

Nov 25, 2023 – 12:54 PM EST

PDB ID	:	8TVU				
EMDB ID	:	EMD-41651				
Title	:	In situ cryo-EM structure of bacteriophage P22 portal protein: head-to-tail				
		protein complex at 3.0A resolution				
Authors	:	Iglesias, S.M.; Cingolani, G.; Feng-Hou, C.				
Deposited on	:	2023-08-18				
Resolution	:	3.00 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	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain					
1	А	725	6%	18%	•	16%		
1	В	725	6% 62%	20%	•	16%		
1	D	725	6% 63%	19%	•	16%		
1	F	725	6%	18%	•	16%		
1	Н	725	6%	19%	•	16%		
1	J	725	6%	19%	•	16%		
1	L	725	6%	18%	•	16%		
1	N	725	6%	20%	·	16%		



Mol	Chain	Length	Quality of chain	
1	Р	725	6% 63% 20%	• 16%
1	R	725	6% 63% 19%	• 16%
1	Т	725	6% 62% 20%	• 16%
1	W	725	6% 64% 17%	• 16%
2	C	166	79%	11% • 8%
2	E	166	78%	13% 8%
2	G	166	79%	13% 8%
2	I	166	77%	14% • 8%
2	K	166	81%	10% 8%
2	M	166	79%	13% 8%
2	0	166	78%	12% • 8%
2	0	166	79%	13% 8%
2	S	166	78%	13% • 8%
2	V	166	77%	13% • 8%
2	X	166	80%	11% 8%
2	a	166	87%	5% 8%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 72840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	Λ	608	Total	С	Ν	0	S	0	0
1	A	008	4904	3088	843	952	21	0	0
1	D	609	Total	С	Ν	0	S	0	0
1	D	008	4904	3088	843	952	21	0	0
1	Л	608	Total	С	Ν	0	S	0	0
1	D	008	4904	3088	843	952	21	0	0
1	F	608	Total	С	Ν	0	S	0	0
1	T,	008	4904	3088	843	952	21	0	0
1	Ц	608	Total	С	Ν	0	\mathbf{S}	0	0
1	11	008	4904	3088	843	952	21	0	0
1	т	608	Total	С	Ν	0	S	0	0
1	J	008	4904	3088	843	952	21	0	0
1	T	608	Total	Total C N O S	0	0			
1		008	4904	3088	843	952	21	0	0
1	N	608	Total	С	Ν	Ο	\mathbf{S}	0	0
1	11	000	4904	3088	843	952	21	0	0
1	р	608	Total	С	Ν	Ο	\mathbf{S}	0	0
1	T	000	4904	3088	843	952	21	0	0
1	В	608	Total	С	Ν	Ο	\mathbf{S}	0	0
1	10	000	4904	3088	843	952	21	0	0
1	Т	608	Total	С	Ν	Ο	\mathbf{S}	0	0
	L	000	4904	3088	843	952	21	U	U
1	W	608	Total	С	Ν	0	S	0	0
	vv	000	4904	3088	843	952	21	0	U

• Molecule 1 is a protein called Portal protein.

• Molecule 2 is a protein called Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms				AltConf	Trace		
9	0	159	Total	С	Ν	Ο	S	0	0	
	152	1166	731	200	229	6	0	0		
9	С	159	Total	С	Ν	0	S	0	0	
	152	1166	731	200	229	6	0	0		
9	F	159	Total	С	Ν	0	S	0	0	
	Ц	Ľ	152	1166	731	200	229	6	0	0



Mol	Chain	Residues		At	oms			AltConf	Trace												
9	С	159	Total	С	Ν	0	S	0	0												
2	G	152	1166	731	200	229	6	0	0												
9	Т	159	Total	С	Ν	0	\mathbf{S}	0	0												
2	1	152	1166	731	200	229	6	0	0												
9	K	159	Total	С	Ν	0	\mathbf{S}	0	0												
2	Т	152	1166	731	200	229	6	0	0												
9	М	159	Total	С	Ν	0	\mathbf{S}	0	0												
2	111	111	IVI	111		1/1	1/1	111	111	11/1	1/1	1/1	111	152	1166	731	200	229	6	0	0
9	0	159	Total	С	Ν	0	\mathbf{S}	0	0												
2	0	152	1166	731	200	229	6	0	0												
9	0	159	Total	С	Ν	0	S	0	0												
	Q	152	1166	731	200	229	6	0	0												
9	S	159	Total	С	Ν	Ο	\mathbf{S}	0	0												
2	0	102	1166	731	200	229	6	0	0												
9	V	159	Total	С	Ν	0	S	0	Ο												
2 V	102	1166	731	200	229	6	0	0													
2	v	159	Total	С	Ν	0	S	0	0												
2 X	152	1166	731	200	229	6		0													

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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: Portal protein









• Molecule 1: Portal protein







N627 N627 N627 N621 1633 1634 1634 N635 N635 N635 N635 N635 N635 N635 N635 N635 N641 N645 N645













• Molecule 1: Portal protein







A637 K638 K638 C640 A641 A641 A642 A642 A642 A642 A1A A1A A1A A1A A1A A1A A1A A1A A1A A1	ASP LEEU SER CLYS CLYS CLN SER ARG CLN CLU CLYS SER ALA CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	ARG GLU GLU ASP ASP ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
THR LHTS LHTS GLN ARG ARG ARA ASN TLE GLN GLN GLN GLN GLN GLN GLN SER ASN VAL	GLU THR PRO GLN	
• Molecule 2: Peptidoglycan hyd	rolase gp4	
Chain a:	87%	5% 8%
M1 M4 D63 E69 E112 E112 F1 40 F1 40 F1 40 F1 40 F1 40 G1 N A1 A ASN ASN ASN ASN	THR THR PRO PRO ASP GLU GLY GLY GLY	
• Molecule 2: Peptidoglycan hyd	rolase gp4	
Chain C:	79%	11% • 8%
M1 13 02 07 07 08 81 13 13 13 13 13 13 13 13 13 13 13 13 13	F84 R90 E112 E112 F140 F140 P150 C115 C115 C115 C115 C115 C115 C115 C	SER THR PRO PRO ASP GLU GLU GLU GLV GLV
• Molecule 2: Peptidoglycan hyd	rolase gp4	
Chain E:	78%	13% 8%
M1 15 15 15 15 15 15 15 15 15 15 15 15 15	F84 R90 P94 F113 L114 L113 L113 R125 R125 F140 F140 F146	A GLN ALA ASP SER THR THR THR HIS ASP GLU GLU GLV GLV GLV
• Molecule 2: Peptidoglycan hyd	rolase gp4	
Chain G:	79%	13% 8%
M1 02 03 06 06 08 03 03 06 06 06 06 06 06 06 06 06 06 06 06 06	F84 D94 E112 E112 E112 F133 M138 F133 M146 M146 M146 G1N G1N	ASM ASP SER THR THR PRO PRO ASN GLY GLY GLY GLY
• Molecule 2: Peptidoglycan hyd	rolase gp4	
Chain I:	77%	14% • 8%
M1 12 12 12 13 13 13 13 13 13 13 13 14 14 15 13 13 14 14 14 14 14 14 14 14 14 14 14 14 14	881 189 180 112 112 112 112 112 112 112 112 112 11	GLA ALA ALA ALA ALA ALA FRO FRO FRO CLU ASP GLY GLY GLY GLY
• Molecule 2: Peptidoglycan hyd	rolase gp4	
Chain K:	81%	10% 8%
	2221 2221 2221 2221 2221 2221 2221 222	
	X	

• Molecule 2: Peptidoglycan hydrolase gp4



Chain M:	79%	13% 8%
M1 02 13 15 15 15 15 15 15 15 15 15 15 16 16 16 16 16 16 16 16 16 16 16 16 16	81 84 84 84 80 812 812 111 111 111 111 111 812 812 8131 8131	W146 P160 C118 C118 C118 ASN ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
• Molecule 2: Peptidogly	ycan hydrolase gp4	
Chain O:	78%	12% • 8%
M1 92 13 13 13 13 13 13 13 13 13 13 13 13 13	G70 577 581 789 784 7890 8112 8112 8112 8113 7140 7140	P150 G151 G151 ALA ALA ASP ASP PTHR HTS ASP PTHR ASN GLY GLY GLY
• Molecule 2: Peptidogly	ycan hydrolase gp4	
Chain Q:	79%	13% 8%
M 13 02 13 15 15 15 15 15 23 15 23 15 23 15 23 15 23	M44 M44 D63 D63 S81 S81 D84 D84 E112 L113 L113 L113 L113 L113 L113 L113 L	N1 46 P1 50 P1 50 C1 N ASN ASN ASN ASP ASN ASP ASN ASP ASN ASP ASN ASP ASN ASP ASN ASP ASN ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
• Molecule 2: Peptidogly	ycan hydrolase gp4	
Chain S:	78%	13% • 8%
M1 13 13 13 13 13 13 15 15 15 15 15 15 15 15 15 15 15 15 15	D63 S77 S81 F84 F84 E112 E112 R126 R126 R126 R131 T134	ALSS 1133 140 146 146 146 146 146 146 146 146
• Molecule 2: Peptidogly	ycan hydrolase gp4	
Chain V:	77%	13% • 8%
M1 02 13 13 13 13 13 13 13 13 13 13 13 13 13	D83 D71 S77 S77 S81 S81 F84 F84 F86 F86 F12 F12 K125	RIA F140 F140 F140 F160 G161 G161 ALN ALN ALN ALN ALN ALN ALN ALN ALN ALN
• Molecule 2: Peptidogly	ycan hydrolase gp4	
Chain X:	80%	11% • 8%
M1 02 02 02 02 02 03 03 03 03 03 04 03 06 3	881 881 881 884 844 844 844 844 844 844	ALA N146 B152 GLN ASN ASP ASP PRO ASP CLV GLV GLV GLV GLV GLY



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	38151	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	1.08	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	40.783	Depositor
Minimum map value	-21.767	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	512.9599, 512.9599, 512.9599	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^{\circ}$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.165818, 1.165818, 1.165818	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		Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	0/5004	0.49	0/6786	
1	В	0.26	0/5004	0.49	0/6786	
1	D	0.26	0/5004	0.50	0/6786	
1	F	0.26	0/5004	0.49	0/6786	
1	Н	0.26	0/5004	0.50	0/6786	
1	J	0.26	0/5004	0.49	0/6786	
1	L	0.26	0/5004	0.50	0/6786	
1	Ν	0.26	0/5004	0.49	0/6786	
1	Р	0.26	0/5004	0.50	0/6786	
1	R	0.26	0/5004	0.49	0/6786	
1	Т	0.26	0/5004	0.49	0/6786	
1	W	0.26	0/5004	0.49	0/6786	
2	С	0.26	0/1191	0.50	0/1614	
2	Ε	0.28	0/1191	0.50	0/1614	
2	G	0.26	0/1191	0.49	0/1614	
2	Ι	0.27	0/1191	0.49	0/1614	
2	Κ	0.26	0/1191	0.47	0/1614	
2	М	0.27	0/1191	0.49	0/1614	
2	0	0.27	0/1191	0.49	0/1614	
2	Q	0.26	0/1191	0.48	0/1614	
2	S	0.26	0/1191	0.49	0/1614	
2	V	0.26	0/1191	0.49	0/1614	
2	Х	0.26	0/1191	0.49	0/1614	
2	a	0.26	0/1191	0.49	0/1614	
All	All	0.26	0/74340	0.49	0/100800	

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	L	0	1



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Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	171	ARG	Sidechain
1	W	249	ARG	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	4904	0	4771	93	0
1	В	4904	0	4771	105	0
1	D	4904	0	4771	107	0
1	F	4904	0	4771	94	0
1	Н	4904	0	4771	101	0
1	J	4904	0	4771	102	0
1	L	4904	0	4771	98	0
1	Ν	4904	0	4771	106	0
1	Р	4904	0	4771	108	0
1	R	4904	0	4771	105	0
1	Т	4904	0	4771	111	0
1	W	4904	0	4771	99	0
2	С	1166	0	1133	9	0
2	Ε	1166	0	1133	9	0
2	G	1166	0	1133	9	0
2	Ι	1166	0	1133	13	0
2	Κ	1166	0	1133	7	0
2	М	1166	0	1133	9	0
2	0	1166	0	1133	12	0
2	Q	1166	0	1133	8	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	1166	0	1133	11	0
2	V	1166	0	1133	13	0
2	Х	1166	0	1133	9	0
2	а	1166	0	1133	0	0
All	All	72840	0	70848	1077	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 8.

All (1077) 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:588:GLU:HA	1:D:591:GLN:HE22	1.38	0.88
1:P:620:ALA:HB2	1:R:622:LEU:HD23	1.56	0.87
1:H:588:GLU:HA	1:H:591:GLN:HE22	1.39	0.86
1:B:588:GLU:HA	1:B:591:GLN:HE22	1.39	0.86
1:T:79:LEU:HA	1:T:95:MET:HE1	1.57	0.86
1:H:79:LEU:HA	1:H:95:MET:HE1	1.58	0.86
1:H:620:ALA:HB2	1:L:622:LEU:HD23	1.59	0.85
1:L:550:GLN:HE22	1:L:581:VAL:HG21	1.45	0.80
1:A:609:VAL:HB	1:B:611:ALA:HB1	1.65	0.78
1:F:609:VAL:HB	1:H:611:ALA:HB1	1.66	0.78
1:L:609:VAL:HB	1:W:611:ALA:HB1	1.68	0.76
1:D:550:GLN:HE22	1:D:581:VAL:HG21	1.50	0.76
2:V:16:LYS:NZ	2:X:39:ASP:OD2	2.20	0.75
1:N:577:ILE:HD13	1:N:589:GLU:HB3	1.69	0.75
1:D:249:ARG:HH12	1:D:513:ARG:HH12	1.35	0.74
1:T:81:ARG:HH21	1:W:560:LEU:HD22	1.52	0.74
1:N:611:ALA:HB1	1:R:609:VAL:HB	1.69	0.74
1:P:550:GLN:HE22	1:P:581:VAL:HG21	1.50	0.74
1:B:609:VAL:O	1:D:615:LEU:HD21	1.88	0.74
1:T:615:LEU:HD21	1:W:609:VAL:O	1.89	0.73
1:A:182:ASN:OD1	1:B:171:ARG:NH2	2.22	0.72
1:L:135:GLN:NE2	1:W:296:GLU:OE2	2.23	0.72
2:C:39:ASP:OD2	2:E:16:LYS:NZ	2.22	0.72
1:R:367:ASP:OD1	2:S:125:ARG:NH2	2.22	0.72
1:N:171:ARG:NH2	1:R:182:ASN:OD1	2.23	0.72
1:T:171:ARG:NH2	1:W:182:ASN:OD1	2.23	0.71
1:D:609:VAL:HB	1:F:611:ALA:HB1	1.70	0.71
2:K:16:LYS:NZ	2:O:39:ASP:OD2	2.22	0.71
1:A:611:ALA:HB1	1:J:609:VAL:HB	1.72	0.71



