE3	1:O:659:PHE:HE1	1.80	0.47
2:R:27:TRP:CE2	2:R:29:ALA:HB2	2.49	0.47
3:A:394:LEU:H	3:A:394:LEU:HG	1.44	0.47
4:I:539:ILE:HD12	4:I:542:ARG:HH21	1.80	0.47
3:N:261:LEU:HG	3:N:587:TYR:CZ	2.49	0.47
3:N:442:TYR:HB2	3:N:449:TRP:CZ3	2.50	0.47



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
3:P:226:SER:HB3	3:P:259:PRO:HB3	1.95	0.47
3:P:431:ILE:HB	3:P:442:TYR:HB3	1.96	0.47
1:C:248:VAL:HG11	1:C:257:GLU:HG3	1.95	0.47
1:F:614:GLU:HA	1:F:617:GLN:HG2	1.96	0.47
3:A:253:MET:HG2	3:A:258:LYS:HA	1.97	0.47
3:B:442:TYR:HB2	3:B:449:TRP:CZ3	2.50	0.47
4:I:459:LYS:HD2	4:I:570:LEU:HD13	1.96	0.47
3:P:297:LYS:O	3:P:592:GLU:CB	2.63	0.47
1:C:609:GLU:HG3	1:C:610:LYS:H	1.80	0.47
1:M:121:ASP:O	3:P:58:ALA:HB1	2.15	0.47
1:M:217:PHE:HA	1:M:220:GLU:HG2	1.96	0.47
1:O:531:ALA:HB3	2:Q:27:TRP:CE3	2.49	0.47
3:A:61:MET:SD	3:B:29:LEU:HG	2.55	0.47
3:N:308:VAL:HG12	3:N:323:GLY:HA3	1.97	0.47
1:F:326:LYS:HA	1:F:329:VAL:HG22	1.97	0.47
1:O:59:ARG:CD	3:N:75:ARG:HB2	2.42	0.47
2:R:45:CYS:HB2	2:R:54:ILE:HG12	1.96	0.47
4:G:539:ILE:HD12	4:G:542:ARG:HH21	1.80	0.47
4:I:592:LYS:HD2	4:I:592:LYS:HA	1.43	0.47
3:N:24:PHE:CZ	3:P:57:ARG:NE	2.73	0.47
3:N:301:PRO:HG2	3:N:360:TRP:HB2	1.97	0.47
1:C:348:LEU:HA	1:C:351:ARG:HG2	1.97	0.47
1:F:269:ILE:HG22	1:F:273:MET:HB2	1.97	0.47
1:F:559:LEU:O	1:F:592:LEU:N	2.39	0.47
1:F:687:GLU:O	1:F:690:GLU:HG3	2.15	0.47
1:O:93:VAL:CG1	1:0:156:CYS:SG	3.02	0.47
1:O:269:ILE:HG22	1:O:303:PHE:CE2	2.50	0.47
3:A:525:VAL:HG12	3:A:536:VAL:HG21	1.97	0.47
4:G:544:ARG:O	4:G:547:GLU:HG3	2.15	0.47
3:B:251:LYS:HA	3:B:251:LYS:HD3	1.53	0.47
3:P:427:VAL:HG11	3:P:504:VAL:HG21	1.95	0.47
1:C:125:TYR:CE1	3:A:109:CYS:O	2.68	0.46
1:C:532:PHE:CB	2:E:27:TRP:CH2	2.98	0.46
1:F:217:PHE:HA	1:F:220:GLU:HG2	1.96	0.46
1:C:532:PHE:CB	2:E:27:TRP:HH2	2.28	0.46
1:M:225:LEU:HD13	1:M:272:HIS:CG	2.49	0.46
1:M:609:GLU:HG3	1:M:610:LYS:H	1.80	0.46
1:M:644:LEU:HD11	1:M:659:PHE:HB3	1.96	0.46
2:D:94:CYS:HB2	2:D:101:TRP:HB2	1.96	0.46
3:B:586:LEU:HD13	3:B:591:LEU:HD11	1.97	0.46
3:N:274:ALA:HB1	3:N:575:LEU:HD22	1.96	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:N:296:TYR:HB3	3:N:591:LEU:HD22	1.97	0.46
3:P:300:SER:HA	3:P:360:TRP:NE1	2.30	0.46
1:C:478:SER:HA	1:C:481:ASN:ND2	2.29	0.46
1:F:273:MET:HG3	1:F:303:PHE:HE2	1.81	0.46
1:O:54:PHE:HB2	3:N:59:MET:HE1	1.93	0.46
1:O:525:PRO:HB3	1:O:603:MET:HG3	1.97	0.46
4:G:482:THR:O	4:G:485:GLU:HG3	2.15	0.46
1:C:605:PHE:HE2	1:C:611:TYR:HB2	1.80	0.46
1:C:646:LYS:HE3	1:C:659:PHE:HE1	1.80	0.46
1:F:88:LYS:HA	1:F:88:LYS:HD3	1.61	0.46
1:F:93:VAL:CG1	1:F:156:CYS:SG	3.02	0.46
1:M:68:LYS:HA	1:M:68:LYS:HD3	1.76	0.46
1:M:646:LYS:HE3	1:M:659:PHE:HE1	1.80	0.46
1:M:687:GLU:O	1:M:690:GLU:HG3	2.15	0.46
1:O:82:THR:O	1:O:86:ILE:HG23	2.16	0.46
1:C:80:VAL:O	1:C:83:GLU:HB3	2.15	0.46
1:C:254:LYS:H	1:C:254:LYS:HG3	1.47	0.46
1:M:83:GLU:HG2	1:M:87:ASN:HD21	1.80	0.46
1:M:476:ASP:HB3	1:M:508:LEU:HB3	1.96	0.46
2:R:98:ASN:HD22	2:R:98:ASN:HA	1.50	0.46
3:A:282:LEU:HD22	3:A:282:LEU:HA	1.75	0.46
3:B:280:CYS:HB3	3:B:281:SER:H	1.54	0.46
1:F:68:LYS:CE	3:B:142:LEU:HA	2.44	0.46
1:M:91:GLU:H	1:M:91:GLU:HG3	1.36	0.46
1:O:609:GLU:HG3	1:O:610:LYS:H	1.80	0.46
3:B:459:ARG:HB3	3:B:476:GLY:HA3	1.98	0.46
3:N:416:PRO:HG2	3:N:440:TYR:CD1	2.50	0.46
3:P:154:ARG:CZ	3:P:357:GLN:NE2	2.79	0.46
1:F:254:LYS:H	1:F:254:LYS:HG3	1.50	0.46
4:H:544:ARG:O	4:H:547:GLU:HG3	2.15	0.46
1:C:85:LEU:H	1:C:85:LEU:HG	1.45	0.46
1:C:269:ILE:O	1:C:273:MET:N	2.48	0.46
1:C:486:GLU:HG3	1:C:490:HIS:CE1	2.51	0.46
1:F:58:TYR:O	1:F:59:ARG:C	2.54	0.46
1:F:605:PHE:HE2	1:F:611:TYR:HB2	1.79	0.46
1:O:260:ILE:O	1:O:264:VAL:HG12	2.16	0.46
1:0:753:TYR:HA	1:O:767:VAL:HG23	1.96	0.46
4:G:453:ASN:HA	4:G:577:ARG:NH1	2.29	0.46
3:N:352:TRP:HB3	3:N:363:LYS:CE	2.46	0.46
4:J:544:ARG:O	4:J:547:GLU:HG3	2.15	0.46
3:P:253:MET:HG2	3:P:258:LYS:HA	1.97	0.46



Λtom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:259:PRO:O	1:C:262:LYS:HB2	2.16	0.46
1:M:703:ILE:HD11	1:M:744:ARG:HD3	1.98	0.46
1:O:550:LEU:H	1:O:550:LEU:HG	1.51	0.46
2:R:61:ALA:O	2:R:62:SER:C	2.53	0.46
3:A:499:VAL:HB	3:A:512:ALA:HB3	1.98	0.46
3:P:526:ARG:NH2	3:P:577:ARG:O	2.39	0.46
1:F:646:LYS:HE3	1:F:659:PHE:HE1	1.80	0.46
1:O:55:GLU:OE1	3:N:66:GLU:HG3	2.16	0.46
2:Q:96:LEU:HD13	2:Q:96:LEU:HA	1.76	0.46
3:B:308:VAL:HG12	3:B:323:GLY:HA3	1.97	0.46
3:N:286:VAL:HG11	3:N:573:TRP:HH2	1.80	0.46
1:F:82:THR:O	1:F:86:ILE:HG23	2.16	0.45
1:M:560:ASN:HD22	2:R:25:LYS:HD2	1.81	0.45
1:M:723:VAL:HA	1:M:726:VAL:HG12	1.98	0.45
1:O:531:ALA:HB3	2:Q:27:TRP:CZ3	2.51	0.45
3:B:416:PRO:HG2	3:B:440:TYR:CD1	2.50	0.45
3:N:188:VAL:N	3:N:262:GLY:HA3	2.31	0.45
1:C:269:ILE:O	1:C:270:SER:C	2.54	0.45
1:F:473:MET:HG3	1:F:513:TRP:CZ2	2.51	0.45
1:F:526:PRO:HD2	1:F:603:MET:CE	2.45	0.45
1:F:609:GLU:HG3	1:F:610:LYS:H	1.80	0.45
2:R:41:ASN:HD21	2:R:46:ARG:HG2	1.81	0.45
3:A:272:ILE:HB	3:A:580:ARG:HB2	1.97	0.45
3:B:188:VAL:N	3:B:262:GLY:HA3	2.31	0.45
3:B:261:LEU:HD12	3:B:264:THR:OG1	2.17	0.45
4:H:502:GLU:O	4:H:505:SER:OG	2.25	0.45
3:P:297:LYS:CB	3:P:592:GLU:OE1	2.55	0.45
1:C:279:MET:HE3	1:C:279:MET:HB3	1.84	0.45
1:M:97:LEU:HD22	1:M:160:HIS:CD2	2.51	0.45
1:M:467:THR:HA	1:M:470:LEU:HB2	1.98	0.45
1:O:632:GLN:HG3	1:O:633:SER:N	2.30	0.45
1:0:687:GLU:0	1:O:690:GLU:HG3	2.15	0.45
3:A:311:VAL:HG11	3:A:382:ILE:HG23	1.98	0.45
3:B:291:GLN:H	3:B:291:GLN:HG3	1.55	0.45
4:H:454:THR:O	4:H:458:GLU:HG2	2.16	0.45
3:N:57:ARG:NH2	3:P:24:PHE:CZ	2.79	0.45
4:J:481:ARG:HA	4:J:484:ILE:HG22	1.99	0.45
3:P:237:LEU:HB3	3:P:241:ASP:HB2	1.99	0.45
1:C:68:LYS:HE2	1:C:68:LYS:HB2	1.44	0.45
1:M:365:LEU:O	1:M:368:GLN:HG3	2.17	0.45
1:O:390:LEU:HD13	1:O:390:LEU:HA	1.72	0.45


	A4	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:O:419:PHE:HZ	1:O:425:LYS:HG3	1.82	0.45	
1:0:88:LYS:HD3	1:O:88:LYS:HA	1.61	0.45	
3:A:283:TYR:HD1	3:A:283:TYR:HA	1.71	0.45	
3:B:301:PRO:HG2	3:B:360:TRP:HB2	1.97	0.45	
3:B:571:VAL:HA	3:B:597:LYS:HG3	1.99	0.45	
4:J:539:ILE:HD12	4:J:542:ARG:HH21	1.80	0.45	
1:F:632:GLN:HG3	1:F:633:SER:N	2.30	0.45	
3:A:352:TRP:HH2	3:A:409:TRP:HH2	1.65	0.45	
3:N:251:LYS:HD3	3:N:251:LYS:HA	1.53	0.45	
3:N:459:ARG:HB3	3:N:476:GLY:HA3	1.98	0.45	
3:P:274:ALA:HB1	3:P:575:LEU:HD22	1.97	0.45	
1:C:488:ARG:NH2	1:C:503:LEU:H	2.14	0.45	
1:F:723:VAL:HA	1:F:726:VAL:HG12	1.99	0.45	
4:G:454:THR:O	4:G:458:GLU:HG2	2.17	0.45	
4:G:581:LEU:HD12	4:G:581:LEU:HA	1.74	0.45	
3:B:455:ARG:HH22	3:B:459:ARG:H	1.65	0.45	
4:I:529:ASP:OD1	4:I:529:ASP:N	2.50	0.45	
3:N:261:LEU:HD12	3:N:264:THR:OG1	2.17	0.45	
1:C:265:GLU:O	1:C:270:SER:N	2.47	0.45	
1:O:54:PHE:CE2	3:N:64:LEU:HD12	2.52	0.45	
3:B:237:LEU:HB3	3:B:241:ASP:HB2	1.99	0.45	
3:N:127:LYS:HA	3:N:127:LYS:HD3	1.42	0.45	
1:C:560:ASN:HD22	2:E:25:LYS:HD2	1.81	0.45	
1:C:714:ARG:NH1	1:C:725:GLU:OE2	2.50	0.45	
1:F:323:GLU:HG2	1:F:326:LYS:HZ1	1.81	0.45	
1:F:365:LEU:O	1:F:368:GLN:HG3	2.17	0.45	
1:M:71:GLU:H	1:M:71:GLU:HG2	1.51	0.45	
1:O:365:LEU:O	1:O:368:GLN:HG3	2.16	0.45	
1:O:436:LEU:HD23	1:O:439:ARG:HH11	1.82	0.45	
3:A:497:VAL:HG23	3:A:514:ASN:HD21	1.78	0.45	
4:H:480:LYS:HD3	4:H:480:LYS:HA	1.52	0.45	
1:F:436:LEU:HD23	1:F:439:ARG:HH11	1.82	0.45	
1:F:559:LEU:HD22	1:F:602:LEU:HD23	1.99	0.45	
1:M:714:ARG:NH1	1:M:725:GLU:OE2	2.50	0.45	
1:O:714:ARG:NH1	1:O:725:GLU:OE2	2.50	0.45	
2:E:98:ASN:HD22	2:E:98:ASN:HA	1.50	0.45	
3:A:573:TRP:CD1	3:A:597:LYS:HG2	2.50	0.45	
4:G:529:ASP:N	4:G:529:ASP:OD1	2.50	0.45	
3:P:307:LYS:HD3	3:P:372:LYS:HE3	1.99	0.45	
1:C:58:TYR:OH	3:A:112:GLN:OE1	2.28	0.44	
1:C:559:LEU:HD22	1:C:602:LEU:HD23	1.99	0.44	



Atom-1	Atom-2	Interatomic	Clash	
		distance (A)	overlap (A)	
1:F:723:VAL:HG11	1:F:742:LYS:HZ3	1.81	0.44	
1:M:76:GLY:O	1:M:80:VAL:HG23	2.17	0.44	
1:M:258:GLU:HA	1:M:261:VAL:HG22	1.99	0.44	
1:O:723:VAL:HA	1:O:726:VAL:HG12	1.99	0.44	
4:H:529:ASP:OD1	4:H:529:ASP:N	2.50	0.44	
3:N:237:LEU:HB3	3:N:241:ASP:HB2	1.99	0.44	
3:N:455:ARG:HH22	3:N:459:ARG:H	1.65	0.44	
3:N:586:LEU:HD13	3:N:591:LEU:HD11	1.97	0.44	
3:P:316:ASN:ND2	3:P:585:LYS:O	2.39	0.44	
1:C:502:ASP:O	2:E:26:LYS:HA	2.17	0.44	
1:0:338:PRO:HA	1:O:341:TYR:HB3	1.99	0.44	
3:N:102:GLU:OE1	3:N:102:GLU:N	2.41	0.44	
4:J:529:ASP:OD1	4:J:529:ASP:N	2.50	0.44	
1:C:87:ASN:O	1:C:89:VAL:N	2.51	0.44	
1:F:66:LEU:C	1:F:68:LYS:N	2.67	0.44	
1:F:185:ASN:HA	1:F:188:GLN:HG2	2.00	0.44	
2:E:41:ASN:HD21	2:E:46:ARG:HG2	1.81	0.44	
3:A:287:CYS:HB2	3:A:298:LEU:HG	2.00	0.44	
4:G:459:LYS:HA	4:G:462:GLU:HG3	2.00	0.44	
4:I:454:THR:O	4:I:458:GLU:HG2	2.17	0.44	
4:J:486:ALA:O	4:J:489:GLU:HG3	2.18	0.44	
3:P:374:SER:HB2	3:P:385:ILE:HB	2.00	0.44	
1:C:185:ASN:HA	1:C:188:GLN:HG2	1.99	0.44	
1:M:265:GLU:HG3	1:M:306:VAL:HA	2.00	0.44	
1:O:351:ARG:HA	1:O:354:ARG:HG2	1.99	0.44	
1:O:479:ILE:HD13	1:O:479:ILE:HA	1.83	0.44	
2:E:47:ASN:O	2:E:48:HIS:HB2	2.18	0.44	
2:E:84:ILE:HD12	2:E:101:TRP:CZ2	2.52	0.44	
2:R:79:PHE:HB2	2:R:84:ILE:CG2	2.46	0.44	
3:B:474:ILE:HG23	3:B:499:VAL:HG22	1.99	0.44	
3:N:474:ILE:HG23	3:N:499:VAL:HG22	1.99	0.44	
1:C:72:LYS:O	1:C:76:GLY:N	2.50	0.44	
1:C:323:GLU:HG2	1:C:326:LYS:HZ3	1.81	0.44	
1:C:436:LEU:HD23	1:C:439:ARG:HH11	1.82	0.44	
1:F:712:LYS:NZ	1:F:767:VAL:O	2.40	0.44	
1:M:436:LEU:HD23	1:M:439:ARG:HH11	1.82	0.44	
1:O:185:ASN:HA	1:O:188:GLN:HG2	2.00	0.44	
2:R:79:PHE:CG	2:R:84:ILE:CG2	3.00	0.44	
3:B:348:ASN:ND2	3:B:366:MET:O	2.32	0.44	
3:B:370:ARG:HH21	3:B:400:GLU:HG2	1.83	0.44	
4:I:486:ALA:O	4:I:489:GLU:HG3	2.18	0.44	