	the office of the second	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:620:ALA:HB2	1:B:622:LEU:HG	1.73	0.71	
1:J:418:LEU:HD23	1:J:446:THR:HG22	1.73	0.70	
1:T:519:ASP:OD1	1:W:525:GLN:NE2	2.23	0.70	
2:I:39:ASP:OD2	2:M:16:LYS:NZ	2.24	0.70	
1:A:525:GLN:NE2	1:B:519:ASP:OD1	2.25	0.70	
1:B:177:HIS:ND1	1:B:221:GLU:OE1	2.23	0.69	
1:T:622:LEU:HD23	1:W:620:ALA:HB2	1.75	0.69	
1:T:177:HIS:ND1	1:T:221:GLU:OE1	2.23	0.69	
1:D:249:ARG:NH2	1:D:470:ASP:OD1	2.26	0.68	
1:H:591:GLN:O	1:H:595:GLU:HG3	1.93	0.68	
1:N:519:ASP:OD1	1:R:525:GLN:NE2	2.27	0.67	
1:H:609:VAL:HB	1:L:611:ALA:HB1	1.74	0.67	
1:P:576:LEU:HB3	1:P:582:LYS:HG3	1.75	0.67	
1:B:135:GLN:NE2	1:D:296:GLU:OE2	2.27	0.67	
1:B:205:ASN:ND2	1:D:312:ASP:OD2	2.28	0.67	
1:P:182:ASN:OD1	1:R:171:ARG:NH2	2.28	0.67	
1:N:177:HIS:ND1	1:N:221:GLU:OE1	2.24	0.66	
1:F:525:GLN:NE2	1:H:519:ASP:OD1	2.29	0.66	
1:F:557:PHE:HZ	1:F:582:LYS:HZ3	1.42	0.66	
1:L:182:ASN:OD1	1:W:171:ARG:NH2	2.28	0.66	
1:A:171:ARG:NH2	1:J:182:ASN:OD1	2.28	0.66	
1:P:615:LEU:HD21	1:T:609:VAL:O	1.96	0.66	
1:P:609:VAL:O	1:R:615:LEU:HD21	1.95	0.66	
1:T:591:GLN:O	1:T:595:GLU:HG3	1.95	0.66	
1:H:205:ASN:ND2	1:L:312:ASP:OD2	2.28	0.66	
1:H:177:HIS:ND1	1:H:221:GLU:OE2	2.23	0.66	
2:Q:16:LYS:NZ	2:V:39:ASP:OD2	2.26	0.66	
1:H:135:GLN:NE2	1:L:296:GLU:OE1	2.29	0.66	
1:F:249:ARG:NH2	1:F:470:ASP:OD1	2.29	0.66	
1:A:249:ARG:NH2	1:A:470:ASP:OD1	2.29	0.65	
1:J:296:GLU:OE2	1:N:135:GLN:NE2	2.29	0.65	
1:N:622:LEU:HD12	1:R:616:LEU:HD12	1.77	0.65	
1:L:134:ASP:HB3	1:W:271:ILE:HG23	1.79	0.65	
1:L:418:LEU:HD23	1:L:446:THR:HG22	1.80	0.64	
1:P:418:LEU:HD23	1:P:446:THR:HG22	1.79	0.64	
1:D:587:PRO:HA	1:D:590:GLN:HB2	1.80	0.64	
1:B:620:ALA:HB2	1:D:622:LEU:HG	1.78	0.64	
1:T:577:ILE:HG12	1:T:589:GLU:HB3	1.78	0.64	
1:J:312:ASP:OD2	1:N:205:ASN:ND2	2.31	0.63	
1:R:177:HIS:ND1	1:R:221:GLU:OE1	2.30	0.63	
1:D:418:LEU:HD23	1:D:446:THR:HG22	1.80	0.63	



	tus page	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:J:615:LEU:HD21	1:N:609:VAL:O	1.99	0.63	
1:P:37:ARG:NH1	1:P:120:GLU:OE1	2.32	0.63	
1:D:37:ARG:NH1	1:D:120:GLU:OE1	2.31	0.62	
1:J:37:ARG:NH1	1:J:120:GLU:OE1	2.32	0.62	
1:L:37:ARG:NH1	1:L:120:GLU:OE1	2.32	0.62	
1:L:587:PRO:HA	1:L:590:GLN:HB2	1.81	0.62	
1:P:587:PRO:HA	1:P:590:GLN:HB2	1.82	0.62	
1:J:587:PRO:HA	1:J:590:GLN:HB2	1.82	0.62	
1:N:367:ASP:OD1	2:O:125:ARG:NH2	2.30	0.62	
1:D:134:ASP:HB3	1:F:271:ILE:HG23	1.81	0.62	
1:H:367:ASP:OD1	2:I:125:ARG:NH2	2.31	0.62	
1:R:234:ILE:HD13	1:R:244:VAL:HG13	1.83	0.61	
1:T:367:ASP:OD1	2:V:125:ARG:NH2	2.29	0.61	
1:T:7:ARG:NH2	1:T:224:GLU:OE2	2.34	0.61	
1:R:33:LEU:O	1:R:37:ARG:HB2	2.00	0.61	
1:P:134:ASP:HB3	1:R:271:ILE:HG23	1.83	0.61	
1:T:312:ASP:OD2	1:W:205:ASN:ND2	2.33	0.61	
1:P:306:GLU:OE2	1:T:65:ARG:NE	2.33	0.61	
1:A:33:LEU:O	1:A:37:ARG:HB2	2.01	0.61	
1:W:33:LEU:O	1:W:37:ARG:HB2	2.01	0.61	
1:H:61:ARG:NH2	1:L:317:GLU:OE1	2.34	0.61	
1:P:249:ARG:NH2	1:P:470:ASP:OD1	2.33	0.61	
1:H:7:ARG:NH2	1:H:224:GLU:OE2	2.34	0.60	
1:D:6:ASN:HB3	1:D:9:GLU:HB2	1.82	0.60	
1:J:6:ASN:HB3	1:J:9:GLU:HB2	1.83	0.60	
1:L:33:LEU:O	1:L:37:ARG:HB2	2.01	0.60	
1:R:40:GLN:NE2	1:R:58:ASP:OD1	2.35	0.60	
1:W:234:ILE:HD13	1:W:244:VAL:HG13	1.84	0.60	
1:F:33:LEU:O	1:F:37:ARG:HB2	2.01	0.60	
1:W:550:GLN:HE22	1:W:581:VAL:HG21	1.65	0.60	
1:B:367:ASP:OD1	2:C:125:ARG:NH2	2.32	0.60	
1:P:33:LEU:O	1:P:37:ARG:HB2	2.01	0.60	
1:P:557:PHE:HZ	1:P:582:LYS:HZ3	1.48	0.60	
1:F:205:ASN:ND2	1:H:312:ASP:OD2	2.34	0.60	
1:F:182:ASN:OD1	1:H:171:ARG:NH2	2.35	0.60	
1:D:33:LEU:O	1:D:37:ARG:HB2	2.02	0.60	
1:N:33:LEU:O	1:N:37:ARG:HB2	2.02	0.60	
1:R:550:GLN:NE2	1:R:581:VAL:HG21	2.16	0.60	
1:J:33:LEU:O	1:J:37:ARG:HB2	2.02	0.60	
1:P:6:ASN:HB3	1:P:9:GLU:HB2	1.82	0.60	
1:F:556:TYR:OH	1:H:542:THR:OG1	2.20	0.59	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:N:7:ARG:NH2	1:N:224:GLU:OE2	2.34	0.59
1:H:33:LEU:O	1:H:37:ARG:HB2	2.02	0.59
1:B:33:LEU:O	1:B:37:ARG:HB2	2.02	0.59
1:P:135:GLN:NE2	1:R:296:GLU:OE2	2.30	0.59
1:B:7:ARG:NH2	1:B:224:GLU:OE2	2.34	0.59
1:J:317:GLU:OE1	1:N:61:ARG:NH2	2.36	0.59
1:W:40:GLN:NE2	1:W:58:ASP:OD1	2.35	0.58
1:A:234:ILE:HD13	1:A:244:VAL:HG22	1.85	0.58
1:R:249:ARG:NH2	1:R:470:ASP:OD1	2.36	0.58
1:D:61:ARG:NH2	1:F:317:GLU:OE1	2.36	0.58
1:T:274:ARG:HG3	1:T:274:ARG:HH11	1.68	0.58
2:V:71:ASP:OD1	2:V:71:ASP:N	2.34	0.58
1:F:92:ASP:OD1	1:F:93:VAL:N	2.37	0.58
1:T:33:LEU:O	1:T:37:ARG:HB2	2.02	0.58
1:F:577:ILE:HD12	1:F:589:GLU:HB3	1.85	0.58
1:L:61:ARG:NH2	1:W:317:GLU:OE1	2.37	0.58
1:T:37:ARG:NH1	1:T:120:GLU:OE1	2.37	0.58
1:A:317:GLU:OE1	1:J:61:ARG:NH2	2.37	0.58
1:L:6:ASN:HB3	1:L:9:GLU:HB2	1.85	0.58
1:B:588:GLU:HA	1:B:591:GLN:NE2	2.12	0.58
1:F:40:GLN:NE2	1:F:58:ASP:OD1	2.37	0.58
1:W:24:GLU:O	1:W:28:GLU:HG3	2.04	0.58
1:W:7:ARG:NH2	1:W:224:GLU:OE2	2.37	0.57
1:H:157:ILE:HB	1:H:174:THR:HG23	1.86	0.57
1:H:236:GLN:HB3	1:H:264:ILE:HG13	1.85	0.57
1:H:588:GLU:HA	1:H:591:GLN:NE2	2.15	0.57
1:A:7:ARG:NH2	1:A:224:GLU:OE2	2.37	0.57
1:A:92:ASP:OD1	1:A:93:VAL:N	2.37	0.57
1:D:576:LEU:HB3	1:D:582:LYS:HG3	1.86	0.57
1:N:37:ARG:NH1	1:N:120:GLU:OE1	2.37	0.57
2:S:3:ILE:HG23	2:S:8:ASP:HB3	1.86	0.57
1:J:7:ARG:NH2	1:J:224:GLU:OE2	2.38	0.57
1:P:61:ARG:NH2	1:R:317:GLU:OE1	2.37	0.57
1:W:236:GLN:HB3	1:W:264:ILE:HG13	1.85	0.57
1:N:550:GLN:NE2	1:N:581:VAL:HG21	2.20	0.57
1:R:7:ARG:NH2	1:R:224:GLU:OE2	2.37	0.57
1:A:24:GLU:O	1:A:28:GLU:HG3	2.05	0.57
1:B:37:ARG:NH1	1:B:120:GLU:OE1	2.37	0.57
1:J:81:ARG:HH21	$1:N:560:LEU:HD2\overline{2}$	1.69	0.57
1:A:556:TYR:OH	1:B:542:THR:OG1	2.23	0.57
1:W:15:PHE:HD1	1:W:174:THR:HG21	1.70	0.57



Atom-1	Atom-2	Interatomic	Clash
1.D.40.CI N.NE2	1.D.50.ACD.OD1		Overlap (A)
1.D.40.GLN.NE2	1.D.36.ASI .0D1	2.38	0.57
1.F.94.CLU.O	1.F.174.11IIX.IIG21	2.04	0.57
1.H.27.ADC.NH1	1.F.20.GLU.IIGJ	2.04	0.57
1.11.37.ANG.M11 1.1.940.ABC.MH2	1.II.120.GLU.OLI 1.I.470.ASP:OD1	2.31	0.57
1.L.249.AIG.MI2	1.L.470.ASI .ODI	2.30	0.57
1.N.230.GLN.HD3	1.N.204.1LE.IIG15	1.60	0.57
1.F.011.ALA.U	1.F.015.LEU.IID25	2.04	0.57
1.F.7.ADC.NH2	1.1.01.ARG.NH2 1.F.994.CLU.OF9	2.31	0.57
1.D.206.CLU.OE2	1:F:224:GLU:UE2	2.31	0.50
1:P:290:GLU:UE2	1:1:130:GLN:NEZ	2.38	0.50
1:A:40:GLN:NEZ	1:A:58:ASP:ODI	2.38	0.50
1:A:296:GLU:UE2	1:J:135:GLN:NE2	2.30	0.56
1:B:236:GLN:HB3	1:B:264:ILE:HG13	1.87	0.56
1:H:40:GLN:NE2	1:H:58:ASP:ODI	2.38	0.56
1:L:587:PRO:0	1:L:591:GLN:NE2	2.38	0.56
2:0:16:LYS:NZ	2:S:39:ASP:OD2	2.26	0.56
1:R:15:PHE:HD1	1:R:174:THR:HG21	1.69	0.56
1:N:40:GLN:NE2	1:N:58:ASP:OD1	2.38	0.56
1:R:24:GLU:O	1:R:28:GLU:HG3	2.04	0.56
2:X:7:GLY:O	2:X:11:ARG:HG3	2.06	0.56
2:G:7:GLY:O	2:G:11:ARG:HG3	2.06	0.56
2:Q:39:ASP:OD1	2:S:15:ARG:NH2	2.38	0.56
1:T:157:ILE:HB	1:T:174:THR:HG23	1.88	0.56
2:X:3:ILE:HG23	2:X:8:ASP:HB3	1.88	0.56
1:A:15:PHE:HD1	1:A:174:THR:HG21	1.70	0.56
1:N:157:ILE:HB	1:N:174:THR:HG23	1.86	0.56
1:T:236:GLN:HB3	1:T:264:ILE:HG13	1.87	0.56
1:T:40:GLN:NE2	1:T:58:ASP:OD1	2.39	0.56
1:B:182:ASN:OD1	1:D:171:ARG:NH2	2.38	0.56
2:G:3:ILE:HG23	2:G:8:ASP:HB3	1.87	0.56
1:J:510:ILE:HG23	1:J:512:GLY:H	1.71	0.56
1:J:587:PRO:O	1:J:591:GLN:NE2	2.38	0.56
1:W:376:ARG:HG2	1:W:377:THR:HG23	1.87	0.56
1:B:61:ARG:NH2	1:D:317:GLU:OE1	2.39	0.56
1:B:576:LEU:HB3	1:B:582:LYS:HG3	1.88	0.56
1:D:7:ARG:NH2	1:D:224:GLU:OE2	2.38	0.56
1:J:171:ARG:NH2	1:N:182:ASN:OD1	2.39	0.56
1:N:454:ALA:HB1	1:N:520:VAL:HG21	1.89	0.56
1:R:376:ARG:HG2	1:R:377:THR:HG23	1.88	0.56
1:B:157:ILE:HB	1:B:174:THR:HG23	1.86	0.55
2:G:39:ASP:OD2	2:I:16:LYS:NZ	2.29	0.55



	A t amo 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:P:7:ARG:NH2	1:P:224:GLU:OE2	2.38	0.55	
1:P:15:PHE:HD1	1:P:174:THR:HG21	1.71	0.55	
1:P:625:ALA:O	1:P:629:THR:HG23	2.07	0.55	
2:S:7:GLY:O	2:S:11:ARG:HG3	2.06	0.55	
1:L:7:ARG:NH2	1:L:224:GLU:OE2	2.38	0.55	
1:B:454:ALA:HB1	1:B:520:VAL:HG21	1.89	0.55	
1:F:620:ALA:HB2	1:H:622:LEU:HD23	1.88	0.55	
1:P:587:PRO:O	1:P:591:GLN:NE2	2.39	0.55	
1:F:249:ARG:HH12	1:F:513:ARG:HH12	1.54	0.55	
1:P:76:ILE:HG22	1:P:457:MET:HG3	1.89	0.55	
1:H:251:ILE:HG23	1:H:252:LYS:HG2	1.89	0.55	
1:L:577:ILE:HD12	1:L:589:GLU:HB3	1.89	0.55	
1:P:588:GLU:HA	1:P:591:GLN:NE2	2.22	0.55	
1:T:605:ASP:O	1:T:609:VAL:HG12	2.06	0.55	
1:W:37:ARG:NH1	1:W:120:GLU:OE1	2.40	0.55	
1:F:37:ARG:NH1	1:F:120:GLU:OE1	2.40	0.55	
1:J:577:ILE:HD12	1:J:589:GLU:HB3	1.88	0.55	
1:P:249:ARG:HH12	1:P:513:ARG:HH12	1.55	0.55	
1:R:37:ARG:NH1	1:R:120:GLU:OE1	2.39	0.55	
1:H:550:GLN:NE2	1:H:581:VAL:HG21	2.22	0.55	
1:J:625:ALA:O	1:J:629:THR:HG23	2.07	0.55	
1:L:510:ILE:HG23	1:L:512:GLY:H	1.70	0.55	
1:N:578:GLN:HG2	1:N:596:ALA:HB2	1.89	0.55	
1:A:561:ASP:OD2	1:A:569:ARG:NH2	2.40	0.55	
1:B:560:LEU:HD22	1:D:81:ARG:HH21	1.71	0.55	
1:D:510:ILE:HG23	1:D:512:GLY:H	1.70	0.55	
1:D:625:ALA:O	1:D:629:THR:HG23	2.07	0.55	
1:W:23:ASP:OD2	1:W:27:ARG:NH1	2.40	0.55	
1:J:203:ASN:OD1	1:J:218:GLN:NE2	2.41	0.54	
1:J:632:LEU:HD13	1:N:631:SER:HB3	1.89	0.54	
1:L:203:ASN:OD1	1:L:218:GLN:NE2	2.41	0.54	
1:A:37:ARG:NH1	1:A:120:GLU:OE1	2.40	0.54	
1:L:220:ALA:HB3	1:L:281:ILE:HG13	1.89	0.54	
1:N:249:ARG:NH2	1:N:470:ASP:OD1	2.40	0.54	
1:D:15:PHE:HD1	1:D:174:THR:HG21	1.72	0.54	
1:L:76:ILE:HG22	1:L:457:MET:HG3	1.90	0.54	
1:L:588:GLU:HA	1:L:591:GLN:NE2	2.22	0.54	
1:P:620:ALA:HB3	1:R:621:GLU:OE2	2.08	0.54	
1:T:220:ALA:HB3	1:T:281:ILE:HG13	1.90	0.54	
1:T:454:ALA:HB1	1:T:520:VAL:HG21	1.88	0.54	
1:B:251:ILE:HG23	1:B:252:LYS:HG2	1.89	0.54	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:F:561:ASP:0D2	1:F:569:ARG:NH2	2.41	0.54
1:L:025:ALA:O	1:L:629:THR:HG23	2.07	0.54
1:R:561:ASP:OD2	1:R:569:ARG:NH2	2.41	0.54
1:J:220:ALA:HB3	1:J:281:ILE:HG13	1.89	0.54
1:L:157:ILE:HB	1:L:174:THR:HG23	1.90	0.54
1:P:157:ILE:HB	1:P:174:THR:HG23	1.90	0.54
1:P:510:ILE:HG23	1:P:512:GLY:H	1.71	0.54
1:R:23:ASP:OD2	1:R:27:ARG:NH1	2.40	0.54
1:W:76:ILE:HG22	1:W:457:MET:HG3	1.90	0.54
1:W:561:ASP:OD2	1:W:569:ARG:NH2	2.41	0.54
1:A:236:GLN:HB3	1:A:264:ILE:HG13	1.90	0.54
1:A:625:ALA:O	1:A:629:THR:HG23	2.07	0.54
1:H:557:PHE:HZ	1:H:582:LYS:HZ3	1.55	0.54
1:D:157:ILE:HB	1:D:174:THR:HG23	1.90	0.54
1:N:92:ASP:OD1	1:N:92:ASP:N	2.36	0.54
1:R:610:GLN:O	1:R:614:VAL:HG23	2.07	0.54
1:A:632:LEU:HD12	1:J:627:ASN:HB3	1.90	0.54
1:D:203:ASN:OD1	1:D:218:GLN:NE2	2.41	0.54
1:F:76:ILE:HG22	1:F:457:MET:HG3	1.90	0.54
2:G:131:ARG:NH1	1:W:53:TYR:O	2.41	0.54
1:H:625:ALA:O	1:H:629:THR:HG23	2.08	0.54
1:J:588:GLU:HA	1:J:591:GLN:NE2	2.23	0.54
1:W:577:ILE:HD12	1:W:589:GLU:HB3	1.88	0.54
1:H:454:ALA:HB1	1:H:520:VAL:HG21	1.89	0.53
1:H:578:GLN:HG2	1:H:596:ALA:HB2	1.90	0.53
1:P:203:ASN:OD1	1:P:218:GLN:NE2	2.41	0.53
1:P:454:ALA:HB1	1:P:520:VAL:HG21	1.90	0.53
1:R:76:ILE:HG22	1:R:457:MET:HG3	1.90	0.53
1:T:323:THR:HB	1:T:412:VAL:HG13	1.90	0.53
1:A:542:THR:HG1	1:J:556:TYR:HH	1.56	0.53
1:B:15:PHE:HD1	1:B:174:THR:HG21	1.74	0.53
1:J:157:ILE:HB	1:J:174:THR:HG23	1.90	0.53
1:J:258:LEU:HB3	1:J:263:PHE:HB2	1.90	0.53
1:D:228:LYS:NZ	1:D:228:LYS:HB3	2.23	0.53
1:H:560:LEU:HD22	1:L:81:ABG:HH21	1.72	0.53
1:N:15:PHE:HD1	1:N:174:THR:HG21	1.73	0.53
1:R:625:ALA:O	1:R:629:THR:HG23	2.09	0.53
1:D:76:ILE:HG22	1:D:457:MET:HG3	1.89	0.53
1:F:625:ALA:O	$1 \cdot F \cdot 629 \cdot THR \cdot HG23$	2.07	0.53
1.H.576.LEU.HR3	1.H.582.LVS.HG3	1.88	0.53
1:L:454:ALA:HB1	1:L:520:VAL:HG21	1.90	0.53



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:T:251:ILE:HG23	1:T:252:LYS:HG2	1.91	0.53
1:A:249:ARG:HH12	1:A:513:ARG:HH12	1.57	0.53
1:B:550:GLN:NE2	1:B:581:VAL:HG21	2.22	0.53
1:D:251:ILE:HG23	1:D:252:LYS:HG2	1.91	0.53
1:J:15:PHE:HD1	1:J:174:THR:HG21	1.72	0.53
1:L:258:LEU:HB3	1:L:263:PHE:HB2	1.90	0.53
1:N:576:LEU:HB3	1:N:582:LYS:HG3	1.91	0.53
1:A:76:ILE:HG22	1:A:457:MET:HG3	1.90	0.53
1:B:76:ILE:HG22	1:B:457:MET:HG3	1.89	0.53
1:J:190:LYS:HE3	1:J:191:TYR:HE1	1.73	0.53
1:J:454:ALA:HB1	1:J:520:VAL:HG21	1.91	0.53
1:A:53:TYR:O	2:S:131:ARG:NH1	2.40	0.53
1:B:631:SER:HB3	1:D:632:LEU:HD13	1.91	0.53
2:G:94:ASP:OD1	2:I:16:LYS:NZ	2.41	0.53
1:H:220:ALA:HB3	1:H:281:ILE:HG13	1.90	0.53
1:L:228:LYS:NZ	1:L:228:LYS:HB3	2.23	0.53
1:N:625:ALA:O	1:N:629:THR:HG23	2.08	0.53
1:R:236:GLN:HB3	1:R:264:ILE:HG13	1.90	0.53
1:F:23:ASP:OD2	1:F:27:ARG:NH1	2.41	0.53
1:J:76:ILE:HG22	1:J:457:MET:HG3	1.89	0.53
1:N:251:ILE:HG23	1:N:252:LYS:HG2	1.91	0.53
1:T:625:ALA:O	1:T:629:THR:HG23	2.09	0.53
1:W:625:ALA:O	1:W:629:THR:HG23	2.08	0.53
1:B:220:ALA:HB3	1:B:281:ILE:HG13	1.90	0.53
1:D:454:ALA:HB1	1:D:520:VAL:HG21	1.91	0.53
1:N:323:THR:HB	1:N:412:VAL:HG13	1.91	0.53
1:P:228:LYS:NZ	1:P:228:LYS:HB3	2.23	0.53
1:T:76:ILE:HG22	1:T:457:MET:HG3	1.91	0.53
1:T:249:ARG:NH2	1:T:470:ASP:OD1	2.42	0.53
1:T:578:GLN:HG2	1:T:596:ALA:HB2	1.91	0.53
1:L:65:ARG:NE	1:W:306:GLU:OE2	2.41	0.53
1:N:632:LEU:HD12	1:R:627:ASN:HB3	1.91	0.53
1:P:561:ASP:OD2	1:P:569:ARG:NH2	2.42	0.53
1:T:557:PHE:HE1	1:T:573:ASN:HA	1.73	0.53
1:T:611:ALA:O	1:T:615:LEU:HD23	2.09	0.53
1:F:620:ALA:HB3	1:H:621:GLU:OE2	2.09	0.52
1:L:15:PHE:HD1	1:L:174:THR:HG21	1.72	0.52
1:N:220:ALA:HB3	1:N:281:ILE:HG13	1.90	0.52
1:P:577:ILE:HD12	1:P:589:GLU:HB3	1.90	0.52
1:B:575:GLN:O	1:B:579:MET:HG3	2.09	0.52
1:J:228:LYS:NZ	1:J:228:LYS:HB3	2.23	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:L:171:ARG:HH21	1:L:171:ARG:HB2	1.74	0.52
1:A:306:GLU:OE2	1:J:65:ARG:NE	2.41	0.52
1:A:550:GLN:HE22	1:A:581:VAL:HG11	1.75	0.52
1:L:251:ILE:HG23	1:L:252:LYS:HG2	1.91	0.52
1:T:15:PHE:HD1	1:T:174:THR:HG21	1.74	0.52
1:W:557:PHE:HZ	1:W:582:LYS:HZ2	1.57	0.52
1:D:182:ASN:OD1	1:F:171:ARG:NH2	2.41	0.52
2:G:134:THR:O	2:G:138:ASN:ND2	2.42	0.52
1:H:323:THR:HB	1:H:412:VAL:HG13	1.92	0.52
2:S:81:SER:HA	2:S:84:PHE:CE2	2.45	0.52
1:T:611:ALA:HB1	1:W:609:VAL:HB	1.91	0.52
1:W:220:ALA:HB3	1:W:281:ILE:HG13	1.92	0.52
1:H:15:PHE:HD1	1:H:174:THR:HG21	1.73	0.52
1:P:65:ARG:NE	1:R:306:GLU:OE2	2.41	0.52
1:R:157:ILE:HB	1:R:174:THR:HG23	1.92	0.52
1:A:577:ILE:HD12	1:A:589:GLU:HB3	1.91	0.52
1:B:246:TYR:HB2	1:B:249:ARG:HG3	1.90	0.52
1:D:65:ARG:NE	1:F:306:GLU:OE2	2.41	0.52
1:N:146:ARG:NH2	1:N:460:ASP:OD2	2.43	0.52
1:P:251:ILE:HG23	1:P:252:LYS:HG2	1.92	0.52
1:R:577:ILE:HD12	1:R:589:GLU:HB3	1.92	0.52
1:H:76:ILE:HG22	1:H:457:MET:HG3	1.91	0.52
1:W:605:ASP:O	1:W:609:VAL:HG23	2.09	0.52
1:A:23:ASP:OD2	1:A:27:ARG:NH1	2.43	0.52
1:J:612:GLN:O	1:J:616:LEU:HG	2.10	0.52
1:W:367:ASP:OD1	2:X:125:ARG:NH2	2.43	0.52
1:B:323:THR:HB	1:B:412:VAL:HG13	1.92	0.52
1:J:251:ILE:HG23	1:J:252:LYS:HG2	1.92	0.52
1:B:578:GLN:HG2	1:B:596:ALA:HB2	1.92	0.51
1:A:157:ILE:HB	1:A:174:THR:HG23	1.92	0.51
1:T:281:ILE:HG22	1:T:286:VAL:HG22	1.93	0.51
1:B:625:ALA:O	1:B:629:THR:HG23	2.09	0.51
1:D:220:ALA:HB3	1:D:281:ILE:HG13	1.91	0.51
1:R:53:TYR:O	2:X:131:ARG:NH1	2.40	0.51
1:T:274:ARG:HG3	1:T:274:ARG:NH1	2.25	0.51
1:W:157:ILE:HB	1:W:174:THR:HG23	1.93	0.51
2:E:81:SER:HA	2:E:84:PHE:CE2	2.45	0.51
1:F:157:ILE:HB	1:F:174:THR:HG23	1.93	0.51
1:A:220:ALA:HB3	1:A:281:ILE:HG13	1.92	0.51
1:F:236:GLN:HB3	1:F:264:ILE:HG13	1.91	0.51
1:F:560:LEU:HD22	1:H:81:ARG:HH21	1.75	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:N:317:GLU:OE1	1:R:61:ARG:NH2	2.44	0.51
1:T:632:LEU:HD13	1:W:631:SER:HB3	1.93	0.51
1:D:631:SER:HB3	1:F:632:LEU:HD13	1.93	0.51
1:H:609:VAL:O	1:L:615:LEU:HD21	2.10	0.51
1:J:611:ALA:HB1	1:N:609:VAL:HB	1.92	0.51
1:B:605:ASP:O	1:B:609:VAL:HG23	2.10	0.51
1:J:306:GLU:OE2	1:N:65:ARG:NE	2.44	0.51
2:M:81:SER:HA	2:M:84:PHE:CE2	2.46	0.51
1:N:622:LEU:HD23	1:R:620:ALA:HB2	1.92	0.51
1:R:226:VAL:HG12	1:R:228:LYS:HG3	1.92	0.51
1:A:631:SER:HB3	1:B:632:LEU:HD13	1.93	0.51
1:H:631:SER:HB3	1:L:632:LEU:HD13	1.93	0.51
1:P:632:LEU:HD13	1:T:631:SER:HB3	1.93	0.51
1:F:234:ILE:HD13	1:F:244:VAL:HG13	1.92	0.50
1:N:542:THR:OG1	1:R:556:TYR:OH	2.24	0.50
1:P:631:SER:HB3	1:R:632:LEU:HD13	1.93	0.50
2:I:131:ARG:NH1	1:T:53:TYR:O	2.43	0.50
1:L:191:TYR:CD2	1:L:280:ILE:HD11	2.46	0.50
1:N:76:ILE:HG22	1:N:457:MET:HG3	1.91	0.50
1:T:561:ASP:OD2	1:T:569:ARG:NH2	2.44	0.50
1:A:632:LEU:HD13	1:J:631:SER:HB3	1.94	0.50
1:P:191:TYR:CD2	1:P:280:ILE:HD11	2.47	0.50
2:X:81:SER:HA	2:X:84:PHE:CE2	2.46	0.50
1:A:205:ASN:ND2	1:B:312:ASP:OD2	2.45	0.50
2:C:46:GLU:OE2	2:C:90:ARG:NH2	2.44	0.50
1:W:550:GLN:NE2	1:W:581:VAL:HG21	2.27	0.50
2:C:131:ARG:NH1	1:H:53:TYR:O	2.43	0.50
2:G:81:SER:HA	2:G:84:PHE:CE2	2.46	0.50
1:W:226:VAL:HG12	1:W:228:LYS:HG3	1.93	0.50
1:W:76:ILE:HG23	1:W:520:VAL:HG13	1.94	0.50
1:A:587:PRO:HA	1:A:590:GLN:HB3	1.94	0.50
1:H:575:GLN:O	1:H:579:MET:HG3	2.12	0.50
1:N:281:ILE:HG22	1:N:286:VAL:HG22	1.93	0.50
2:S:134:THR:O	2:S:138:ASN:ND2	2.45	0.50
2:X:134:THR:O	2:X:138:ASN:ND2	2.45	0.50
1:A:271:ILE:HG23	1:J:134:ASP:HB3	1.94	0.50
1:H:323:THR:HG22	1:H:415:VAL:HG13	1.94	0.50
1:L:561:ASP:OD2	1:L:569:ARG:NH2	2.45	0.50
1:D:281:ILE:HG22	1:D:286:VAL:HG22	1.94	0.50
1:N:203:ASN:ND2	1:N:205:ASN:O	2.45	0.50
1:P:605:ASP:O	1:P:609:VAL:HG23	2.12	0.50