A 1 -		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:265:GLU:HA	1:C:269:ILE:CG1	2.47	0.44	
1:C:723:VAL:HA	1:C:726:VAL:HG12	1.99	0.44	
1:C:73:LEU:HD12	1:C:73:LEU:HA	1.79	0.44	
1:C:488:ARG:HH22	1:C:502:ASP:HA	1.83	0.44	
1:F:714:ARG:NH1	1:F:725:GLU:OE2	2.50	0.44	
1:M:41:ILE:HD12	1:M:80:VAL:HG11	2.00	0.44	
3:A:310:THR:HG22	3:A:580:ARG:HD3	2.00	0.44	
3:B:366:MET:HG2	3:B:409:TRP:CZ2	2.53	0.44	
4:I:481:ARG:HA	4:I:484:ILE:HG22	1.99	0.44	
4:I:548:ASP:O	4:I:551:LYS:HG3	2.18	0.44	
3:N:370:ARG:HH21	3:N:400:GLU:HG2	1.83	0.44	
4:J:548:ASP:O	4:J:551:LYS:HG3	2.18	0.44	
1:C:472:GLY:HA3	1:C:512:TYR:CE2	2.52	0.44	
1:M:263:VAL:HA	1:M:266:ARG:HB2	1.98	0.44	
1:M:390:LEU:HD13	1:M:390:LEU:HA	1.72	0.44	
2:Q:45:CYS:HB2	2:Q:54:ILE:HG12	1.98	0.44	
4:G:486:ALA:O	4:G:489:GLU:HG3	2.18	0.44	
3:N:265:LYS:HD3	3:N:587:TYR:CD1	2.53	0.44	
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.78	0.44	
1:C:365:LEU:O	1:C:368:GLN:HG3	2.17	0.44	
1:M:262:LYS:O	1:M:265:GLU:HG2	2.18	0.44	
1:M:351:ARG:HA	1:M:354:ARG:HG2	1.99	0.44	
3:B:170:MET:O	3:B:209:ARG:NH2	2.38	0.44	
3:B:272:ILE:HD12	3:B:310:THR:HG22	1.99	0.44	
1:C:488:ARG:HH21	1:C:503:LEU:H	1.66	0.43	
1:M:84:HIS:CE1	1:M:88:LYS:HG2	2.53	0.43	
1:M:559:LEU:HD22	1:M:602:LEU:HD23	1.99	0.43	
2:R:47:ASN:O	2:R:48:HIS:HB2	2.18	0.43	
3:B:247:GLN:H	3:B:247:GLN:HG2	1.69	0.43	
3:N:272:ILE:HD12	3:N:310:THR:HG22	1.99	0.43	
3:P:462:ALA:HA	3:P:475:GLY:HA3	2.00	0.43	
1:F:553:HIS:HA	1:F:597:PHE:CE1	2.53	0.43	
1:M:553:HIS:HA	1:M:597:PHE:CE1	2.53	0.43	
1:O:647:GLU:HB2	1:O:648:PRO:HD3	2.01	0.43	
2:R:72:TRP:HB2	2:R:105:LYS:O	2.17	0.43	
3:B:109:CYS:O	3:B:112:GLN:NE2	2.52	0.43	
1:C:351:ARG:HA	1:C:354:ARG:HG2	1.99	0.43	
1:C:446:VAL:HG23	1:C:447:SER:H	1.83	0.43	
1:F:647:GLU:HB2	1:F:648:PRO:HD3	2.00	0.43	
1:M:185:ASN:HA	1:M:188:GLN:HG2	1.99	0.43	
1:M:277:VAL:HG11	1:M:312:THR:OG1	2.18	0.43	



	bus page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:M:484:MET:SD	1:M:504:THR:HA	2.58	0.43	
1:O:265:GLU:HG2	1:O:266:ARG:N	2.32	0.43	
1:0:480:SER:HB2	1:O:506:ARG:HE	1.84	0.43	
1:O:497:SER:C	1:O:499:GLY:H	2.21	0.43	
1:O:524:ILE:H	1:O:524:ILE:HG12	1.53	0.43	
1:O:553:HIS:HA	1:O:597:PHE:CE1	2.53	0.43	
3:A:503:ASP:HB2	3:A:508:GLU:H	1.84	0.43	
1:C:54:PHE:CB	3:A:59:MET:SD	3.07	0.43	
1:C:527:ALA:HB3	1:C:528:PRO:HD3	2.00	0.43	
1:F:390:LEU:HD13	1:F:390:LEU:HA	1.71	0.43	
1:M:423:GLN:HG2	1:M:424:GLU:H	1.83	0.43	
1:O:622:ILE:CG1	1:O:627:LEU:HB2	2.49	0.43	
2:R:71:ALA:CB	2:R:84:ILE:CD1	2.86	0.43	
4:H:548:ASP:O	4:H:551:LYS:HG3	2.18	0.43	
3:P:265:LYS:HB3	3:P:265:LYS:HE3	1.66	0.43	
1:C:88:LYS:HG3	1:C:89:VAL:HG13	1.99	0.43	
1:M:647:GLU:HB2	1:M:648:PRO:HD3	2.00	0.43	
1:O:378:LEU:HD12	1:O:378:LEU:HA	1.73	0.43	
1:O:527:ALA:HB3	1:O:528:PRO:HD3	2.00	0.43	
2:R:100:GLU:O	2:R:101:TRP:HB3	2.18	0.43	
3:B:94:LEU:HD21	3:B:116:VAL:HG13	2.00	0.43	
3:B:287:CYS:SG	3:B:296:TYR:HB2	2.58	0.43	
3:N:24:PHE:CZ	3:P:57:ARG:CD	2.97	0.43	
3:N:265:LYS:HA	3:N:265:LYS:HD2	1.88	0.43	
4:J:459:LYS:HA	4:J:462:GLU:HG3	1.99	0.43	
4:J:534:ARG:HD2	3:P:257:PHE:CD2	2.54	0.43	
1:C:525:PRO:HB3	1:C:603:MET:HG3	2.01	0.43	
1:C:647:GLU:HB2	1:C:648:PRO:HD3	2.00	0.43	
1:O:54:PHE:CZ	3:N:64:LEU:HD12	2.52	0.43	
1:O:423:GLN:HG2	1:O:424:GLU:H	1.83	0.43	
1:O:559:LEU:HD22	1:O:602:LEU:HD23	1.99	0.43	
3:A:8:GLN:H	3:A:8:GLN:HG2	1.49	0.43	
3:A:225:LEU:HB3	3:A:229:THR:HG23	2.01	0.43	
3:A:442:TYR:H	3:A:442:TYR:HD2	1.67	0.43	
4:H:486:ALA:O	4:H:489:GLU:HG3	2.18	0.43	
4:J:467:TYR:HD1	4:J:467:TYR:HA	1.73	0.43	
3:P:22:LYS:HE3	3:P:91:THR:HG23	2.00	0.43	
3:P:319:TYR:HB3	3:P:350:PHE:CE2	2.54	0.43	
1:C:264:VAL:O	1:C:265:GLU:C	2.56	0.43	
1:C:354:ARG:HA	1:C:357:LEU:HG	2.01	0.43	
1:F:622:ILE:CG1	1:F:627:LEU:HB2	2.49	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:751:ARG:HD3	1:F:751:ARG:HA	1.88	0.43	
1:M:73:LEU:O	1:M:74:TYR:C	2.54	0.43	
1:M:86:ILE:HA	1:M:150:GLN:NE2	2.33	0.43	
3:A:257:PHE:CD2	4:G:534:ARG:HD2	2.54	0.43	
3:A:403:ASP:HB2	3:A:408:GLU:H	1.84	0.43	
4:G:436:VAL:HG11	4:G:445:VAL:HG13	2.01	0.43	
3:P:392:GLY:HA3	3:P:395:ASN:HB3	2.00	0.43	
1:C:553:HIS:HA	1:C:597:PHE:CE1	2.53	0.43	
1:F:446:VAL:HG23	1:F:447:SER:H	1.84	0.43	
1:F:756:ARG:HA	1:F:764:TYR:CE1	2.54	0.43	
1:M:446:VAL:HG23	1:M:447:SER:H	1.84	0.43	
1:O:526:PRO:HD2	1:O:603:MET:CE	2.49	0.43	
3:P:305:LEU:H	3:P:305:LEU:HD23	1.84	0.43	
1:C:480:SER:HB2	1:C:506:ARG:CB	2.28	0.43	
1:F:354:ARG:HA	1:F:357:LEU:HG	2.01	0.43	
1:0:154:TYR:HB3	1:O:157:ILE:HG22	2.01	0.43	
1:O:500:GLY:HA2	1:O:503:LEU:HD23	2.01	0.43	
3:A:472:PHE:CD1	3:A:499:VAL:HG12	2.54	0.43	
4:G:480:LYS:HB3	4:G:549:LEU:HD21	2.00	0.43	
3:B:265:LYS:HD3	3:B:587:TYR:CD1	2.53	0.43	
1:C:181:GLY:HA2	1:C:184:ARG:HG2	2.01	0.43	
1:C:559:LEU:O	1:C:592:LEU:N	2.39	0.43	
1:C:598:GLN:HG2	1:C:634:LEU:HG	2.01	0.43	
1:F:351:ARG:HA	1:F:354:ARG:HG2	1.99	0.43	
1:F:545:GLY:HA2	1:O:493:ALA:HB2	2.00	0.43	
1:M:700:LYS:HG2	1:M:744:ARG:HD2	2.00	0.43	
2:R:87:TRP:CZ2	2:R:91:ARG:HB3	2.54	0.43	
3:N:109:CYS:O	3:N:112:GLN:NE2	2.52	0.43	
3:P:291:GLN:H	3:P:291:GLN:HG2	1.48	0.43	
1:O:280:GLU:HB3	1:O:281:ASN:H	1.74	0.42	
3:A:351:TYR:HB3	3:A:360:TRP:HB3	2.01	0.42	
3:P:251:LYS:H	3:P:251:LYS:HG2	1.66	0.42	
1:C:63:THR:O	1:C:66:LEU:HB2	2.20	0.42	
1:0:125:TYR:O	1:O:129:VAL:HG22	2.19	0.42	
1:O:446:VAL:HG23	1:O:447:SER:H	1.83	0.42	
1:O:467:THR:HA	1:O:470:LEU:HB2	2.01	0.42	
4:G:548:ASP:O	4:G:551:LYS:HG3	2.18	0.42	
3:B:352:TRP:HB3	3:B:363:LYS:CE	2.46	0.42	
3:N:554:TYR:HB2	3:N:561:TRP:CZ3	2.54	0.42	
3:P:391:GLY:H	3:P:396:ARG:HG3	1.84	0.42	
1:C:486:GLU:O	1:C:490:HIS:ND1	2.35	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:F:248:VAL:HG23	1:F:252:LEU:HD22	2.00	0.42	
1:M:154:TYR:HB3	1:M:157:ILE:HG22	2.02	0.42	
1:M:259:PRO:O	1:M:262:LYS:HB2	2.19	0.42	
1:O:254:LYS:H	1:O:254:LYS:HG3	1.48	0.42	
3:B:437:ASN:O	3:B:455:ARG:N	2.40	0.42	
1:C:125:TYR:O	1:C:129:VAL:HG22	2.19	0.42	
1:C:524:ILE:HB	1:C:529:ARG:HG2	2.01	0.42	
1:F:181:GLY:HA2	1:F:184:ARG:HG2	2.01	0.42	
1:M:181:GLY:HA2	1:M:184:ARG:HG2	2.01	0.42	
1:O:97:LEU:HD22	1:O:97:LEU:HA	1.90	0.42	
1:O:559:LEU:O	1:O:592:LEU:N	2.39	0.42	
1:O:622:ILE:HG13	1:O:627:LEU:HB2	2.01	0.42	
3:A:57:ARG:NH2	3:B:20:GLN:NE2	2.67	0.42	
3:P:442:TYR:HB2	3:P:449:TRP:CZ3	2.54	0.42	
1:C:323:GLU:HA	1:C:326:LYS:HZ3	1.83	0.42	
1:F:89:VAL:HG11	1:F:151:VAL:CG2	2.45	0.42	
1:F:269:ILE:H	1:F:269:ILE:HG12	1.49	0.42	
1:F:323:GLU:HA	1:F:326:LYS:HZ1	1.83	0.42	
1:F:423:GLN:HG2	1:F:424:GLU:H	1.83	0.42	
1:O:181:GLY:HA2	1:O:184:ARG:HG2	2.01	0.42	
3:A:175:ASP:HA	3:A:178:ILE:HG12	2.01	0.42	
4:H:459:LYS:HE2	4:H:573:LEU:HD12	2.02	0.42	
4:I:524:ILE:HD12	4:I:524:ILE:HA	1.89	0.42	
3:P:276:SER:HA	3:P:573:TRP:HE1	1.85	0.42	
3:P:307:LYS:HB3	3:P:371:ILE:HG23	2.00	0.42	
3:P:554:TYR:HB2	3:P:561:TRP:CE3	2.55	0.42	
1:C:510:THR:HG23	2:E:76:ASN:HD21	1.84	0.42	
1:C:532:PHE:N	2:E:27:TRP:HZ3	2.17	0.42	
1:F:526:PRO:HD2	1:F:603:MET:HE1	2.02	0.42	
1:M:82:THR:O	1:M:83:GLU:C	2.55	0.42	
1:O:354:ARG:HA	1:O:357:LEU:HG	2.01	0.42	
2:D:84:ILE:HD13	2:D:84:ILE:O	2.20	0.42	
4:G:480:LYS:HA	4:G:480:LYS:HD3	1.55	0.42	
4:G:527:ASN:HA	4:G:530:LYS:HE3	2.02	0.42	
3:B:223:ASP:HB2	3:B:257:PHE:HE1	1.84	0.42	
1:C:37:LEU:HD21	1:C:60:ASN:CB	2.50	0.42	
1:F:173:ARG:HH12	1:F:213:SER:HA	1.84	0.42	
2:E:39:VAL:O	2:E:39:VAL:CG1	2.53	0.42	
2:Q:50:MET:HB2	2:Q:51:ASP:H	1.67	0.42	
3:A:431:ILE:H	3:A:431:ILE:HG13	1.56	0.42	
3:A:500:GLU:HA	3:A:511:MET:HG2	2.01	0.42	