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:T:74:ASN:HD22	1:T:450:GLN:HE22	1.60	0.50
2:K:81:SER:HA	2:K:84:PHE:CE2	2.47	0.49
1:P:81:ARG:HH21	1:T:560:LEU:HD22	1.76	0.49
1:B:587:PRO:HA	1:B:590:GLN:HB3	1.94	0.49
1:F:627:ASN:HB3	1:H:632:LEU:HD12	1.94	0.49
1:F:631:SER:HB3	1:H:632:LEU:HD13	1.94	0.49
1:H:249:ARG:NH2	1:H:470:ASP:OD1	2.45	0.49
2:Q:81:SER:HA	2:Q:84:PHE:CE2	2.47	0.49
1:J:588:GLU:HA	1:J:591:GLN:HE21	1.78	0.49
1:J:591:GLN:HA	1:J:594:VAL:HB	1.93	0.49
1:N:632:LEU:HD13	1:R:631:SER:HB3	1.94	0.49
1:P:591:GLN:HA	1:P:594:VAL:HB	1.94	0.49
1:R:76:ILE:HG23	1:R:520:VAL:HG13	1.94	0.49
1:D:611:ALA:O	1:D:615:LEU:HD23	2.12	0.49
1:P:220:ALA:HB3	1:P:281:ILE:HG13	1.94	0.49
1:W:296:GLU:OE1	1:W:514:TYR:OH	2.29	0.49
1:D:191:TYR:CD2	1:D:280:ILE:HD11	2.47	0.49
1:L:244:VAL:HB	1:L:511:ARG:HB2	1.95	0.49
1:P:244:VAL:HB	1:P:511:ARG:HB2	1.95	0.49
1:A:610:GLN:O	1:A:614:VAL:HG23	2.13	0.49
1:B:609:VAL:HB	1:D:611:ALA:HB1	1.95	0.49
1:L:627:ASN:HB3	1:W:632:LEU:HD12	1.95	0.49
1:L:631:SER:HB3	1:W:632:LEU:HD13	1.94	0.49
1:N:74:ASN:HD22	1:N:450:GLN:HE22	1.60	0.49
1:N:81:ARG:HH21	1:R:560:LEU:HD22	1.77	0.49
1:D:258:LEU:HB3	1:D:263:PHE:HB2	1.94	0.49
1:F:578:GLN:HG2	1:F:596:ALA:HB2	1.95	0.49
1:J:550:GLN:HE21	1:J:550:GLN:HA	1.77	0.49
1:L:76:ILE:HG23	1:L:520:VAL:HG13	1.95	0.49
1:L:591:GLN:HA	1:L:594:VAL:HB	1.93	0.49
1:B:323:THR:HG22	1:B:415:VAL:HG13	1.94	0.49
1:F:323:THR:HG22	1:F:415:VAL:HG13	1.93	0.49
1:L:281:ILE:HG22	1:L:286:VAL:HG22	1.95	0.49
1:L:620:ALA:HB3	1:W:621:GLU:OE1	2.13	0.49
1:R:468:VAL:HG22	1:R:472:TYR:CD2	2.48	0.49
1:A:61:ARG:NH2	1:B:317:GLU:OE1	2.46	0.49
1:D:556:TYR:OH	1:F:542:THR:OG1	2.29	0.49
1:D:591:GLN:O	1:D:595:GLU:HG3	2.13	0.49
1:J:281:ILE:HG22	1:J:286:VAL:HG22	1.94	0.49
1:L:225:VAL:HG13	1:L:276:VAL:HG22	1.95	0.49
2:0:7:GLY:0	2:O:11:ARG:HG3	2.12	0.49



	• us puge	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:468:VAL:HG22	1:A:472:TYR:CD2	2.48	0.49
1:B:249:ARG:NH2	1:B:470:ASP:OD1	2.45	0.49
1:F:550:GLN:OE1	1:F:581:VAL:HG21	2.13	0.49
1:L:556:TYR:OH	1:W:542:THR:OG1	2.29	0.49
1:P:78:VAL:HG13	1:P:518:THR:HG23	1.95	0.49
1:D:323:THR:HB	1:D:412:VAL:HG13	1.94	0.48
1:D:557:PHE:HZ	1:D:582:LYS:HZ2	1.60	0.48
1:L:616:LEU:HD21	1:W:622:LEU:HD12	1.95	0.48
1:A:620:ALA:HB3	1:B:621:GLU:OE2	2.12	0.48
1:B:297:HIS:HB2	1:B:463:ILE:HG12	1.95	0.48
1:F:550:GLN:HA	1:F:550:GLN:HE21	1.79	0.48
1:H:74:ASN:HD22	1:H:450:GLN:HE22	1.59	0.48
1:H:605:ASP:O	1:H:609:VAL:HG23	2.13	0.48
1:J:88:PRO:HB2	1:N:561:ASP:OD2	2.13	0.48
1:N:297:HIS:HB2	1:N:463:ILE:HG12	1.95	0.48
1:N:605:ASP:O	1:N:609:VAL:HG23	2.13	0.48
1:T:317:GLU:OE1	1:W:61:ARG:NH2	2.46	0.48
1:A:560:LEU:HD22	1:B:81:ARG:HH21	1.77	0.48
1:A:578:GLN:HG2	1:A:596:ALA:HB2	1.95	0.48
1:B:53:TYR:O	2:O:131:ARG:NH1	2.43	0.48
1:F:61:ARG:NH2	1:H:317:GLU:OE1	2.46	0.48
1:H:65:ARG:NE	1:L:306:GLU:OE1	2.46	0.48
1:H:281:ILE:HG22	1:H:286:VAL:HG22	1.95	0.48
1:L:588:GLU:HA	1:L:591:GLN:HE21	1.77	0.48
2:O:69:GLU:OE2	2:O:70:GLY:N	2.46	0.48
1:P:632:LEU:HD12	1:T:627:ASN:HB3	1.95	0.48
1:F:76:ILE:HG23	1:F:520:VAL:HG13	1.96	0.48
1:H:297:HIS:HB2	1:H:463:ILE:HG12	1.95	0.48
1:A:76:ILE:HG23	1:A:520:VAL:HG13	1.95	0.48
1:A:323:THR:HG22	1:A:415:VAL:HG13	1.96	0.48
1:A:510:ILE:HG23	1:A:512:GLY:H	1.78	0.48
1:D:577:ILE:HD12	1:D:589:GLU:HB3	1.95	0.48
1:F:550:GLN:HA	1:F:550:GLN:NE2	2.29	0.48
1:F:562:GLY:H	1:F:565:VAL:HG12	1.77	0.48
1:N:582:LYS:HB3	1:N:582:LYS:HE3	1.68	0.48
1:P:627:ASN:HB3	1:R:632:LEU:HD12	1.95	0.48
1:A:618:GLY:HA2	1:J:617:GLN:HG3	1.96	0.48
1:D:468:VAL:HG22	1:D:472:TYR:CD2	2.48	0.48
1:J:249:ARG:HE	1:J:275:ARG:HH22	1.61	0.48
1:W:468:VAL:HG22	1:W:472:TYR:CD2	2.48	0.48
1:B:510:ILE:HG23	1:B:512:GLY:H	1.79	0.48



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:627:ASN:HB3	1:D:632:LEU:HD12	1.96	0.48
1:J:76:ILE:HG23	1:J:520:VAL:HG13	1.96	0.48
1:P:271:ILE:HG23	1:T:134:ASP:HB3	1.95	0.48
1:T:323:THR:HG22	1:T:415:VAL:HG13	1.95	0.48
1:D:76:ILE:HG23	1:D:520:VAL:HG13	1.95	0.48
1:P:499:LEU:HA	1:P:505:GLN:HA	1.96	0.48
1:W:586:THR:HG22	1:W:588:GLU:OE1	2.14	0.48
1:B:92:ASP:OD1	1:B:92:ASP:N	2.36	0.47
1:B:281:ILE:HG22	1:B:286:VAL:HG22	1.95	0.47
1:D:244:VAL:HB	1:D:511:ARG:HB2	1.95	0.47
1:F:468:VAL:HG22	1:F:472:TYR:CD2	2.48	0.47
1:H:274:ARG:HG3	1:H:274:ARG:HH11	1.79	0.47
1:J:78:VAL:HG13	1:J:518:THR:HG23	1.96	0.47
1:L:499:LEU:HA	1:L:505:GLN:HA	1.96	0.47
1:P:76:ILE:HG23	1:P:520:VAL:HG13	1.96	0.47
1:R:562:GLY:H	1:R:565:VAL:HG12	1.77	0.47
1:D:588:GLU:HA	1:D:591:GLN:NE2	2.17	0.47
1:D:627:ASN:HB3	1:F:632:LEU:HD12	1.96	0.47
1:A:226:VAL:HG12	1:A:228:LYS:HG3	1.95	0.47
1:F:510:ILE:HG23	1:F:512:GLY:H	1.79	0.47
1:H:561:ASP:OD2	1:L:88:PRO:HB2	2.13	0.47
1:J:499:LEU:HA	1:J:505:GLN:HA	1.96	0.47
1:B:65:ARG:NE	1:D:306:GLU:OE2	2.47	0.47
1:D:225:VAL:HG13	1:D:276:VAL:HG22	1.96	0.47
1:R:454:ALA:HB1	1:R:520:VAL:HG21	1.96	0.47
1:P:237:ASP:OD2	1:P:476:ARG:NH1	2.48	0.47
1:W:253:ASP:HB3	1:W:504:LYS:HE2	1.97	0.47
1:H:627:ASN:HB3	1:L:632:LEU:HD12	1.96	0.47
2:I:46:GLU:OE2	2:I:90:ARG:NH2	2.47	0.47
1:R:323:THR:HG22	1:R:415:VAL:HG13	1.97	0.47
1:R:591:GLN:HA	1:R:594:VAL:HB	1.97	0.47
1:A:504:LYS:H	1:A:504:LYS:HG3	1.52	0.47
2:C:69:GLU:OE2	2:C:70:GLY:N	2.48	0.47
1:H:587:PRO:HA	1:H:590:GLN:HB3	1.95	0.47
1:J:234:ILE:HD13	1:J:244:VAL:HG13	1.96	0.47
1:P:451:ASP:OD2	1:T:72:ARG:HD2	2.15	0.47
1:R:23:ASP:OD1	1:R:26:ARG:NH1	2.48	0.47
1:T:510:ILE:HG23	1:T:512:GLY:H	1.79	0.47
1:T:636:ALA:HB2	1:W:634:ILE:HD13	1.97	0.47
1:W:323:THR:HG22	1:W:415:VAL:HG13	1.95	0.47
1:W:454:ALA:HB1	1:W:520:VAL:HG21	1.95	0.47



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:B:561:ASP:OD2	1:D:88:PRO:HB2	2.13	0.47
1:D:239:VAL:HG12	1:D:240:THR:HG22	1.97	0.47
2:E:3:ILE:HG23	2:E:8:ASP:HB3	1.96	0.47
1:F:226:VAL:HG12	1:F:228:LYS:HG3	1.95	0.47
1:H:510:ILE:HG23	1:H:512:GLY:H	1.80	0.47
1:H:609:VAL:HG12	1:L:615:LEU:HD23	1.96	0.47
1:N:274:ARG:HG3	1:N:274:ARG:HH11	1.79	0.47
1:P:246:TYR:HB2	1:P:249:ARG:HG3	1.97	0.47
1:D:59:VAL:HG12	1:D:327:GLN:OE1	2.15	0.47
1:D:78:VAL:HG13	1:D:518:THR:HG23	1.95	0.47
1:H:72:ARG:HD2	1:L:451:ASP:OD2	2.15	0.47
1:H:634:ILE:HD13	1:L:636:ALA:HB2	1.97	0.47
1:P:323:THR:HB	1:P:412:VAL:HG13	1.96	0.47
1:P:609:VAL:HB	1:R:611:ALA:HB1	1.95	0.47
1:T:297:HIS:HB2	1:T:463:ILE:HG12	1.95	0.47
1:A:135:GLN:NE2	1:B:296:GLU:OE2	2.37	0.47
1:A:454:ALA:HB1	1:A:520:VAL:HG21	1.97	0.47
1:B:504:LYS:H	1:B:504:LYS:HG3	1.52	0.47
1:J:225:VAL:HG13	1:J:276:VAL:HG22	1.97	0.47
1:N:622:LEU:HA	1:R:620:ALA:HB2	1.96	0.47
2:O:16:LYS:NZ	2:S:94:ASP:OD1	2.44	0.47
2:0:81:SER:HA	2:O:84:PHE:CE2	2.50	0.47
1:P:225:VAL:HG13	1:P:276:VAL:HG22	1.96	0.47
1:P:281:ILE:HG22	1:P:286:VAL:HG22	1.97	0.47
1:P:621:GLU:OE1	1:T:620:ALA:HB3	2.15	0.47
2:Q:3:ILE:HG23	2:Q:8:ASP:HB3	1.97	0.47
1:F:220:ALA:HB3	1:F:281:ILE:HG13	1.96	0.46
1:H:246:TYR:HB2	1:H:249:ARG:HG3	1.96	0.46
2:I:3:ILE:HG23	2:I:8:ASP:HB3	1.97	0.46
1:J:53:TYR:O	2:Q:131:ARG:NH1	2.48	0.46
2:K:3:ILE:HG23	2:K:8:ASP:HB3	1.97	0.46
1:L:323:THR:HB	1:L:412:VAL:HG13	1.95	0.46
1:N:53:TYR:O	2:V:131:ARG:NH1	2.43	0.46
1:N:76:ILE:HG23	1:N:520:VAL:HG13	1.97	0.46
1.N.468.VAL/HG22	1·N·472·TYB·CD2	2.51	0.46
1:P:279:SER:OG	1:P:289:ASP:O	2.24	0.46
1:R:587:PRO·HA	1:R:590:GLN·HB3	1.97	0.46
2:V:81:SEB:HA	2:V:84:PHE:CE2	2.50	0.46
1·B·274·ABG·HG3	1·B·274·ARG·HH11	1.79	0.46
1.B.468.VAL. HG22	1.B.472.TVR·CD2	2.50	0.10
1:B:552:LEU:HD21	1:D:542:THR:HG23	1.96	0.46



	t i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:627:ASN:OD1	1:D:629:THR:HG22	2.16	0.46
1:F:186:ASP:OD2	1:H:171:ARG:NE	2.48	0.46
2:I:81:SER:HA	2:I:84:PHE:CE2	2.50	0.46
1:J:323:THR:HB	1:J:412:VAL:HG13	1.97	0.46
1:J:636:ALA:HB2	1:N:634:ILE:HD13	1.97	0.46
2:M:131:ARG:NH1	1:P:53:TYR:O	2.47	0.46
1:R:510:ILE:HG23	1:R:512:GLY:H	1.80	0.46
2:E:46:GLU:OE1	2:E:90:ARG:NH2	2.46	0.46
1:F:591:GLN:HA	1:F:594:VAL:HB	1.97	0.46
1:N:323:THR:HG22	1:N:415:VAL:HG13	1.96	0.46
1:N:510:ILE:HG23	1:N:512:GLY:H	1.80	0.46
1:T:468:VAL:HG22	1:T:472:TYR:CD2	2.50	0.46
1:B:591:GLN:HA	1:B:594:VAL:HB	1.98	0.46
2:I:69:GLU:OE2	2:I:70:GLY:N	2.48	0.46
1:J:451:ASP:OD2	1:N:72:ARG:HD2	2.15	0.46
1:L:78:VAL:HG13	1:L:518:THR:HG23	1.96	0.46
1:N:246:TYR:HB2	1:N:249:ARG:HG3	1.97	0.46
1:P:588:GLU:HA	1:P:591:GLN:HE21	1.79	0.46
1:F:274:ARG:HB2	1:F:296:GLU:HG2	1.97	0.46
1:L:239:VAL:HG12	1:L:240:THR:HG22	1.97	0.46
1:P:234:ILE:HD13	1:P:244:VAL:HG13	1.97	0.46
1:T:146:ARG:NH2	1:T:460:ASP:OD2	2.48	0.46
1:A:591:GLN:HA	1:A:594:VAL:HB	1.97	0.46
1:B:146:ARG:NH2	1:B:460:ASP:OD2	2.49	0.46
1:J:504:LYS:H	1:J:504:LYS:HG3	1.52	0.46
1:P:258:LEU:HB3	1:P:263:PHE:HB2	1.97	0.46
1:T:81:ARG:NH2	1:W:560:LEU:HD22	2.27	0.46
1:T:632:LEU:HD12	1:W:627:ASN:HB3	1.96	0.46
2:C:3:ILE:HG23	2:C:8:ASP:HB3	1.97	0.46
1:D:591:GLN:HA	1:D:594:VAL:HB	1.97	0.46
1:R:78:VAL:HG13	1:R:518:THR:HG23	1.98	0.46
1:T:106:THR:OG1	1:T:146:ARG:O	2.33	0.46
1:T:271:ILE:HG23	1:W:134:ASP:HB3	1.97	0.46
1:T:562:GLY:H	1:T:565:VAL:HG13	1.80	0.46
1:A:323:THR:HB	1:A:412:VAL:HG13	1.97	0.46
1:A:627:ASN:HB3	1:B:632:LEU:HD12	1.98	0.46
2:C:81:SER:HA	2:C:84:PHE:CE2	2.50	0.46
1:J:23:ASP:OD2	1:J:27:ARG:NH1	2.49	0.46
1:J:23:ASP:OD1	1:J:26:ARG:NH1	2.49	0.46
2:M:3:ILE:HG23	2:M:8:ASP:HB3	1.96	0.46
2:O:16:LYS:HD2	2:O:16:LYS:HA	1.58	0.46