	ous puge	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
4:G:521:ILE:HD12	4:G:521:ILE:HA	1.84	0.42	
3:B:97:ASN:OD1	3:B:100:THR:OG1	2.32	0.42	
3:B:261:LEU:HD11	3:B:590:CYS:SG	2.60	0.42	
1:F:467:THR:HA	1:F:470:LEU:HB2	2.01	0.42	
1:F:622:ILE:HG13	1:F:627:LEU:HB2	2.01	0.42	
1:M:274:LYS:HD2	1:M:274:LYS:HA	1.32	0.42	
1:M:548:LEU:HD22	2:R:32:LEU:O	2.20	0.42	
1:O:390:LEU:HG	1:O:681:GLN:HG2	2.01	0.42	
3:A:298:LEU:HD22	3:A:353:PHE:CE2	2.55	0.42	
3:A:320:ILE:HB	3:A:360:TRP:CZ3	2.55	0.42	
4:G:438:LYS:HD2	4:G:438:LYS:HA	1.74	0.42	
4:G:459:LYS:O	4:G:462:GLU:HG3	2.20	0.42	
4:I:459:LYS:HE2	4:I:573:LEU:HD12	2.02	0.42	
3:N:261:LEU:HD11	3:N:590:CYS:SG	2.60	0.42	
1:C:65:VAL:HG11	1:C:125:TYR:CE2	2.54	0.42	
1:C:404:THR:OG1	1:C:407:GLU:OE2	2.20	0.42	
1:M:89:VAL:O	1:M:90:ARG:C	2.55	0.42	
1:M:173:ARG:HH12	1:M:213:SER:HA	1.84	0.42	
2:E:79:PHE:HB2	2:E:84:ILE:HG23	2.02	0.42	
3:A:61:MET:CE	3:B:30:PHE:CE2	3.02	0.42	
3:A:298:LEU:HA	3:A:298:LEU:HD23	1.80	0.42	
3:N:223:ASP:HB2	3:N:257:PHE:HE1	1.84	0.42	
1:M:592:LEU:HD23	1:M:672:VAL:HG13	2.02	0.42	
1:O:173:ARG:HH12	1:O:213:SER:HA	1.84	0.42	
2:R:52:LEU:HA	2:R:52:LEU:HD13	1.75	0.42	
1:C:423:GLN:HG2	1:C:424:GLU:H	1.83	0.41	
1:F:90:ARG:HA	1:F:90:ARG:HD3	1.50	0.41	
1:F:154:TYR:HB3	1:F:157:ILE:HG22	2.01	0.41	
1:M:598:GLN:HG2	1:M:634:LEU:HG	2.01	0.41	
1:O:464:CYS:HA	1:O:467:THR:OG1	2.20	0.41	
2:E:52:LEU:HD11	2:E:59:ASN:HA	2.02	0.41	
3:A:451:GLU:H	3:A:451:GLU:HG2	1.52	0.41	
3:N:427:VAL:HG21	3:N:471:ILE:HG12	2.02	0.41	
3:P:175:ASP:HA	3:P:178:ILE:HG12	2.01	0.41	
3:P:225:LEU:HB3	3:P:229:THR:HG23	2.01	0.41	
1:C:96:SER:O	1:C:97:LEU:C	2.56	0.41	
1:C:173:ARG:HH12	1:C:213:SER:HA	1.84	0.41	
1:F:54:PHE:O	1:F:57:LEU:HB2	2.19	0.41	
1:F:531:ALA:HB1	2:D:27:TRP:HZ3	1.75	0.41	
1:M:77:LEU:O	1:M:78:ARG:C	2.53	0.41	
1:M:94:LEU:HD12	1:M:94:LEU:HA	1.77	0.41	