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:Q:5:THR:OG1	2:Q:8:ASP:OD1	2.33	0.46
1:W:23:ASP:OD1	1:W:26:ARG:NH1	2.48	0.46
1:B:203:ASN:ND2	1:B:205:ASN:O	2.49	0.46
1:J:237:ASP:OD2	1:J:476:ARG:NH1	2.48	0.46
1:L:237:ASP:OD2	1:L:476:ARG:NH1	2.49	0.46
1:L:249:ARG:HH12	1:L:513:ARG:HH12	1.64	0.46
1:L:578:GLN:HG2	1:L:596:ALA:HB2	1.98	0.46
1:A:622:LEU:HD23	1:J:620:ALA:HB2	1.97	0.46
1:B:634:ILE:HD13	1:D:636:ALA:HB2	1.98	0.46
1:F:225:VAL:HG13	1:F:276:VAL:HG22	1.98	0.46
1:F:504:LYS:H	1:F:504:LYS:HG3	1.52	0.46
2:O:3:ILE:HG23	2:O:8:ASP:HB3	1.97	0.46
1:R:239:VAL:HG12	1:R:240:THR:HG22	1.98	0.46
1:R:578:GLN:HG2	1:R:596:ALA:HB2	1.97	0.46
1:T:76:ILE:HG23	1:T:520:VAL:HG13	1.97	0.46
1:D:237:ASP:OD2	1:D:476:ARG:NH1	2.49	0.45
1:F:78:VAL:HG13	1:F:518:THR:HG23	1.98	0.45
2:K:5:THR:OG1	2:K:8:ASP:OD1	2.34	0.45
1:P:612:GLN:O	1:P:616:LEU:HG	2.16	0.45
1:R:225:VAL:HG13	1:R:276:VAL:HG22	1.97	0.45
1:W:232:ALA:HB3	1:W:271:ILE:HD12	1.97	0.45
1:W:557:PHE:HZ	1:W:582:LYS:NZ	2.14	0.45
1:A:225:VAL:HG13	1:A:276:VAL:HG22	1.98	0.45
1:A:507:LEU:HD23	1:A:507:LEU:H	1.80	0.45
1:F:179:MET:HE1	1:F:187:PHE:CD1	2.51	0.45
1:H:78:VAL:HG13	1:H:518:THR:HG23	1.98	0.45
1:H:620:ALA:HB3	1:L:621:GLU:OE2	2.16	0.45
1:L:234:ILE:HD13	1:L:244:VAL:HG13	1.97	0.45
1:N:171:ARG:NE	1:R:186:ASP:OD2	2.50	0.45
1:T:550:GLN:NE2	1:T:581:VAL:HG21	2.30	0.45
1:T:582:LYS:HE3	1:T:582:LYS:HB3	1.50	0.45
1:W:179:MET:HE1	1:W:187:PHE:CD1	2.51	0.45
1:W:588:GLU:HA	1:W:591:GLN:OE1	2.15	0.45
1:A:253:ASP:HB3	1:A:504:LYS:HE2	1.99	0.45
1:F:587:PRO:O	1:F:590:GLN:HB3	2.16	0.45
1:J:244:VAL:HB	1:J:511:ARG:HB2	1.98	0.45
1:T:33:LEU:HD22	1:T:37:ARG:HH11	1.81	0.45
1:N:106:THR:OG1	1:N:146:ARG:O	2.34	0.45
1:A:179:MET:HE1	1:A:187:PHE:CD1	2.51	0.45
1:A:239:VAL:HG12	1:A:240:THR:HG22	1.98	0.45
2:C:16:LYS:HA	2:C:16:LYS:HD2	1.57	0.45



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:562:GLY:H	1:D:565:VAL:HG22	1.82	0.45
1:F:454:ALA:HB1	1:F:520:VAL:HG21	1.97	0.45
1:H:468:VAL:HG22	1:H:472:TYR:CD2	2.50	0.45
1:J:323:THR:HG22	1:J:415:VAL:HG13	1.98	0.45
1:N:239:VAL:HG12	1:N:240:THR:HG22	1.98	0.45
1:T:78:VAL:HG13	1:T:518:THR:HG23	1.98	0.45
1:W:78:VAL:HG13	1:W:518:THR:HG23	1.97	0.45
1:W:225:VAL:HG13	1:W:276:VAL:HG22	1.99	0.45
1:W:510:ILE:HG23	1:W:512:GLY:H	1.80	0.45
1:B:577:ILE:HD12	1:B:589:GLU:HB3	1.99	0.45
2:E:5:THR:OG1	2:E:8:ASP:OD1	2.35	0.45
1:F:507:LEU:HD23	1:F:507:LEU:H	1.81	0.45
1:H:76:ILE:HG23	1:H:520:VAL:HG13	1.99	0.45
1:J:578:GLN:HG2	1:J:596:ALA:HB2	1.99	0.45
1:N:312:ASP:OD2	1:R:205:ASN:ND2	2.48	0.45
1:T:615:LEU:CD2	1:W:609:VAL:HG12	2.46	0.45
1:B:76:ILE:HG23	1:B:520:VAL:HG13	1.98	0.45
1:B:78:VAL:HG13	1:B:518:THR:HG23	1.98	0.45
1:B:562:GLY:H	1:B:565:VAL:HG13	1.81	0.45
1:P:636:ALA:HB2	1:T:634:ILE:HD13	1.99	0.45
1:R:179:MET:HE1	1:R:187:PHE:CD1	2.52	0.45
1:R:281:ILE:HG22	1:R:286:VAL:HG22	1.97	0.45
1:R:507:LEU:HD23	1:R:507:LEU:H	1.81	0.45
1:W:281:ILE:HG22	1:W:286:VAL:HG22	1.98	0.45
1:H:239:VAL:HG12	1:H:240:THR:HG22	1.98	0.45
2:M:46:GLU:OE1	2:M:90:ARG:NH2	2.46	0.45
1:T:244:VAL:HB	1:T:511:ARG:HB2	1.98	0.45
1:B:72:ARG:HD2	1:D:451:ASP:OD2	2.16	0.45
1:F:281:ILE:HG22	1:F:286:VAL:HG22	1.97	0.45
1:J:468:VAL:HG22	1:J:472:TYR:CD2	2.52	0.45
1:N:562:GLY:H	1:N:565:VAL:HG13	1.81	0.45
1:R:323:THR:HB	1:R:412:VAL:HG13	1.97	0.45
1:T:530:GLN:O	1:T:534:GLU:HG3	2.17	0.45
1:B:186:ASP:OD2	1:D:171:ARG:NE	2.50	0.45
1:D:499:LEU:HA	1:D:505:GLN:HA	1.98	0.45
1:F:33:LEU:HD22	1:F:37:ARG:HH11	1.81	0.45
1:H:582:LYS:HE3	1:H:582:LYS:HB3	1.64	0.45
1:J:542:THR:HG23	1:N:552:LEU:HD21	1.98	0.45
1:W:33:LEU:HD22	1:W:37:ARG:HH11	1.81	0.45
1:A:78:VAL:HG13	1:A:518:THR:HG23	1.98	0.44
1:F:134:ASP:HB3	1:H:271:ILE:HG23	1.98	0.44



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:171:ARG:NE	1:N:186:ASP:OD2	2.50	0.44
1:L:389:LEU:HD23	1:L:389:LEU:HA	1.82	0.44
1:N:18:ASP:OD2	1:N:172:HIS:NE2	2.46	0.44
1:R:220:ALA:HB3	1:R:281:ILE:HG13	1.99	0.44
1:T:179:MET:HE1	1:T:187:PHE:CD1	2.52	0.44
1:T:587:PRO:HA	1:T:590:GLN:HB3	1.99	0.44
1:D:186:ASP:OD2	1:F:171:ARG:NE	2.51	0.44
2:E:114:LEU:HD12	2:E:114:LEU:HA	1.83	0.44
1:H:33:LEU:HD22	1:H:37:ARG:HH11	1.81	0.44
2:M:5:THR:OG1	2:M:8:ASP:OD1	2.35	0.44
1:N:78:VAL:HG13	1:N:518:THR:HG23	1.99	0.44
2:O:46:GLU:OE2	2:O:90:ARG:NH2	2.50	0.44
1:R:232:ALA:HB3	1:R:271:ILE:HD12	1.99	0.44
1:R:253:ASP:HB3	1:R:504:LYS:HE2	1.99	0.44
1:T:246:TYR:HB2	1:T:249:ARG:HG3	1.98	0.44
1:A:622:LEU:HA	1:J:620:ALA:HB2	1.99	0.44
1:B:239:VAL:HG12	1:B:240:THR:HG22	1.97	0.44
1:B:557:PHE:HZ	1:B:582:LYS:HZ3	1.62	0.44
1:D:191:TYR:HE2	1:D:278:LYS:HZ2	1.66	0.44
1:L:33:LEU:HD22	1:L:37:ARG:HH11	1.82	0.44
2:M:124:LYS:HB2	2:M:124:LYS:HE2	1.65	0.44
1:N:566:GLU:HA	1:N:569:ARG:NH2	2.32	0.44
1:A:87:ARG:NH1	1:A:89:ASP:OD1	2.50	0.44
1:A:281:ILE:HG22	1:A:286:VAL:HG22	1.98	0.44
1:D:235:TYR:C	1:D:243:PRO:HD2	2.37	0.44
1:D:507:LEU:HD23	1:D:507:LEU:H	1.82	0.44
1:H:274:ARG:HG3	1:H:274:ARG:NH1	2.33	0.44
1:J:191:TYR:CD2	1:J:280:ILE:HD11	2.52	0.44
1:N:179:MET:HE1	1:N:187:PHE:CD1	2.53	0.44
1:N:575:GLN:O	1:N:579:MET:HG3	2.17	0.44
1:P:23:ASP:OD1	1:P:26:ARG:NH1	2.51	0.44
1:P:33:LEU:HD22	1:P:37:ARG:HH11	1.82	0.44
1:P:239:VAL:HG12	1:P:240:THR:HG22	1.99	0.44
1:P:323:THR:HG22	1:P:415:VAL:HG13	1.98	0.44
1:T:329:LEU:HD23	1:T:329:LEU:HA	1.86	0.44
1:W:587:PRO:HA	1:W:590:GLN:HB3	1.99	0.44
1:B:566:GLU:HA	1:B:569:ARG:NH2	2.32	0.44
1:F:87:ARG:NH1	1:F:89:ASP:OD1	2.50	0.44
1:F:253:ASP:HB3	1:F:504:LYS:HE2	2.00	0.44
1:H:627:ASN:OD1	1:L:629:THR:HG22	2.17	0.44
1:N:587:PRO:HA	1:N:590:GLN:HB3	2.00	0.44



	the o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:N:591:GLN:O	1:N:595:GLU:HG3	2.18	0.44
1:T:239:VAL:HG12	1:T:240:THR:HG22	1.98	0.44
1:W:239:VAL:HG12	1:W:240:THR:HG22	1.99	0.44
1:A:33:LEU:HD22	1:A:37:ARG:HH11	1.81	0.44
1:H:179:MET:HE1	1:H:187:PHE:CD1	2.53	0.44
1:H:566:GLU:HA	1:H:569:ARG:NH2	2.31	0.44
1:L:23:ASP:OD1	1:L:26:ARG:NH1	2.50	0.44
1:N:554:LEU:HD22	1:R:567:MET:HE2	2.00	0.44
1:N:586:THR:HB	1:N:589:GLU:HG3	1.99	0.44
1:B:33:LEU:HD22	1:B:37:ARG:HH11	1.81	0.44
1:F:634:ILE:HD13	1:H:636:ALA:HB2	1.99	0.44
1:J:528:LYS:HG2	1:J:532:ARG:HH21	1.83	0.44
1:J:562:GLY:H	1:J:565:VAL:HG22	1.83	0.44
1:T:171:ARG:NE	1:W:186:ASP:OD2	2.51	0.44
1:B:274:ARG:HG3	1:B:274:ARG:NH1	2.33	0.44
1:D:53:TYR:O	2:K:131:ARG:NH1	2.47	0.44
2:E:131:ARG:NH1	1:L:53:TYR:O	2.48	0.44
1:F:559:LEU:HD23	1:F:559:LEU:HA	1.85	0.44
1:N:588:GLU:HA	1:N:591:GLN:OE1	2.17	0.44
1:P:578:GLN:HG2	1:P:596:ALA:HB2	2.00	0.44
1:P:634:ILE:HD13	1:R:636:ALA:HB2	2.00	0.44
1:W:507:LEU:HD23	1:W:507:LEU:H	1.81	0.44
2:X:16:LYS:HD2	2:X:16:LYS:HA	1.78	0.44
1:H:591:GLN:HA	1:H:594:VAL:HB	1.99	0.44
1:J:629:THR:HG22	1:N:627:ASN:OD1	2.17	0.44
1:N:504:LYS:H	1:N:504:LYS:HG3	1.52	0.44
1:N:621:GLU:OE1	1:R:620:ALA:HB3	2.16	0.44
1:A:134:ASP:HB3	1:B:271:ILE:HG23	1.99	0.43
1:D:190:LYS:HE2	1:D:191:TYR:CE1	2.53	0.43
1:D:528:LYS:HG2	1:D:532:ARG:HH21	1.83	0.43
1:D:578:GLN:HG2	1:D:596:ALA:HB2	1.99	0.43
1:F:616:LEU:HD21	1:H:622:LEU:HD12	1.99	0.43
2:I:124:LYS:HB2	2:I:124:LYS:HE2	1.78	0.43
1:J:239:VAL:HG12	1:J:240:THR:HG22	1.99	0.43
1:N:33:LEU:HD22	1:N:37:ARG:HH11	1.81	0.43
1:N:91:ALA:O	1:N:95:MET:HB2	2.19	0.43
1:A:297:HIS:HB2	1:A:463:ILE:HG12	2.01	0.43
1:H:552:LEU:HD21	1:L:542:THR:HG23	2.00	0.43
1:J:561:ASP:OD1	1:J:569:ARG:NH1	2.51	0.43
1:L:528:LYS:HG2	1:L:532:ARG:HH21	1.83	0.43
1:P:163:LYS:HB3	1:T:150:HIS:CD2	2.54	0.43


Atom-1	Atom-2	Interatomic	Clash	
1.D.528.IVS.HC2	1.D.529.ADC.HH91		0.43	
1.1.526.D15.HG2	1.1.552.ARG.IIII21	2.05	0.43	
1.1.330.1110.011 1.R.33.1 FU-HD99	1.R.342.11.0.001	1.21	0.43	
1.W.560.I FILH	1.W.560.I FU.HD92	1.01	0.43	
1.W.J00.LEU.II	1.W.300.LEU.IID23	1.83	0.43	
1.D.010.11DE.11G12	1.D.311.AIG.II	2.00	0.43	
1.1.239. VAL.IIG12	1.Г.240.1ПП.ПG22 1.І.27. А Р.С.НЦ11	2.00	0.43	
1.J.35.LEU.HD22	1.J.57.ANG.IIIII 1. L.02.WAL.N	1.00	0.43	
1.J.:92:A5P:0D1	1:J:95:VAL:N	2.31	0.43	
1:L:190:L15:ПЕЭ	1:L:191:11K:UE1	2.00	0.43	
1:L:240:1 Y K:HB2	1:L:249:ARG:HG3	2.00	0.43	
1:1:559:LEU:HD23	1:1:559:LEU:HA	1.85	0.43	
1:F:278:LYS:HB3	1:F:278:LYS:HE3	1.88	0.43	
1:P:557:PHE:HZ	1:P:582:LYS:NZ	2.14	0.43	
1:R:59:VAL:HG13	1:R:412:VAL:HG11	2.00	0.43	
1:R:178:SER:OG	1:R:218:GLN:NE2	2.51	0.43	
1:W:323:THR:HB	1:W:412:VAL:HG13	1.99	0.43	
1:B:298:ILE:HA	1:B:299:PRO:HD3	1.89	0.43	
1:P:510:ILE:HG12	1:P:511:ARG:H	1.83	0.43	
1:T:588:GLU:HA	1:T:591:GLN:OE1	2.17	0.43	
1:W:298:ILE:HA	1:W:299:PRO:HD3	1.89	0.43	
1:H:150:HIS:CD2	1:L:163:LYS:HB3	2.54	0.43	
1:N:80:TYR:HB2	1:N:95:MET:HG2	2.00	0.43	
1:P:468:VAL:HG22	1:P:472:TYR:CD2	2.54	0.43	
1:B:106:THR:OG1	1:B:146:ARG:O	2.34	0.43	
1:B:150:HIS:CD2	1:D:163:LYS:HB3	2.54	0.43	
1:J:163:LYS:HB3	1:N:150:HIS:CD2	2.53	0.43	
1:J:348:LYS:HB2	1:N:372:TYR:CE2	2.54	0.43	
1:T:557:PHE:HZ	1:T:582:LYS:HZ3	1.67	0.43	
1:W:578:GLN:HG2	1:W:596:ALA:HB2	2.00	0.43	
1:H:106:THR:OG1	1:H:146:ARG:O	2.32	0.43	
1:J:274:ARG:NH1	1:J:274:ARG:HG3	2.33	0.43	
1:L:541:LYS:HE2	1:L:541:LYS:HB3	1.80	0.43	
1:L:591:GLN:O	1:L:595:GLU:HG3	2.18	0.43	
1:P:629:THR:HG22	1:T:627:ASN:OD1	2.17	0.43	
1:R:389:LEU:HD23	1:R:389:LEU:HA	1.80	0.43	
1:B:91:ALA:O	1:B:95:MET:HB2	2.19	0.43	
1:D:274:ARG:NH1	1:D:274:ARG:HG3	2.33	0.43	
1:F:577:ILE:HD11	1:F:582:LYS:HE2	2.00	0.43	
1:F:587:PRO:HA	1:F:590:GLN:HB3	2.00	0.43	
1:H:184:TRP:CZ2	1:H:199:PRO:HD3	2.54	0.43	
1:H:530:GLN:O	1:H:534:GLU:HG3	2.19	0.43	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:L:510:ILE:HG12	1:L:511:ARG:H	1.83	0.43
1:T:346:LYS:H	1:T:346:LYS:HG2	1.56	0.43
1:B:228:LYS:NZ	1:B:228:LYS:HB3	2.34	0.43
1:B:372:TYR:CE2	1:D:348:LYS:HB2	2.54	0.43
1:D:33:LEU:HD22	1:D:37:ARG:HH11	1.83	0.43
1:D:234:ILE:HD13	1:D:244:VAL:HG13	1.99	0.43
1:J:551:LEU:HD11	1:N:556:TYR:OH	2.18	0.43
1:N:274:ARG:HG3	1:N:274:ARG:NH1	2.33	0.43
1:P:627:ASN:OD1	1:R:629:THR:HG22	2.18	0.43
1:R:297:HIS:HB3	1:R:459:ARG:NH2	2.34	0.43
1:T:561:ASP:OD1	1:T:569:ARG:NH1	2.51	0.43
1:A:562:GLY:H	1:A:565:VAL:HG12	1.84	0.42
1:B:249:ARG:HH12	1:B:513:ARG:HH12	1.67	0.42
1:D:184:TRP:CZ2	1:D:199:PRO:HD3	2.54	0.42
1:F:499:LEU:HA	1:F:505:GLN:HA	2.01	0.42
1:N:228:LYS:NZ	1:N:228:LYS:HB3	2.34	0.42
1:N:306:GLU:OE2	1:R:65:ARG:NE	2.52	0.42
1:P:274:ARG:NH1	1:P:274:ARG:HG3	2.33	0.42
1:P:620:ALA:HB2	1:R:622:LEU:HA	2.01	0.42
1:R:297:HIS:HB2	1:R:463:ILE:HG12	2.01	0.42
1:T:51:LEU:HD12	1:T:51:LEU:HA	1.80	0.42
1:A:67:LEU:HD13	1:A:418:LEU:HD22	2.01	0.42
1:D:586:THR:HG22	1:D:588:GLU:H	1.84	0.42
1:F:42:ASP:OD1	1:F:42:ASP:N	2.48	0.42
2:G:16:LYS:HD2	2:G:16:LYS:HA	1.78	0.42
1:L:184:TRP:CZ2	1:L:199:PRO:HD3	2.55	0.42
1:L:504:LYS:H	1:L:504:LYS:HG3	1.52	0.42
1:B:18:ASP:OD2	1:B:172:HIS:NE2	2.46	0.42
1:P:274:ARG:HG3	1:P:274:ARG:HH11	1.85	0.42
1:R:306:GLU:O	1:R:316:TYR:HA	2.19	0.42
1:T:414:GLU:OE2	1:W:59:VAL:HG22	2.19	0.42
2:V:46:GLU:OE2	2:V:90:ARG:NH2	2.52	0.42
1:W:297:HIS:HB2	1:W:463:ILE:HG12	2.00	0.42
1:W:306:GLU:O	1:W:316:TYR:HA	2.20	0.42
1:A:65:ARG:NE	1:B:306:GLU:OE1	2.52	0.42
1:D:389:LEU:HD23	1:D:389:LEU:HA	1.82	0.42
1:D:561:ASP:OD1	1:D:569:ARG:NH1	2.52	0.42
1:H:562:GLY:H	1:H:565:VAL:HG13	1.83	0.42
1:L:600:LYS:HB2	1:L:600:LYS:HE2	1.88	0.42
1:P:184:TRP:CZ2	1:P:199:PRO:HD3	2.54	0.42
1:P:559:LEU:HD23	1:P:559:LEU:HA	1.85	0.42



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance (Å)	overlap (Å)
1:P:611:ALA:HB1	1:T:609:VAL:HG13	2.00	0.42
1:F:67:LEU:HD13	1:F:418:LEU:HD22	2.01	0.42
1:F:329:LEU:HD23	1:F:329:LEU:HA	1.84	0.42
1:H:504:LYS:H	1:H:504:LYS:HG3	1.52	0.42
1:J:559:LEU:HD23	1:J:559:LEU:HA	1.88	0.42
1:L:190:LYS:HE3	1:L:191:TYR:HE1	1.85	0.42
1:N:307:TRP:HZ3	1:R:113:ILE:HD11	1.84	0.42
1:P:348:LYS:HB2	1:T:372:TYR:CE2	2.54	0.42
1:W:297:HIS:HB3	1:W:459:ARG:NH2	2.34	0.42
1:A:458:ARG:HG2	1:A:518:THR:HG22	2.02	0.42
1:A:499:LEU:HA	1:A:505:GLN:HA	2.01	0.42
1:B:184:TRP:CZ2	1:B:199:PRO:HD3	2.54	0.42
1:F:113:ILE:HD11	1:H:307:TRP:HZ3	1.84	0.42
1:F:298:ILE:HA	1:F:299:PRO:HD3	1.89	0.42
1:J:274:ARG:HG3	1:J:274:ARG:HH11	1.85	0.42
1:R:329:LEU:HD23	1:R:329:LEU:HA	1.82	0.42
1:R:458:ARG:HG2	1:R:518:THR:HG22	2.02	0.42
1:W:67:LEU:HD13	1:W:418:LEU:HD22	2.02	0.42
1:A:609:VAL:HG12	1:B:615:LEU:HB2	2.01	0.42
1:B:80:TYR:HB2	1:B:95:MET:HG2	2.00	0.42
1:B:179:MET:HE1	1:B:187:PHE:CD1	2.54	0.42
1:B:530:GLN:O	1:B:534:GLU:HG3	2.20	0.42
1:D:274:ARG:HG3	1:D:274:ARG:HH11	1.85	0.42
1:D:559:LEU:HD23	1:D:559:LEU:HA	1.86	0.42
1:F:306:GLU:O	1:F:316:TYR:HA	2.20	0.42
1:H:587:PRO:O	1:H:590:GLN:HB3	2.20	0.42
1:J:184:TRP:CZ2	1:J:199:PRO:HD3	2.54	0.42
1:J:632:LEU:HD12	1:N:627:ASN:HB3	2.00	0.42
1:L:282:THR:OG1	1:L:283:CYS:N	2.52	0.42
1:L:507:LEU:H	1:L:507:LEU:HD23	1.84	0.42
1:R:67:LEU:HD13	1:R:418:LEU:HD22	2.01	0.42
1:R:499:LEU:HA	1:R:505:GLN:HA	2.02	0.42
1:T:306:GLU:OE1	1:W:65:ARG:NE	2.53	0.42
1:A:629:THR:HG22	1:J:627:ASN:OD1	2.20	0.42
1:D:92:ASP:OD1	1:D:93:VAL:N	2.52	0.42
1:H:372:TYR:CE2	1:L:348:LYS:HB2	2.54	0.42
1:J:297:HIS:HB2	1:J:463:ILE:HG12	2.02	0.42
1:J:510:ILE:HG12	1:J:511:ARG:H	1.83	0.42
1:L:563:LYS:HA	1:L:563:LYS:HD2	1.84	0.42
1:N:530:GLN:O	1:N:534:GLU:HG3	2.19	0.42
1:A:113:ILE:HD11	1:B:307:TRP:HZ3	1.84	0.42



Atom-1	Atom-2	Interatomic	Clash	
1100111-1	1100111-2	distance (Å)	overlap (Å)	
1:A:235:TYR:C	1:A:243:PRO:HD2	2.40	0.42	
1:A:297:HIS:HB3	1:A:459:ARG:NH2	2.34	0.42	
1:B:559:LEU:HD23	1:B:559:LEU:HA	1.85	0.42	
1:D:323:THR:HG22	1:D:415:VAL:HG13	2.01	0.42	
1:H:228:LYS:NZ	1:H:228:LYS:HB3	2.34	0.42	
1:H:586:THR:HG22	1:H:588:GLU:OE1	2.19	0.42	
1:P:190:LYS:HD2	1:P:191:TYR:CE1	2.55	0.42	
1:R:577:ILE:HD11	1:R:582:LYS:HE2	2.02	0.42	
1:R:600:LYS:HB2	1:R:600:LYS:HE2	1.87	0.42	
1:T:88:PRO:O	1:W:561:ASP:HB2	2.20	0.42	
1:T:629:THR:HG22	1:W:627:ASN:OD1	2.19	0.42	
1:W:458:ARG:HG2	1:W:518:THR:HG22	2.02	0.42	
1:B:582:LYS:HB3	1:B:582:LYS:HE3	1.65	0.42	
1:D:59:VAL:HG23	1:F:414:GLU:OE2	2.20	0.42	
1:D:249:ARG:HH12	1:D:513:ARG:NH1	2.08	0.42	
1:F:627:ASN:OD1	1:H:629:THR:HG22	2.20	0.42	
2:I:7:GLY:O	2:I:11:ARG:HG3	2.20	0.42	
1:J:507:LEU:H	1:J:507:LEU:HD23	1.84	0.42	
1:L:468:VAL:HG22	1:L:472:TYR:CD2	2.53	0.42	
1:T:184:TRP:CZ2	1:T:199:PRO:HD3	2.54	0.42	
1:T:307:TRP:HZ3	1:W:113:ILE:HD11	1.84	0.42	
1:A:337:ASN:HB2	1:B:404:MET:HE2	2.02	0.41	
2:C:7:GLY:O	2:C:11:ARG:HG3	2.20	0.41	
1:F:184:TRP:CZ2	1:F:199:PRO:HD3	2.55	0.41	
1:F:600:LYS:HA	1:F:603:GLN:OE1	2.19	0.41	
1:N:184:TRP:CZ2	1:N:199:PRO:HD3	2.55	0.41	
2:S:124:LYS:HE2	2:S:124:LYS:HB2	1.73	0.41	
1:A:184:TRP:CZ2	1:A:199:PRO:HD3	2.55	0.41	
1:A:398:PRO:HB3	1:J:395:PRO:HD2	2.02	0.41	
1:B:587:PRO:O	1:B:590:GLN:HB3	2.21	0.41	
1:D:395:PRO:HD2	1:F:398:PRO:HB3	2.02	0.41	
1:D:582:LYS:HE2	1:D:582:LYS:HB3	1.62	0.41	
1:L:186:ASP:OD2	1:W:171:ARG:NE	2.53	0.41	
1:L:323:THR:HG22	1:L:415:VAL:HG13	2.02	0.41	
1:N:310:VAL:HG22	1:R:37:ARG:HD3	2.02	0.41	
1:N:621:GLU:OE1	1:R:617:GLN:HA	2.18	0.41	
1:P:298:ILE:HA	1:P:299:PRO:HD3	1.88	0.41	
1:P:542:THR:HG23	1:T:552:LEU:HD21	2.01	0.41	
2:V:124:LYS:HB2	2:V:124:LYS:HE2	1.79	0.41	
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.80	0.41	
1:A:600:LYS:HA	1:A:603:GLN:OE1	2.20	0.41	