Atom-1	Atom-2	Interatomic	Clash	
1100111-1	1100111-2	distance (Å)	$\operatorname{overlap}\left(\mathrm{\AA}\right)$	
1:M:269:ILE:O	1:M:270:SER:C	2.58	0.41	
1:M:275:THR:O	:M:275:THR:O 1:M:279:MET:HB2		0.41	
1:M:354:ARG:HA	1:M:357:LEU:HG	2.01	0.41	
1:F:558:ASP:OD1	1:F:671:ARG:NH2	2.54	0.41	
1:M:37:LEU:HD21	1:M:60:ASN:CB	2.50	0.41	
3:A:454:MET:H	3:A:454:MET:HG2	1.70	0.41	
3:B:554:TYR:HB2	3:B:561:TRP:CZ3	2.54	0.41	
1:C:680:LYS:HB3	1:C:680:LYS:HE3	1.32	0.41	
1:M:265:GLU:O	1:M:269:ILE:HB	2.21	0.41	
3:A:307:LYS:HA	3:A:372:LYS:HG3	2.02	0.41	
4:I:480:LYS:HA	4:I:480:LYS:HD3	1.52	0.41	
4:I:534:ARG:HA	4:I:537:GLU:HG2	2.03	0.41	
4:J:527:ASN:HA	4:J:530:LYS:HE3	2.02	0.41	
4:J:534:ARG:HA	4:J:537:GLU:HG2	2.03	0.41	
1:F:710:ILE:HG21	1:F:729:GLN:HE22	1.86	0.41	
1:M:326:LYS:HA	1:M:329:VAL:HG22	2.01	0.41	
1:M:374:PHE:O	1:M:378:LEU:HB2	2.21	0.41	
1:M:437:ALA:HA	1:M:513:TRP:HZ3	1.85	0.41	
3:A:53:SER:HB2	3:A:113:VAL:HG22	2.03	0.41	
3:A:297:LYS:HD2	3:A:297:LYS:HA	1.87	0.41	
3:A:350:PHE:HD1	3:A:352:TRP:CZ3	2.39	0.41	
4:J:459:LYS:O	4:J:462:GLU:HG3	2.20	0.41	
3:P:127:LYS:HA	3:P:127:LYS:HD3	1.49	0.41	
1:C:383:ARG:H	1:C:383:ARG:HG2	1.67	0.41	
1:O:52:LEU:O	3:N:66:GLU:OE2	2.38	0.41	
2:E:94:CYS:HA	2:E:95:PRO:HD3	1.87	0.41	
2:R:54:ILE:HA	2:R:57:GLN:HE21	1.85	0.41	
3:N:46:LYS:NZ	3:N:67:SER:O	2.53	0.41	
3:N:109:CYS:HA	3:N:117:LEU:HD11	2.03	0.41	
3:P:390:VAL:HA	3:P:396:ARG:HG3	2.03	0.41	
1:C:81:VAL:HG23	1:C:82:THR:N	2.35	0.41	
1:C:154:TYR:HB3	1:C:157:ILE:HG22	2.01	0.41	
1:C:484:MET:HE1	1:C:504:THR:HG22	1.94	0.41	
1:F:520:PRO:HG3	1:F:553:HIS:CE1	2.55	0.41	
1:M:87:ASN:HB2	1:M:88:LYS:H	1.61	0.41	
1:M:761:ARG:H	1:M:761:ARG:HG2	1.75	0.41	
2:E:34:ALA:HA	2:E:76:ASN:HD22	1.86	0.41	
3:A:46:LYS:NZ	3:A:67:SER:O	2.54	0.41	
4:G:566:ILE:HD12	4:G:566:ILE:HA	1.74	0.41	
1:M:288:LEU:O	1:M:351:ARG:NH2	2.42	0.41	
1:O:560:ASN:HA	1:O:591:ILE:HG13	2.03	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:B:427:VAL:HG21	3:B:471:ILE:HG12	2.02	0.41	
4:H:481:ARG:HA	4:H:484:ILE:HG22	2.03	0.41	
1:C:263:VAL:O	1:C:266:ARG:HB2	2.21	0.41	
1:F:698:ASP:HA	1:F:701:HIS:CD2	2.56	0.41	
1:M:593:GLN:HE21	1:M:593:GLN:HB3	1.71	0.41	
2:E:84:ILE:CD1	2:E:101:TRP:HZ2	2.33	0.41	
2:R:37:ILE:HD13	2:R:72:TRP:CH2	2.56	0.41	
3:A:352:TRP:CH2	3:A:409:TRP:HH2	2.39	0.41	
3:A:352:TRP:HH2	3:A:409:TRP:CH2	2.38	0.41	
3:A:519:ARG:HA	4:I:440:ASP:CB	2.50	0.41	
3:B:363:LYS:O	3:B:364:THR:C	2.59	0.41	
4:H:534:ARG:HA	4:H:537:GLU:HG2	2.02	0.41	
4:I:593:LYS:HD2	4:I:593:LYS:HA	1.35	0.41	
3:N:7:ARG:HD3	3:P:93:ASN:HB2	2.03	0.41	
3:N:57:ARG:NE	3:P:24:PHE:HZ	2.13	0.41	
3:N:593:GLU:H	3:N:593:GLU:HG2	1.46	0.41	
1:C:262:LYS:HA	1:C:262:LYS:HD3	1.89	0.41	
1:C:274:LYS:HA	1:C:274:LYS:HD2	1.47	0.41	
1:M:348:LEU:HA	1:M:351:ARG:HG2	2.02	0.41	
2:D:98:ASN:HD22	2:D:98:ASN:HA	1.71	0.41	
3:B:96:MET:HE3	3:B:96:MET:HB3	1.77	0.41	
3:N:263:MET:H	3:N:263:MET:HG2	1.61	0.41	
3:N:417:CYS:HB2	3:N:419:TRP:CZ2	2.56	0.41	
3:P:459:ARG:HD2	3:P:476:GLY:HA3	2.03	0.41	
1:C:484:MET:SD	1:C:504:THR:CG2	2.95	0.40	
1:F:432:TYR:HE2	1:F:470:LEU:HD21	1.86	0.40	
1:F:531:ALA:HB3	2:D:27:TRP:CE3	2.53	0.40	
1:M:524:ILE:HB	1:M:529:ARG:HG3	2.03	0.40	
1:M:750:GLU:H	1:M:750:GLU:HG2	1.56	0.40	
1:O:336:LYS:HB2	1:O:337:ASN:H	1.64	0.40	
2:E:97:ASP:N	2:E:97:ASP:OD1	2.54	0.40	
3:B:108:ALA:O	3:B:112:GLN:N	2.54	0.40	
3:B:417:CYS:HB2	3:B:419:TRP:CZ2	2.56	0.40	
3:N:108:ALA:O	3:N:112:GLN:N	2.53	0.40	
3:P:353:PHE:HB2	3:P:360:TRP:CH2	2.56	0.40	
1:C:207:ALA:HB3	1:C:208:PRO:HD3	2.04	0.40	
1:F:503:LEU:HD21	2:D:27:TRP:HE3	1.86	0.40	
1:O:710:ILE:HG21	1:O:729:GLN:HE22	1.86	0.40	
1:0:717:MET:HG2	1:O:764:TYR:HE2	1.85	0.40	
2:E:54:ILE:HA	2:E:57:GLN:HE21	1.86	0.40	
3:A:61:MET:HE3	3:B:30:PHE:CD2	2.56	0.40	



	lo de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:123:TYR:HA	3:A:126:LYS:HE2	2.03	0.40
3:A:271:PHE:HB3	3:A:274:ALA:HB2	2.02	0.40
3:P:435:THR:O	3:P:455:ARG:NH2	2.38	0.40
1:C:710:ILE:HG21	1:C:729:GLN:HE22	1.85	0.40
1:F:420:ARG:NH1	1:F:461:GLU:OE2	2.55	0.40
1:M:207:ALA:HB3	1:M:208:PRO:HD3	2.04	0.40
1:M:622:ILE:CG1	1:M:627:LEU:HB2	2.52	0.40
1:0:558:ASP:OD1	1:O:671:ARG:NH2	2.54	0.40
2:D:97:ASP:OD1	2:D:97:ASP:N	2.54	0.40
2:R:94:CYS:HA	2:R:95:PRO:HD3	1.87	0.40
2:Q:89:LYS:HD2	2:Q:89:LYS:HA	1.56	0.40
3:A:357:GLN:H	3:A:357:GLN:HG2	1.50	0.40
1:C:524:ILE:HB	1:C:529:ARG:HG3	2.03	0.40
1:C:556:SER:OG	2:E:28:ASN:ND2	2.55	0.40
1:C:560:ASN:HA	1:C:591:ILE:HG13	2.03	0.40
1:C:622:ILE:CG1	1:C:627:LEU:HB2	2.52	0.40
1:F:550:LEU:H	1:F:550:LEU:HG	1.41	0.40
1:F:592:LEU:HD23	1:F:672:VAL:HG13	2.02	0.40
1:M:560:ASN:HA	1:M:591:ILE:HG13	2.03	0.40
1:O:271:LYS:HE3	1:0:271:LYS:HB2	1.76	0.40
1:0:288:LEU:O	1:O:351:ARG:NH2	2.42	0.40
1:O:334:GLU:H	1:O:334:GLU:HG2	1.56	0.40
3:B:273:GLU:OE2	3:B:307:LYS:N	2.55	0.40
3:P:81:THR:HG21	3:P:103:GLN:HG3	2.04	0.40
3:P:272:ILE:HD12	3:P:310:THR:HG22	2.03	0.40
1:C:524:ILE:O	1:C:529:ARG:NE	2.54	0.40
1:F:334:GLU:H	1:F:334:GLU:HG2	1.51	0.40
1:F:464:CYS:HA	1:F:467:THR:OG1	2.20	0.40
1:F:553:HIS:HA	1:F:597:PHE:HE1	1.87	0.40
1:M:168:MET:HA	1:M:171:ARG:HG2	2.04	0.40
1:M:548:LEU:HD22	1:M:548:LEU:HA	1.92	0.40
1:M:558:ASP:OD1	1:M:671:ARG:NH2	2.54	0.40
1:M:710:ILE:HG21	1:M:729:GLN:HE22	1.86	0.40
4:G:549:LEU:O	4:G:552:GLN:HG3	2.22	0.40
3:B:109:CYS:HA	3:B:117:LEU:HD11	2.03	0.40
4:J:480:LYS:HD3	4:J:480:LYS:HA	1.54	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	Percentiles
1	С	716/768~(93%)	628 (88%)	80 (11%)	8 (1%)	14 52
1	F	716/768~(93%)	633 (88%)	72 (10%)	11 (2%)	10 46
1	М	716/768~(93%)	648 (90%)	62 (9%)	6 (1%)	19 60
1	Ο	716/768~(93%)	646 (90%)	64 (9%)	6 (1%)	19 60
2	D	87/108 (81%)	60 (69%)	17 (20%)	10 (12%)	0 6
2	Е	87/108 (81%)	57 (66%)	18 (21%)	12 (14%)	0 4
2	Q	87/108 (81%)	62 (71%)	19 (22%)	6 (7%)	1 15
2	R	87/108 (81%)	57 (66%)	20 (23%)	10 (12%)	0 6
3	А	561/623~(90%)	480 (86%)	76 (14%)	5 (1%)	17 57
3	В	558/623~(90%)	510 (91%)	44 (8%)	4 (1%)	22 63
3	Ν	558/623~(90%)	512 (92%)	42 (8%)	4 (1%)	22 63
3	Р	547/623~(88%)	505~(92%)	40 (7%)	2(0%)	34 72
4	G	166/724~(23%)	156 (94%)	10 (6%)	0	100 100
4	Н	166/724~(23%)	156 (94%)	10 (6%)	0	100 100
4	Ι	166/724~(23%)	156 (94%)	8 (5%)	2 (1%)	13 50
4	J	166/724~(23%)	155 (93%)	11 (7%)	0	100 100
All	All	6100/8892~(69%)	5421 (89%)	593 (10%)	86 (1%)	15 46