Atom-1	Atom-2	Interatomic	Clash	
	1100111 2	distance (Å)	overlap (Å)	
1:B:586:THR:HG22	1:B:588:GLU:OE1	2.20	0.41	
1:D:37:ARG:HD3	1:F:310:VAL:HG22	2.02	0.41	
1:D:59:VAL:CG1	1:D:412:VAL:HG11	2.50	0.41	
1:F:563:LYS:HD2	1:F:563:LYS:HA	1.84	0.41	
1:H:146:ARG:NH2	1:H:460:ASP:OD2	2.52	0.41	
1:J:541:LYS:HE2	1:N:536:LEU:HD21	2.02	0.41	
1:P:329:LEU:HD23	1:P:329:LEU:HA	1.85	0.41	
1:P:395:PRO:HD2	1:R:398:PRO:HB3	2.02	0.41	
1:P:417:THR:O	1:P:417:THR:OG1	2.38	0.41	
1:R:563:LYS:HA	1:R:563:LYS:HD2	1.84	0.41	
1:W:184:TRP:CZ2	1:W:199:PRO:HD3	2.55	0.41	
1:D:177:HIS:NE2	1:D:221:GLU:OE1	2.53	0.41	
1:F:559:LEU:HD11	1:H:538:LEU:HD21	2.02	0.41	
1:P:249:ARG:HH12	1:P:513:ARG:NH1	2.18	0.41	
1:P:620:ALA:CB	1:R:622:LEU:HA	2.51	0.41	
1:W:249:ARG:HE	1:W:275:ARG:HH22	1.66	0.41	
1:W:504:LYS:H	1:W:504:LYS:HG3	1.52	0.41	
1:W:510:ILE:HG12	1:W:511:ARG:H	1.85	0.41	
1:A:600:LYS:HB2	1:A:600:LYS:HE2	1.89	0.41	
1:B:609:VAL:HG12	1:D:615:LEU:CD2	2.51	0.41	
1:D:249:ARG:NH1	1:D:513:ARG:HH22	2.17	0.41	
1:D:282:THR:OG1	1:D:283:CYS:N	2.53	0.41	
2:K:21:SER:O	2:K:24:THR:HG22	2.20	0.41	
1:L:297:HIS:HB2	1:L:463:ILE:HG12	2.02	0.41	
1:N:538:LEU:HD21	1:R:559:LEU:HD11	2.02	0.41	
1:P:504:LYS:H	1:P:504:LYS:HG3	1.52	0.41	
1:P:507:LEU:HD23	1:P:507:LEU:H	1.84	0.41	
1:P:622:LEU:HD12	1:T:616:LEU:HD21	2.03	0.41	
1:R:510:ILE:HG12	1:R:511:ARG:H	1.85	0.41	
1:T:228:LYS:NZ	1:T:228:LYS:HB3	2.34	0.41	
2:V:3:ILE:HG23	2:V:8:ASP:HB3	2.01	0.41	
2:V:81:SER:HB2	2:X:42:ALA:HB1	2.03	0.41	
1:A:306:GLU:O	1:A:316:TYR:HA	2.20	0.41	
2:K:124:LYS:HB2	2:K:124:LYS:HE2	1.65	0.41	
1:N:209:PHE:CG	1:N:210:PRO:HD2	2.55	0.41	
1:P:37:ARG:HD3	1:R:310:VAL:HG22	2.03	0.41	
1:T:209:PHE:CG	1:T:210:PRO:HD2	2.55	0.41	
2:V:7:GLY:O	2:V:11:ARG:HG3	2.20	0.41	
1:W:577:ILE:HD11	1:W:582:LYS:HE2	2.01	0.41	
1:D:563:LYS:HA	1:D:563:LYS:HD2	1.86	0.41	
1:H:209:PHE:CG	1:H:210:PRO:HD2	2.55	0.41	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:J:146:ARG:NH2	1:J:460:ASP:OD2	2.53	0.41
1:J:561:ASP:OD2	1:J:569:ARG:NH2	2.54	0.41
1:L:634:1LE:HD13	1:W:636:ALA:HB2	2.02	0.41
1:A:37:ARG:HD3	1:B:310:VAL:HG22	2.03	0.41
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.83	0.41
1:A:615:LEU:O	1:A:619:GLN:HG3	2.21	0.41
1:F:65:ARG:NE	1:H:306:GLU:OE2	2.53	0.41
2:G:42:ALA:HB1	2:I:81:SER:HB2	2.03	0.41
1:H:145:ARG:HE	1:H:145:ARG:HB3	1.78	0.41
1:J:298:ILE:HA	1:J:299:PRO:HD3	1.88	0.41
1:L:593:LEU:O	1:L:593:LEU:HD12	2.21	0.41
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.85	0.41
1:P:615:LEU:O	1:P:619:GLN:HG3	2.21	0.41
1:T:232:ALA:HB3	1:T:271:ILE:HD12	2.03	0.41
1:T:249:ARG:HH12	1:T:513:ARG:HH12	1.68	0.41
1:B:209:PHE:CG	1:B:210:PRO:HD2	2.55	0.41
1:B:209:PHE:CD1	1:B:210:PRO:HD2	2.56	0.41
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.90	0.41
1:D:417:THR:O	1:D:417:THR:OG1	2.38	0.41
1:D:561:ASP:OD2	1:D:569:ARG:NH2	2.54	0.41
1:F:386:THR:HG23	1:H:387:GLN:HE21	1.86	0.41
1:H:209:PHE:CD1	1:H:210:PRO:HD2	2.56	0.41
1:J:101:ASP:OD2	1:J:464:TYR:OH	2.26	0.41
1:J:264:ILE:HD12	1:J:264:ILE:O	2.21	0.41
1:J:282:THR:OG1	1:J:283:CYS:N	2.54	0.41
1:J:310:VAL:HG22	1:N:37:ARG:HD3	2.03	0.41
1:L:164:LEU:HD23	1:L:164:LEU:HA	1.92	0.41
1:N:209:PHE:CD1	1:N:210:PRO:HD2	2.56	0.41
1:N:249:ARG:HH12	1:N:513:ARG:HH12	1.67	0.41
1:N:296:GLU:OE2	1:R:135:GLN:NE2	2.38	0.41
1:N:600:LYS:HB2	1:N:600:LYS:HE2	1.89	0.41
2:O:2:GLN:HB2	2:S:38:ASP:OD1	2.21	0.41
1:P:306:GLU:O	1:P:316:TYR:HA	2.21	0.41
1:P:561:ASP:HB2	1:R:88:PRO:O	2.21	0.41
1:R:59:VAL:HG12	1:R:327:GLN:OE1	2.21	0.41
1:R:504:LYS:H	1:R:504:LYS:HG3	1.52	0.41
1:T:92:ASP:OD1	1:T:92:ASP:N	2.37	0.41
2:V:16:LYS:HD2	2:V:16:LYS:HA	1.69	0.41
1:W:499:LEU:HA	1:W:505:GLN:HA	2.02	0.41
1:A:310:VAL:HG22	1:J:37:ARG:HD3	2.03	0.41
1:D:119:ILE:HA	1:D:449:PHE:HE2	1.86	0.41



Atom-1	Atom-2	Interatomic	Clash	
		distance (A)	overlap (A)	
1:D:620:ALA:HB3	1:F:621:GLU:OE1	2.21	0.41	
1:F:135:GLN:NE2	1:H:296:GLU:OE2	2.38	0.41	
1:J:593:LEU:O	1:J:593:LEU:HD12	2.21	0.41	
1:P:297:HIS:HB2	1:P:463:ILE:HG12	2.03	0.41	
1:P:497:VAL:HG12	1:P:507:LEU:HA	2.03	0.41	
1:R:113:ILE:HD13	1:R:150:HIS:CE1	2.56	0.41	
1:T:209:PHE:CD1	1:T:210:PRO:HD2	2.56	0.41	
1:T:557:PHE:CZ	1:T:582:LYS:HD3	2.55	0.41	
1:W:113:ILE:HD13	1:W:150:HIS:CE1	2.56	0.41	
1:A:244:VAL:HB	1:A:511:ARG:HB2	2.03	0.40	
1:A:582:LYS:HE3	1:A:582:LYS:HB3	1.84	0.40	
1:B:134:ASP:HB3	1:D:271:ILE:HG23	2.03	0.40	
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.86	0.40	
1:D:371:TYR:HA	1:F:348:LYS:HB3	2.04	0.40	
2:E:21:SER:O	2:E:24:THR:HG22	2.21	0.40	
1:F:249:ARG:HH12	1:F:513:ARG:NH1	2.17	0.40	
1:F:458:ARG:HG2	1:F:518:THR:HG22	2.02	0.40	
1:H:33:LEU:HD23	1:H:33:LEU:HA	1.92	0.40	
1:H:232:ALA:HB3	1:H:271:ILE:HD12	2.04	0.40	
1:H:564:GLY:C	1:L:554:LEU:HD21	2.41	0.40	
1:L:242:GLU:N	1:L:242:GLU:OE1	2.54	0.40	
2:M:29:GLU:HG2	2:M:30:PRO:HD2	2.03	0.40	
1:N:165:MET:HE2	1:N:165:MET:HB2	1.96	0.40	
1:N:278:LYS:HE3	1:N:278:LYS:HB3	1.90	0.40	
1:P:186:ASP:OD2	1:R:171:ARG:NE	2.54	0.40	
1:R:184:TRP:CZ2	1:R:199:PRO:HD3	2.55	0.40	
1:W:229:LYS:HA	1:W:272:LYS:HA	2.03	0.40	
1:D:23:ASP:OD1	1:D:26:ARG:NH1	2.55	0.40	
2:E:29:GLU:HG2	2:E:30:PRO:HD2	2.03	0.40	
1:L:274:ARG:NH1	1:L:274:ARG:HG3	2.37	0.40	
1:P:541:LYS:HE2	1:T:536:LEU:HD21	2.02	0.40	
1:T:588:GLU:OE1	1:T:588:GLU:N	2.50	0.40	
2:V:29:GLU:HG2	2:V:30:PRO:HD2	2.03	0.40	
1:W:582:LYS:HE3	1:W:582:LYS:HB3	1.82	0.40	
1:B:93:VAL:HG11	1:B:475:PRO:HD2	2.03	0.40	
1:H:190:LYS:HD2	1:H:191:TYR:CE2	2.56	0.40	
2:I:29:GLU:HG2	2:I:30:PRO:HD2	2.04	0.40	
1:J:591:GLN:O	1:J:595:GLU:HG3	2.21	0.40	
1:J:629:THR:HG22	1:N:627:ASN:CG	2.42	0.40	
1:T:190:LYS:HD2	1:T:191:TYR:CE2	2.56	0.40	
1:T:229:LYS:HA	1:T:272:LYS:HA	2.04	0.40	



	Cleah		
Atom-1	Atom-2		Clash
		distance (A)	overlap (A)
1:T:296:GLU:OE2	1:W:135:GLN:NE2	2.38	0.40
1:T:458:ARG:HG2	1:T:518:THR:HG22	2.03	0.40
1:T:599:ALA:O	1:T:603:GLN:NE2	2.54	0.40
1:A:209:PHE:CD1	1:A:210:PRO:HD2	2.57	0.40
1:A:561:ASP:HB2	1:B:88:PRO:O	2.22	0.40
1:A:627:ASN:CG	1:B:629:THR:HG22	2.42	0.40
1:L:627:ASN:OD1	1:W:629:THR:HG22	2.21	0.40
1:N:615:LEU:HB2	1:R:609:VAL:HG12	2.04	0.40
1:P:242:GLU:OE1	1:P:242:GLU:N	2.55	0.40
1:P:593:LEU:O	1:P:593:LEU:HD12	2.21	0.40
2:Q:21:SER:O	2:Q:24:THR:HG22	2.21	0.40
2:Q:29:GLU:HG2	2:Q:30:PRO:HD2	2.03	0.40
1:T:44:TRP:CE3	1:T:208:VAL:HB	2.56	0.40
1:T:504:LYS:H	1:T:504:LYS:HG3	1.52	0.40
1:T:621:GLU:OE1	1:W:620:ALA:HB3	2.21	0.40
1:W:593:LEU:O	1:W:593:LEU:HD12	2.22	0.40
1:F:113:ILE:HD13	1:F:150:HIS:CE1	2.56	0.40
1:J:321:ARG:HE	1:J:321:ARG:HB2	1.75	0.40
1:L:37:ARG:HD3	1:W:310:VAL:HG22	2.03	0.40
1:N:163:LYS:HB3	1:R:150:HIS:CD2	2.57	0.40
1:R:613:GLY:O	1:R:616:LEU:HD23	2.21	0.40
1:T:563:LYS:HA	1:T:563:LYS:HD2	1.85	0.40
1:T:593:LEU:O	1:T:593:LEU:HD12	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	Perce	ntiles
1	А	602/725~(83%)	582 (97%)	20 (3%)	0	100	100
1	В	602/725~(83%)	580 (96%)	22 (4%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	D	602/725~(83%)	582 (97%)	20 (3%)	0	100	100
1	F	602/725~(83%)	582 (97%)	20 (3%)	0	100	100
1	Н	602/725~(83%)	579 (96%)	23 (4%)	0	100	100
1	J	602/725~(83%)	583 (97%)	19 (3%)	0	100	100
1	L	602/725~(83%)	581 (96%)	21 (4%)	0	100	100
1	N	602/725~(83%)	582 (97%)	20 (3%)	0	100	100
1	Р	602/725~(83%)	581 (96%)	21 (4%)	0	100	100
1	R	602/725~(83%)	581 (96%)	21 (4%)	0	100	100
1	Т	602/725~(83%)	582 (97%)	20 (3%)	0	100	100
1	W	602/725~(83%)	583 (97%)	19 (3%)	0	100	100
2	С	150/166~(90%)	144 (96%)	6 (4%)	0	100	100
2	Е	150/166~(90%)	147 (98%)	3 (2%)	0	100	100
2	G	150/166~(90%)	146 (97%)	4 (3%)	0	100	100
2	Ι	150/166~(90%)	144 (96%)	6 (4%)	0	100	100
2	К	150/166~(90%)	147 (98%)	3 (2%)	0	100	100
2	М	150/166~(90%)	147 (98%)	3 (2%)	0	100	100
2	Ο	150/166~(90%)	144 (96%)	6 (4%)	0	100	100
2	Q	150/166~(90%)	147 (98%)	3 (2%)	0	100	100
2	S	150/166~(90%)	146 (97%)	4 (3%)	0	100	100
2	V	150/166~(90%)	144 (96%)	6 (4%)	0	100	100
2	Х	150/166~(90%)	146 (97%)	4 (3%)	0	100	100
2	a	150/166~(90%)	146 (97%)	4 (3%)	0	100	100
All	All	9024/10692 (84%)	8726 (97%)	298 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	А	530/630~(84%)	493~(93%)	37~(7%)	15	47
1	В	530/630~(84%)	494~(93%)	36~(7%)	16	48
1	D	530/630~(84%)	498 (94%)	32~(6%)	19	53
1	F	530/630~(84%)	493~(93%)	37 (7%)	15	47
1	Н	530/630~(84%)	495~(93%)	35~(7%)	16	49
1	J	530/630~(84%)	498 (94%)	32 (6%)	19	53
1	L	530/630~(84%)	499 (94%)	31 (6%)	20	55
1	Ν	530/630~(84%)	495 (93%)	35~(7%)	16	49
1	Р	530/630~(84%)	496 (94%)	34 (6%)	17	51
1	R	530/630~(84%)	494 (93%)	36 (7%)	16	48
1	Т	530/630~(84%)	492 (93%)	38 (7%)	14	45
1	W	530/630~(84%)	493 (93%)	37 (7%)	15	47
2	С	120/131~(92%)	111 (92%)	9 (8%)	13	43
2	Е	120/131~(92%)	112 (93%)	8 (7%)	16	49
2	G	120/131~(92%)	112 (93%)	8 (7%)	16	49
2	Ι	120/131~(92%)	112 (93%)	8 (7%)	16	49
2	Κ	120/131~(92%)	113 (94%)	7~(6%)	20	55
2	М	120/131~(92%)	112 (93%)	8 (7%)	16	49
2	Ο	120/131~(92%)	111 (92%)	9~(8%)	13	43
2	Q	120/131~(92%)	111 (92%)	9 (8%)	13	43
2	S	120/131~(92%)	110 (92%)	10 (8%)	11	39
2	V	120/131~(92%)	109 (91%)	11 (9%)	9	34
2	X	120/131~(92%)	112 (93%)	8 (7%)	16	49
2	a	120/131~(92%)	112 (93%)	8 (7%)	16	49
All	All	7800/9132~(85%)	7277 (93%)	523 (7%)	20	49