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	88	LYS
1	С	268	LEU
1	F	526	PRO
2	D	40	ASP
2	Q	40	ASP
3	Ν	592	GLU



Mol	Chain	Res	Type
1	С	84	HIS
1	С	269	ILE
1	F	269	ILE
1	F	501	VAL
1	М	88	LYS
1	М	501	VAL
2	Е	39	VAL
2	Е	66	GLU
2	Е	94	CYS
2	D	35	TRP
2	D	92	GLN
2	D	94	CYS
2	R	39	VAL
2	R	66	GLU
2	R	94	CYS
2	Q	35	TRP
3	А	302	PRO
3	А	391	GLY
3	А	599	PRO
4	Ι	442	ILE
1	С	78	ARG
1	С	83	GLU
1	С	258	GLU
1	F	50	SER
1	М	278	GLU
1	0	257	GLU
1	0	526	PRO
2	E	35	TRP
2	E	64	THR
2	E	98	ASN
2	R	35	TRP
2	R	64	THR
2	R	98	ASN
3	A	476	GLY
3	В	248	GLY
3	N	248	GLY
1	С	267	GLU
1	F	196	GLU
1	F	270	SER
1	F	279	MET
1	F	330	SER
1	М	277	VAL



Mol	Chain	Res	Type
1	0	258	GLU
2	Е	40	ASP
2	Е	97	ASP
2	D	97	ASP
2	D	98	ASN
2	R	40	ASP
2	R	97	ASP
2	Q	94	CYS
3	N	600	THR
1	F	382	SER
1	М	335	GLY
1	0	266	ARG
2	Е	48	HIS
2	D	39	VAL
2	R	48	HIS
2	Q	46	ARG
3	А	513	ALA
1	F	59	ARG
2	Е	57	GLN
2	Е	101	TRP
2	D	46	ARG
2	D	101	TRP
2	Q	39	VAL
3	В	600	THR
1	0	767	VAL
2	Е	38	VAL
2	R	38	VAL
4	Ι	588	GLY
3	Р	516	PRO
3	Р	571	VAL
3	В	279	PRO
3	В	595	PRO
3	N	279	PRO
1	F	623	PRO
1	М	269	ILE
1	0	623	PRO
2	D	38	VAL
2	Q	38	VAL



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	С	635/693~(92%)	527~(83%)	108 (17%)	2	12
1	F	603/693~(87%)	502 (83%)	101 (17%)	2	12
1	М	604/693~(87%)	506 (84%)	98 (16%)	2	13
1	Ο	628/693~(91%)	525 (84%)	103~(16%)	2	12
2	D	78/90~(87%)	55 (70%)	23~(30%)	0	2
2	Е	78/90~(87%)	61 (78%)	17 (22%)	1	6
2	Q	78/90~(87%)	52~(67%)	26~(33%)	0	2
2	R	78/90~(87%)	63 (81%)	15 (19%)	1	8
3	А	504/560~(90%)	379~(75%)	125~(25%)	0	3
3	В	495/560~(88%)	461 (93%)	34~(7%)	15	40
3	Ν	496/560~(89%)	464 (94%)	32~(6%)	17	42
3	Р	477/560~(85%)	445 (93%)	32 (7%)	16	41
4	G	151/654~(23%)	123~(82%)	28 (18%)	1	9
4	Н	129/654~(20%)	111 (86%)	18 (14%)	3	17
4	Ι	134/654~(20%)	115 (86%)	19 (14%)	3	16
4	J	125/654~(19%)	106 (85%)	19 (15%)	3	14
All	All	5293/7988~(66%)	4495 (85%)	798 (15%)	6	14

All (798) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	35	ASP
1	С	43	GLU
1	С	55	GLU
1	С	65	VAL
1	С	66	LEU
1	С	67	HIS
1	С	68	LYS
1	С	71	GLU



Mol	Chain	Res	Type
1	С	72	LYS
1	С	73	LEU
1	С	78	ARG
1	С	79	GLU
1	С	82	THR
1	С	83	GLU
1	С	85	LEU
1	С	86	ILE
1	С	87	ASN
1	С	90	ARG
1	С	91	GLU
1	С	94	LEU
1	С	96	SER
1	С	98	ASN
1	С	102	LEU
1	С	121	ASP
1	С	204	ASP
1	С	225	LEU
1	С	252	LEU
1	С	254	LYS
1	С	258	GLU
1	С	260	ILE
1	С	261	VAL
1	С	262	LYS
1	С	263	VAL
1	С	266	ARG
1	С	267	GLU
1	С	268	LEU
1	С	270	SER
1	С	273	MET
1	С	274	LYS
1	С	276	ILE
1	C	278	GLU
1	C	279	MET
1	C	280	GLU
1	C	282	SER
1	C	284	LEU
1	C	328	LEU
1	C	334	GLU
1	С	336	LYS
1	С	340	ASP
1	С	341	TYR



Mol	Chain	Res	Type
1	С	342	ILE
1	С	346	LEU
1	С	349	LYS
1	С	353	ASP
1	С	380	LEU
1	С	397	LYS
1	С	405	GLU
1	С	407	GLU
1	С	411	ILE
1	С	420	ARG
1	С	446	VAL
1	С	462	CYS
1	С	465	GLN
1	С	468	SER
1	С	470	LEU
1	С	473	MET
1	С	484	MET
1	С	486	GLU
1	С	491	LEU
1	С	496	VAL
1	С	498	LEU
1	С	501	VAL
1	С	503	LEU
1	С	508	LEU
1	С	509	THR
1	С	510	THR
1	С	513	TRP
1	С	515	THR
1	С	521	LYS
1	С	593	GLN
1	С	596	THR
1	C	600	THR
1	C	602	LEU
1	C	613	PHE
1	С	627	LEU
1	C	632	GLN
1	С	633	SER
1	С	634	LEU
1	C	641	GLN
1	C	653	ILE
1	С	665	PHE
1	С	669	LEU



Mol	Chain	Res	Type
1	С	676	THR
1	С	677	VAL
1	С	680	LYS
1	С	687	GLU
1	С	688	ARG
1	С	697	ASP
1	С	699	ARG
1	С	701	HIS
1	С	702	GLU
1	С	716	LYS
1	С	750	GLU
1	С	751	ARG
1	С	753	TYR
1	С	762	LYS
1	С	763	VAL
1	С	767	VAL
1	F	35	ASP
1	F	43	GLU
1	F	68	LYS
1	F	72	LYS
1	F	77	LEU
1	F	83	GLU
1	F	84	HIS
1	F	86	ILE
1	F	88	LYS
1	F	90	ARG
1	F	94	LEU
1	F	97	LEU
1	F	98	ASN
1	F	99	ASN
1	F	102	LEU
1	F	196	GLU
1	F	198	ARG
1	F	199	SER
1	F	204	ASP
1	F	225	LEU
1	F	254	LYS
1	F	256	THR
1	F	258	GLU
1	F	260	ILE
1	F	262	LYS
1	F	264	VAL



Mol	Chain	Res	Type
1	F	266	ARG
1	F	267	GLU
1	F	268	LEU
1	F	269	ILE
1	F	271	LYS
1	F	273	MET
1	F	274	LYS
1	F	275	THR
1	F	277	VAL
1	F	279	MET
1	F	280	GLU
1	F	282	SER
1	F	284	LEU
1	F	330	SER
1	F	334	GLU
1	F	336	LYS
1	F	339	VAL
1	F	342	ILE
1	F	348	LEU
1	F	349	LYS
1	F	353	ASP
1	F	382	SER
1	F	383	ARG
1	F	384	SER
1	F	390	LEU
1	F	397	LYS
1	F	405	GLU
1	F	407	GLU
1	F	411	ILE
1	F	420	ARG
1	F	446	VAL
1	F	468	SER
1	F	469	LYS
1	F	470	LEU
1	F	473	MET
1	F	478	SER
1	F	479	ILE
1	F	481	ASN
1	F	503	LEU
1	F	504	THR
1	F	505	VAL
1	F	507	VAL



Mol	Chain	Res	Type
1	F	510	THR
1	F	515	THR
1	F	521	LYS
1	F	522	CYS
1	F	523	ASN
1	F	524	ILE
1	F	526	PRO
1	F	550	LEU
1	F	551	GLN
1	F	593	GLN
1	F	596	THR
1	F	600	THR
1	F	602	LEU
1	F	613	PHE
1	F	632	GLN
1	F	634	LEU
1	F	641	GLN
1	F	653	ILE
1	F	665	PHE
1	F	669	LEU
1	F	680	LYS
1	F	683	GLU
1	F	698	ASP
1	F	703	ILE
1	F	716	LYS
1	F	748	LEU
1	F	749	ILE
1	F	750	GLU
1	F	751	ARG
1	F	752	GLU
1	F	757	THR
1	F	761	ARG
1	F	762	LYS
1	М	35	ASP
1	М	43	GLU
1	М	66	LEU
1	М	72	LYS
1	М	79	GLU
1	М	86	ILE
1	М	88	LYS
1	М	91	GLU
1	М	94	LEU