All (523) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	7	ARG
1	А	31	ASN
1	А	42	ASP
1	А	61	ARG
1	А	77	ASP
1	А	116	ARG



Mol	Chain	Res	Type
1	А	130	THR
1	А	165	MET
1	А	174	THR
1	А	178	SER
1	А	192	ASP
1	А	225	VAL
1	А	253	ASP
1	А	273	ARG
1	А	282	THR
1	А	283	CYS
1	А	291	GLN
1	А	367	ASP
1	А	381	SER
1	А	387	GLN
1	А	389	LEU
1	А	450	GLN
1	А	459	ARG
1	А	470	ASP
1	А	476	ARG
1	А	499	LEU
1	А	504	LYS
1	А	507	LEU
1	А	511	ARG
1	А	537	GLU
1	А	541	LYS
1	А	546	THR
1	А	557	PHE
1	А	558	THR
1	А	560	LEU
1	А	608	MET
1	A	630	LEU
2	a	44	MET
2	a	63	ASP
2	a	69	GLU
2	a	77	SER
2	a	112	GLU
2	a	125	ARG
2	a	140	PHE
2	a	146	TRP
1	В	7	ARG
1	В	61	ARG
1	В	106	THR



Mol	Chain	Res	Type
1	В	116	ARG
1	В	128	LEU
1	В	130	THR
1	В	174	THR
1	В	178	SER
1	В	190	LYS
1	В	206	ASP
1	В	236	GLN
1	В	253	ASP
1	В	256	ASP
1	В	273	ARG
1	В	283	CYS
1	В	325	ASP
1	В	346	LYS
1	В	387	GLN
1	В	404	MET
1	В	406	GLU
1	В	413	LYS
1	В	450	GLN
1	В	459	ARG
1	В	473	ASP
1	В	476	ARG
1	В	504	LYS
1	В	507	LEU
1	В	541	LYS
1	В	546	THR
1	В	558	THR
1	В	560	LEU
1	В	567	MET
1	В	569	ARG
1	В	603	GLN
1	В	622	LEU
1	В	630	LEU
2	С	1	MET
2	С	16	LYS
2	С	63	ASP
2	С	77	SER
2	C	112	GLU
2	С	125	ARG
2	С	140	PHE
2	С	146	TRP
2	С	150	PRO



Mol	Chain	Res	Type
1	D	7	ARG
1	D	42	ASP
1	D	77	ASP
1	D	128	LEU
1	D	130	THR
1	D	174	THR
1	D	206	ASP
1	D	221	GLU
1	D	225	VAL
1	D	253	ASP
1	D	256	ASP
1	D	265	LYS
1	D	266	ILE
1	D	273	ARG
1	D	283	CYS
1	D	325	ASP
1	D	371	TYR
1	D	387	GLN
1	D	389	LEU
1	D	450	GLN
1	D	459	ARG
1	D	476	ARG
1	D	504	LYS
1	D	507	LEU
1	D	537	GLU
1	D	546	THR
1	D	558	THR
1	D	560	LEU
1	D	579	MET
1	D	608	MET
1	D	622	LEU
1	D	630	LEU
2	E	44	MET
2	Е	77	SER
2	Е	94	ASP
2	Е	95	TYR
2	Е	112	GLU
2	Е	125	ARG
2	E	140	PHE
2	Е	146	TRP
1	F	7	ARG
1	F	42	ASP



Mol	Chain	Res	Type
1	F	77	ASP
1	F	116	ARG
1	F	130	THR
1	F	165	MET
1	F	174	THR
1	F	178	SER
1	F	192	ASP
1	F	225	VAL
1	F	236	GLN
1	F	243	PRO
1	F	253	ASP
1	F	273	ARG
1	F	282	THR
1	F	283	CYS
1	F	291	GLN
1	F	367	ASP
1	F	381	SER
1	F	387	GLN
1	F	389	LEU
1	F	396	GLU
1	F	450	GLN
1	F	459	ARG
1	F	470	ASP
1	F	476	ARG
1	F	499	LEU
1	F	504	LYS
1	F	507	LEU
1	F	511	ARG
1	F	537	GLU
1	F	541	LYS
1	F	546	THR
1	F	557	PHE
1	F	558	THR
1	F	560	LEU
1	F	608	MET
2	G	44	MET
2	G	63	ASP
2	G	69	GLU
2	G	77	SER
2	G	112	GLU
2	G	125	ARG
2	G	140	PHE



Mol	Chain	Res	Type
2	G	146	TRP
1	Н	7	ARG
1	Н	42	ASP
1	Н	106	THR
1	Н	116	ARG
1	Н	128	LEU
1	Н	130	THR
1	Н	174	THR
1	Н	178	SER
1	Н	190	LYS
1	Н	206	ASP
1	Н	236	GLN
1	Н	243	PRO
1	Н	253	ASP
1	Н	269	ARG
1	Н	273	ARG
1	Н	283	CYS
1	Н	325	ASP
1	Н	346	LYS
1	Н	387	GLN
1	Н	404	MET
1	Н	406	GLU
1	Н	413	LYS
1	Н	459	ARG
1	Н	473	ASP
1	Н	476	ARG
1	Н	504	LYS
1	Н	507	LEU
1	Н	541	LYS
1	Н	546	THR
1	Н	558	THR
1	Н	560	LEU
1	Н	567	MET
1	Н	569	ARG
1	Н	603	GLN
1	Н	630	LEU
2	Ι	1	MET
2	Ι	63	ASP
2	Ι	77	SER
2	Ι	112	GLU
2	Ι	125	ARG
2	Ι	140	PHE



Mol	Chain	Res	Type
2	Ι	146	TRP
2	Ι	150	PRO
1	J	7	ARG
1	J	42	ASP
1	J	77	ASP
1	J	128	LEU
1	J	130	THR
1	J	174	THR
1	J	178	SER
1	J	225	VAL
1	J	253	ASP
1	J	256	ASP
1	J	265	LYS
1	J	266	ILE
1	J	273	ARG
1	J	283	CYS
1	J	325	ASP
1	J	371	TYR
1	J	387	GLN
1	J	459	ARG
1	J	476	ARG
1	J	504	LYS
1	J	507	LEU
1	J	537	GLU
1	J	541	LYS
1	J	546	THR
1	J	558	THR
1	J	560	LEU
1	J	567	MET
1	J	573	ASN
1	J	579	MET
1	J	608	MET
1	J	616	LEU
1	J	630	LEU
2	Κ	44	MET
2	K	94	ASP
2	K	112	GLU
2	K	113	LEU
2	K	125	ARG
2	K	140	PHE
2	K	146	TRP
1	L	7	ARG



Mol	Chain	Res	Type
1	L	42	ASP
1	L	77	ASP
1	L	128	LEU
1	L	130	THR
1	L	165	MET
1	L	171	ARG
1	L	174	THR
1	L	190	LYS
1	L	206	ASP
1	L	225	VAL
1	L	243	PRO
1	L	253	ASP
1	L	256	ASP
1	L	265	LYS
1	L	273	ARG
1	L	283	CYS
1	L	325	ASP
1	L	371	TYR
1	L	387	GLN
1	L	389	LEU
1	L	459	ARG
1	L	476	ARG
1	L	504	LYS
1	L	507	LEU
1	L	546	THR
1	L	558	THR
1	L	560	LEU
1	L	573	ASN
1	L	579	MET
1	L	630	LEU
2	М	44	MET
2	М	63	ASP
2	М	94	ASP
2	М	112	GLU
2	М	125	ARG
2	М	140	PHE
2	М	146	TRP
2	М	150	PRO
1	N	7	ARG
1	N	106	THR
1	N	116	ARG
1	Ν	128	LEU



Mol	Chain	Res	Type
1	Ν	130	THR
1	N	174	THR
1	Ν	178	SER
1	Ν	206	ASP
1	Ν	236	GLN
1	N	243	PRO
1	N	253	ASP
1	N	256	ASP
1	N	261	SER
1	N	269	ARG
1	N	273	ARG
1	N	283	CYS
1	N	325	ASP
1	N	387	GLN
1	Ν	404	MET
1	N	406	GLU
1	N	459	ARG
1	N	473	ASP
1	N	476	ARG
1	N	493	MET
1	N	504	LYS
1	Ν	507	LEU
1	N	541	LYS
1	N	546	THR
1	N	558	THR
1	N	560	LEU
1	Ν	567	MET
1	N	569	ARG
1	N	591	GLN
1	N	603	GLN
1	N	630	LEU
2	0	1	MET
2	0	16	LYS
2	0	63	ASP
2	Ο	77	SER
2	0	112	GLU
2	Ο	125	ARG
2	0	140	PHE
2	0	146	TRP
2	0	150	PRO
1	Р	7	ARG
1	Р	42	ASP



Mol	Chain	Res	Type
1	Р	77	ASP
1	Р	128	LEU
1	Р	130	THR
1	Р	171	ARG
1	Р	174	THR
1	Р	178	SER
1	Р	206	ASP
1	Р	225	VAL
1	Р	243	PRO
1	Р	253	ASP
1	Р	256	ASP
1	Р	265	LYS
1	Р	266	ILE
1	Р	273	ARG
1	Р	283	CYS
1	Р	325	ASP
1	Р	371	TYR
1	Р	387	GLN
1	Р	450	GLN
1	Р	459	ARG
1	Р	476	ARG
1	Р	504	LYS
1	Р	507	LEU
1	Р	537	GLU
1	Р	541	LYS
1	Р	546	THR
1	Р	557	PHE
1	Р	558	THR
1	Р	560	LEU
1	Р	579	MET
1	Р	616	LEU
1	Р	630	LEU
2	Q	44	MET
2	Q	63	ASP
2	Q	94	ASP
2	Q	112	GLU
2	Q	113	LEU
2	Q	125	ARG
2	Q	140	PHE
2	Q	146	TRP
2	Q	150	PRO
1	R	7	ARG



Mol	Chain	Res	Type
1	R	42	ASP
1	R	61	ARG
1	R	77	ASP
1	R	116	ARG
1	R	130	THR
1	R	165	MET
1	R	174	THR
1	R	178	SER
1	R	192	ASP
1	R	205	ASN
1	R	225	VAL
1	R	243	PRO
1	R	253	ASP
1	R	273	ARG
1	R	282	THR
1	R	283	CYS
1	R	381	SER
1	R	387	GLN
1	R	389	LEU
1	R	413	LYS
1	R	450	GLN
1	R	459	ARG
1	R	470	ASP
1	R	476	ARG
1	R	499	LEU
1	R	504	LYS
1	R	507	LEU
1	R	511	ARG
1	R	537	GLU
1	R	541	LYS
1	R	546	THR
1	R	557	PHE
1	R	558	THR
1	R	560	LEU
1	R	603	GLN
2	S	41	GLU
2	S	44	MET
2	S	63	ASP
2	S	77	SER
2	S	94	ASP
2	S	112	GLU
2	S	125	ARG



Mol	Chain	Res	Type
2	S	140	PHE
2	S	146	TRP
2	S	150	PRO
1	Т	7	ARG
1	Т	42	ASP
1	Т	106	THR
1	Т	116	ARG
1	Т	128	LEU
1	Т	130	THR
1	Т	174	THR
1	Т	178	SER
1	Т	190	LYS
1	Т	205	ASN
1	Т	236	GLN
1	Т	243	PRO
1	Т	253	ASP
1	Т	256	ASP
1	Т	261	SER
1	Т	269	ARG
1	Т	273	ARG
1	Т	283	CYS
1	Т	325	ASP
1	Т	346	LYS
1	Т	387	GLN
1	Т	404	MET
1	Т	406	GLU
1	Т	414	GLU
1	Т	459	ARG
1	Т	473	ASP
1	Т	476	ARG
1	Т	504	LYS
1	Т	507	LEU
1	Т	541	LYS
1	Т	546	THR
1	Т	557	PHE
1	Т	558	THR
1	Т	560	LEU
1	Т	591	GLN
1	Т	603	GLN
1	Т	609	VAL
1	Т	630	LEU
2	V	1	MET



Mol	Chain	Res	Type
2	V	16	LYS
2	V	63	ASP
2	V	71	ASP
2	V	77	SER
2	V	95	TYR
2	V	112	GLU
2	V	125	ARG
2	V	140	PHE
2	V	146	TRP
2	V	150	PRO
1	W	7	ARG
1	W	31	ASN
1	W	42	ASP
1	W	61	ARG
1	W	77	ASP
1	W	116	ARG
1	W	130	THR
1	W	174	THR
1	W	178	SER
1	W	192	ASP
1	W	225	VAL
1	W	236	GLN
1	W	243	PRO
1	W	250	ASP
1	W	253	ASP
1	W	273	ARG
1	W	282	THR
1	W	283	CYS
1	W	367	ASP
1	W	381	SER
1	W	387	GLN
1	W	389	LEU
1	W	450	GLN
1	W	459	ARG
1	W	470	ASP
1	W	476	ARG
1	W	499	LEU
1	W	504	LYS
1	W	507	LEU
1	W	511	ARG
1	W	537	GLU
1	W	541	LYS



Mol	Chain	Res	Type
1	W	546	THR
1	W	558	THR
1	W	560	LEU
1	W	591	GLN
1	W	603	GLN
2	Х	44	MET
2	Х	63	ASP
2	Х	77	SER
2	Х	94	ASP
2	Х	112	GLU
2	Х	125	ARG
2	Х	140	PHE
2	Х	146	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	525	GLN
1	А	550	GLN
1	В	591	GLN
1	D	40	GLN
1	D	135	GLN
1	D	218	GLN
1	D	550	GLN
1	D	591	GLN
1	F	525	GLN
1	F	550	GLN
1	Н	74	ASN
1	Н	450	GLN
1	Н	591	GLN
1	J	591	GLN
1	L	218	GLN
1	L	550	GLN
1	L	591	GLN
1	Ν	74	ASN
1	N	450	GLN
1	N	550	GLN
1	Р	550	GLN
1	Р	591	GLN
1	R	525	GLN
1	Т	74	ASN
1	Т	450	GLN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-41651. 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: 220



Y Index: 220



Z Index: 220

6.2.2 Raw map



X Index: 220

Y Index: 220



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



6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 243





Z Index: 183

6.3.2 Raw map



X Index: 196

Y Index: 196



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 3.5. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_41651_msk_1.map (i)





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 1193 $\rm nm^3;$ this corresponds to an approximate mass of 1078 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 0.333 ${\rm \AA^{-1}}$



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 0.333 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.30	2.98
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-41651 and PDB model 8TVU. 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 3.5 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 (3.5).



9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.5510
А	0.8190	0.5470
В	0.8180	0.5470
С	0.8840	0.5690
D	0.8160	0.5470
Е	0.8900	0.5670
F	0.8180	0.5480
G	0.8900	0.5690
Н	0.8180	0.5470
Ι	0.8850	0.5650
J	0.8150	0.5460
К	0.8900	0.5690
L	0.8130	0.5480
М	0.8880	0.5670
N	0.8180	0.5470
0	0.8890	0.5680
Р	0.8140	0.5460
Q	0.8870	0.5680
R	0.8180	0.5470
S	0.8910	0.5680
Т	0.8160	0.5470
V	0.8860	0.5680
W	0.8180	0.5470
Х	0.8910	0.5690
a	0.8920	0.5680