Mol	Chain	Res	Type
1	М	96	SER
1	М	97	LEU
1	М	98	ASN
1	М	99	ASN
1	М	102	LEU
1	М	204	ASP
1	М	225	LEU
1	М	252	LEU
1	М	253	ASP
1	М	254	LYS
1	М	257	GLU
1	М	258	GLU
1	М	262	LYS
1	М	263	VAL
1	М	264	VAL
1	М	267	GLU
1	М	268	LEU
1	М	270	SER
1	М	273	MET
1	М	274	LYS
1	М	275	THR
1	М	278	GLU
1	М	279	MET
1	М	280	GLU
1	М	282	SER
1	М	284	LEU
1	М	336	LYS
1	М	342	ILE
1	М	346	LEU
1	М	349	LYS
1	М	353	ASP
1	М	377	PHE
1	М	378	LEU
1	М	380	LEU
1	М	390	LEU
1	М	397	LYS
1	М	405	GLU
1	М	407	GLU
1	М	411	ILE
1	М	420	ARG
1	М	446	VAL
1	М	457	LYS



Mol	Chain	Res	Type
1	М	458	LEU
1	М	462	CYS
1	М	464	CYS
1	М	465	GLN
1	М	470	LEU
1	М	473	MET
1	М	484	MET
1	М	505	VAL
1	М	508	LEU
1	М	509	THR
1	М	510	THR
1	М	515	THR
1	М	516	GLN
1	М	521	LYS
1	М	522	CYS
1	М	523	ASN
1	М	524	ILE
1	М	547	GLN
1	М	548	LEU
1	М	549	THR
1	М	593	GLN
1	М	596	THR
1	М	600	THR
1	М	602	LEU
1	М	613	PHE
1	М	627	LEU
1	М	632	GLN
1	М	633	SER
1	М	634	LEU
1	М	641	GLN
1	М	653	ILE
1	М	665	PHE
1	М	669	LEU
1	М	680	LYS
1	М	683	GLU
1	М	695	VAL
1	М	698	ASP
1	M	701	HIS
1	М	703	ILE
1	М	716	LYS
1	М	750	GLU
1	М	753	TYR



Mol	Chain	Res	Type
1	М	754	LEU
1	М	761	ARG
1	М	762	LYS
1	М	763	VAL
1	М	767	VAL
1	0	35	ASP
1	0	43	GLU
1	0	55	GLU
1	0	56	GLU
1	0	57	LEU
1	0	68	LYS
1	0	72	LYS
1	0	77	LEU
1	0	83	GLU
1	0	84	HIS
1	0	86	ILE
1	0	88	LYS
1	0	90	ARG
1	0	94	LEU
1	0	97	LEU
1	0	98	ASN
1	0	99	ASN
1	0	102	LEU
1	0	121	ASP
1	0	204	ASP
1	0	225	LEU
1	0	252	LEU
1	0	253	ASP
1	0	254	LYS
1	0	256	THR
1	0	258	GLU
1	0	262	LYS
1	0	264	VAL
1	0	265	GLU
1	Ο	267	GLU
1	Ō	268	LEU
1	0	271	LYS
1	0	273	MET
1	0	274	LYS
1	0	275	THR
1	Ο	276	ILE
1	Ο	284	LEU



Mol	Chain	Res	Type
1	0	328	LEU
1	0	334	GLU
1	0	336	LYS
1	0	339	VAL
1	0	341	TYR
1	0	346	LEU
1	0	349	LYS
1	0	353	ASP
1	Ο	377	PHE
1	0	379	ASN
1	0	381	ASN
1	0	383	ARG
1	Ο	384	SER
1	0	390	LEU
1	0	397	LYS
1	0	405	GLU
1	0	407	GLU
1	Ο	411	ILE
1	0	418	LEU
1	0	420	ARG
1	Ο	421	PHE
1	0	446	VAL
1	Ο	468	SER
1	0	469	LYS
1	0	470	LEU
1	0	473	MET
1	0	478	SER
1	Ο	479	ILE
1	0	481	ASN
1	0	504	THR
1	0	505	VAL
1	0	510	THR
1	0	515	THR
1	0	521	LYS
1	0	523	ASN
1	0	524	ILE
1	Ο	526	PRO
1	0	550	LEU
1	0	551	GLN
1	0	593	GLN
1	0	596	THR
1	0	600	THR



Mol	Chain	Res	Type
1	0	602	LEU
1	0	613	PHE
1	0	632	GLN
1	0	634	LEU
1	0	641	GLN
1	0	653	ILE
1	0	665	PHE
1	0	669	LEU
1	0	680	LYS
1	0	683	GLU
1	0	697	ASP
1	0	701	HIS
1	0	716	LYS
1	0	748	LEU
1	0	749	ILE
1	0	750	GLU
1	0	751	ARG
1	0	752	GLU
1	0	757	THR
1	0	761	ARG
1	0	762	LYS
1	0	763	VAL
1	0	765	THR
1	0	767	VAL
2	Е	28	ASN
2	Е	35	TRP
2	Е	37	ILE
2	Ε	42	CYS
2	Е	47	ASN
2	Ε	49	ILE
2	Е	55	GLU
2	Е	59	ASN
2	Е	74	VAL
2	E	86	ARG
2	E	90	THR
2	Е	91	ARG
2	E	93	VAL
2	Е	98	ASN
2	E	99	ARG
2	E	104	GLN
2	E	105	LYS
2	D	28	ASN



Mol	Chain	Res	Type
2	D	35	TRP
2	D	37	ILE
2	D	39	VAL
2	D	40	ASP
2	D	42	CYS
2	D	46	ARG
2	D	47	ASN
2	D	50	MET
2	D	66	GLU
2	D	84	ILE
2	D	86	ARG
2	D	89	LYS
2	D	91	ARG
2	D	92	GLN
2	D	93	VAL
2	D	98	ASN
2	D	99	ARG
2	D	100	GLU
2	D	101	TRP
2	D	103	PHE
2	D	105	LYS
2	D	108	HIS
2	R	28	ASN
2	R	35	TRP
2	R	37	ILE
2	R	42	CYS
2	R	47	ASN
2	R	49	ILE
2	R	52	LEU
2	R	59	ASN
2	R	86	ARG
2	R	91	ARG
2	R	93	VAL
2	R	98	ASN
2	R	99	ARG
2	R	102	GLU
2	R	104	GLN
2	Q	28	ASN
2	Q	35	TRP
2	Q	37	ILE
2	Q	39	VAL
2	Q	40	ASP



Mol	Chain	Res	Type
2	Q	42	CYS
2	Q	46	ARG
2	Q	47	ASN
2	Q	50	MET
2	Q	59	ASN
2	Q	66	GLU
2	Q	74	VAL
2	Q	84	ILE
2	Q	87	TRP
2	Q	89	LYS
2	Q	90	THR
2	Q	91	ARG
2	Q	92	GLN
2	Q	93	VAL
2	Q	96	LEU
2	Q	98	ASN
2	Q	99	ARG
2	Q	102	GLU
2	Q	105	LYS
2	Q	106	TYR
2	Q	108	HIS
3	А	7	ARG
3	А	8	GLN
3	А	9	ILE
3	А	37	VAL
3	А	53	SER
3	А	54	SER
3	А	128	ILE
3	А	131	GLU
3	A	133	CYS
3	A	241	ASP
3	А	243	SER
3	A	253	MET
3	A	263	MET
3	A	270	ILE
3	A	275	SER
3	A	277	GLU
3	A	278	ASN
3	A	280	CYS
3	A	281	SER
3	A	282	LEU
3	А	283	TYR



Mol	Chain	Res	Type
3	А	286	VAL
3	А	287	CYS
3	А	291	GLN
3	А	297	LYS
3	А	298	LEU
3	А	300	SER
3	А	305	LEU
3	А	307	LYS
3	А	308	VAL
3	А	310	THR
3	А	311	VAL
3	А	313	THR
3	А	315	ASP
3	A	317	ASP
3	А	318	ILE
3	А	324	GLN
3	А	325	VAL
3	А	328	LYS
3	А	344	PHE
3	А	349	CYS
3	А	353	PHE
3	А	356	GLN
3	А	357	GLN
3	А	363	LYS
3	А	367	LEU
3	А	370	ARG
3	А	371	ILE
3	А	372	LYS
3	А	375	LEU
3	А	376	VAL
3	А	377	CYS
3	А	378	CYS
3	А	381	TYR
3	A	388	ASP
3	A	389	SER
3	A	393	GLU
3	А	394	LEU
3	А	396	ARG
3	A	397	ARG
3	А	398	THR
3	A	401	ARG
3	А	404	THR



Mol	Chain	Res	Type
3	А	406	LYS
3	А	411	MET
3	А	412	VAL
3	А	426	VAL
3	А	427	VAL
3	А	431	ILE
3	А	436	LEU
3	А	443	PHE
3	А	445	ARG
3	А	446	SER
3	А	447	ASP
3	А	451	GLU
3	А	452	MET
3	A	454	MET
3	A	455	ARG
3	А	456	GLN
3	А	457	THR
3	А	458	SER
3	А	459	ARG
3	А	470	LYS
3	А	471	ILE
3	А	474	ILE
3	А	477	LEU
3	А	497	VAL
3	А	500	GLU
3	А	503	ASP
3	А	505	ASN
3	А	506	LYS
3	А	509	TRP
3	А	510	LYS
3	А	514	ASN
3	А	515	ILE
3	A	525	VAL
3	A	534	LEU
3	A	538	MET
3	A	539	ARG
3	А	541	THR
3	А	543	LEU
3	A	551	THR
3	A	555	ASP
3	A	557	GLU
3	А	559	ASP



Mol	Chain	Res	Type
3	А	560	ARG
3	А	561	TRP
3	А	562	SER
3	А	563	LEU
3	А	567	ILE
3	А	571	VAL
3	А	574	ASP
3	А	578	ASP
3	А	580	ARG
3	А	582	THR
3	А	583	VAL
3	А	586	LEU
3	А	589	SER
3	А	591	LEU
3	А	592	GLU
3	А	594	SER
3	А	602	LEU
3	А	603	PHE
3	А	604	SER
3	А	605	THR
4	G	433	GLN
4	G	434	ASP
4	G	436	VAL
4	G	437	VAL
4	G	438	LYS
4	G	440	ASP
4	G	453	ASN
4	G	454	THR
4	G	457	GLN
4	G	467	TYR
4	G	476	GLU
4	G	477	ILE
4	G	479	MET
4	G	480	LYS
4	G	481	ARG
4	G	507	GLU
4	G	515	GLU
4	G	521	ILE
4	G	525	MET
4	G	526	HIS
4	G	547	GLU
4	G	551	LYS



Mol	Chain	Res	Type
4	G	561	LYS
4	G	562	ARG
4	G	566	ILE
4	G	581	LEU
4	G	598	LEU
4	G	600	ASN
3	В	7	ARG
3	В	8	GLN
3	В	9	ILE
3	В	19	GLU
3	В	37	VAL
3	В	61	MET
3	В	93	ASN
3	В	96	MET
3	В	114	GLU
3	В	127	LYS
3	В	133	CYS
3	В	134	VAL
3	В	203	GLU
3	В	243	SER
3	В	251	LYS
3	В	275	SER
3	В	277	GLU
3	В	278	ASN
3	В	280	CYS
3	В	282	LEU
3	В	283	TYR
3	В	291	GLN
3	В	305	LEU
3	В	328	LYS
3	В	363	LYS
3	В	374	SER
3	В	397	ARG
3	В	408	GLU
3	В	568	SER
3	В	571	VAL
3	В	572	LEU
3	В	596	TRP
3	В	597	LYS
3	В	601	TYR
4	Н	453	ASN
4	Н	454	THR



Mol	Chain	Res	Type
4	Н	457	GLN
4	Н	467	TYR
4	Н	476	GLU
4	Н	477	ILE
4	Н	480	LYS
4	Н	481	ARG
4	Н	507	GLU
4	Н	515	GLU
4	Н	521	ILE
4	Н	525	MET
4	Н	526	HIS
4	Н	547	GLU
4	Н	551	LYS
4	Н	561	LYS
4	Н	562	ARG
4	Н	566	ILE
4	Ι	453	ASN
4	Ι	454	THR
4	Ι	457	GLN
4	Ι	467	TYR
4	Ι	476	GLU
4	Ι	477	ILE
4	Ι	480	LYS
4	Ι	481	ARG
4	Ι	507	GLU
4	Ι	515	GLU
4	Ι	525	MET
4	Ι	547	GLU
4	Ι	551	LYS
4	Ι	561	LYS
4	Ι	562	ARG
4	Ι	566	ILE
4	Ι	592	LYS
4	Ι	593	LYS
4	Ι	598	LEU
3	N	7	ARG
3	N	8	GLN
3	Ν	11	THR
3	Ν	12	GLU
3	N	37	VAL
3	Ν	114	GLU
3	N	127	LYS



Mol	Chain	Res	Type
3	Ν	128	ILE
3	Ν	133	CYS
3	N	134	VAL
3	N	203	GLU
3	N	243	SER
3	N	251	LYS
3	N	277	GLU
3	N	278	ASN
3	N	280	CYS
3	N	282	LEU
3	N	291	GLN
3	N	305	LEU
3	N	328	LYS
3	N	363	LYS
3	Ν	374	SER
3	N	397	ARG
3	Ν	406	LYS
3	N	407	ASP
3	N	408	GLU
3	N	571	VAL
3	N	572	LEU
3	N	592	GLU
3	N	593	GLU
3	N	597	LYS
3	N	601	TYR
4	J	453	ASN
4	J	454	THR
4	J	457	GLN
4	J	467	TYR
4	J	476	GLU
4	J	477	ILE
4	J	479	MET
4	J	480	LYS
4	J	481	ARG
4	J	507	GLU
4	J	515	GLU
4	J	521	ILE
4	J	525	MET
4	J	526	HIS
4	J	547	GLU
4	J	551	LYS
4	J	561	LYS



Mol	Chain	Res	Type
4	J	562	ARG
4	J	566	ILE
3	Р	7	ARG
3	Р	11	THR
3	Р	37	VAL
3	Р	96	MET
3	Р	127	LYS
3	Р	128	ILE
3	Р	131	GLU
3	Р	133	CYS
3	Р	134	VAL
3	Р	243	SER
3	Р	251	LYS
3	Р	253	MET
3	Р	263	MET
3	Р	265	LYS
3	Р	275	SER
3	Р	277	GLU
3	Р	282	LEU
3	Р	291	GLN
3	Р	324	GLN
3	Р	346	THR
3	Р	350	PHE
3	Р	396	ARG
3	Р	406	LYS
3	Р	407	ASP
3	Р	408	GLU
3	Р	540	GLU
3	Р	568	SER
3	Р	570	ARG
3	Р	571	VAL
3	Р	572	LEU
3	Р	589	SER
3	Р	601	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	99	ASN
1	С	106	ASN
1	С	110	ASN
1	С	134	ASN



Mol	Chain	Res	Type
1	С	163	GLN
1	С	218	GLN
1	С	222	GLN
1	С	324	GLN
1	С	361	ASN
1	С	381	ASN
1	С	465	GLN
1	С	606	ASN
1	С	618	GLN
1	С	641	GLN
1	С	657	HIS
1	F	106	ASN
1	F	110	ASN
1	F	134	ASN
1	F	163	GLN
1	F	218	GLN
1	F	324	GLN
1	F	361	ASN
1	F	606	ASN
1	F	618	GLN
1	F	641	GLN
1	F	657	HIS
1	F	718	GLN
1	F	719	HIS
1	М	84	HIS
1	М	87	ASN
1	М	110	ASN
1	М	134	ASN
1	М	150	GLN
1	М	160	HIS
1	М	163	GLN
1	M	218	GLN
1	M	324	GLN
1	М	361	ASN
1	М	381	ASN
1	M	606	ASN
1	М	618	GLN
1	М	641	GLN
1	M	657	HIS
1	М	718	GLN
1	М	719	HIS
1	0	106	ASN



Mol	Chain	Res	Type
1	Ο	110	ASN
1	0	134	ASN
1	0	150	GLN
1	0	163	GLN
1	0	218	GLN
1	0	222	GLN
1	0	281	ASN
1	0	324	GLN
1	0	361	ASN
1	0	381	ASN
1	0	606	ASN
1	0	618	GLN
1	0	641	GLN
1	0	657	HIS
1	0	718	GLN
1	0	719	HIS
2	Е	28	ASN
2	Е	41	ASN
2	Е	47	ASN
2	Е	57	GLN
2	Е	98	ASN
2	D	28	ASN
2	D	48	HIS
2	D	98	ASN
2	R	28	ASN
2	R	41	ASN
2	R	98	ASN
2	Q	28	ASN
2	Q	48	HIS
2	Q	98	ASN
3	А	10	ASN
3	А	230	GLN
3	А	306	HIS
3	А	514	ASN
4	G	450	HIS
4	G	453	ASN
4	G	455	GLN
4	G	457	GLN
4	G	564	ASN
4	G	572	GLN
3	В	20	GLN
3	В	93	ASN



Mol	Chain	Res	Type
3	В	230	GLN
3	В	356	GLN
3	В	357	GLN
4	Н	453	ASN
4	Н	455	GLN
4	Н	457	GLN
4	Н	564	ASN
4	Н	572	GLN
4	Ι	453	ASN
4	Ι	455	GLN
4	Ι	457	GLN
4	Ι	564	ASN
4	Ι	572	GLN
4	Ι	591	GLN
4	Ι	595	ASN
3	N	112	GLN
3	N	230	GLN
3	N	356	GLN
3	N	357	GLN
4	J	453	ASN
4	J	455	GLN
4	J	457	GLN
4	J	564	ASN
4	J	572	GLN
3	Р	230	GLN
3	Р	278	ASN
3	Р	356	GLN
3	Р	357	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.


5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

5.7 Other polymers (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-34453. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 96



Y Index: 96



Z Index: 96

6.2.2 Raw map



X Index: 96

Y Index: 96

Z Index: 96

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



6.3 Largest variance slices (i)

6.3.1 Primary map







Y Index: 106



Z Index: 68

6.3.2 Raw map



X Index: 102

Y Index: 108



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



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

6.4.1 Primary map



6.4.2 Raw map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 108428 nm^3 ; this corresponds to an approximate mass of 97946 kDa.

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



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.133 ${\rm \AA}^{-1}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.133 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	7.52	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	8.58	10.89	8.79	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.58 differs from the reported value 7.52 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34453 and PDB model 8H37. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.001).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9740	0.0570	
А	0.9950	0.0600	
В	0.9880	0.0440	1 0
C	0.9930	0.1050	1.0
D	0.9200	0.0200	
Е	0.9710	0.0270	
F	0.9950	0.0940	
G	0.9610	0.0420	
Н	0.9320	0.0330	
I	0.7700	-0.0150	
J	0.8140	-0.0430	
М	0.9860	0.0840	0.0
N	0.9800	0.0250	<0.0
0	0.9870	0.0720	
P	0.9890	0.0280	
Q	0.9810	0.0150	
R	0.9490	-0.0020	

