

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2023 – 10:11 PM JST

PDB ID	:	7WRW
Title	:	Structure of Deinococcus radiodurans HerA
Authors	:	Cheng, K.
Deposited on	:	2022-01-27
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp 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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain					
-		010	5%					
	А	618	63%	29%	• 6%			
			4%					
1	В	618	69%	24%	• 6%			
			3%					
1	С	618	71%	21%	• 6%			
			4%					
1	D	618	64%	28%	• 6%			
			6%					
1	Ε	618	63%	29%	• 6%			
			7%					
1	F	618	61%	32%	• 6%			



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 27153 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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		Ate	oms			ZeroOcc	AltConf	Trace
1	Р	591	Total	С	Ν	Ο	S	0	0	0
	D	301	4518	2867	798	844	9	0	0	0
1	C	592	Total	С	Ν	0	S	0	0	0
1	U	000	4527	2872	800	846	9	0	0	0
1	Б	592	Total	С	Ν	0	S	0	0	0
	Г	000	4527	2872	800	846	9	0	0	0
1	П	592	Total	С	Ν	0	S	0	0	0
1		000	4527	2872	800	846	9	0	0	0
1	F	592	Total	С	Ν	0	S	0	0	0
	Ľ	000	4527	2872	800	846	9	0	0	0
1	Δ	592	Total	С	Ν	Ο	S	0	0	0
	A	000	4527	2872	800	846	9		0	U

• Molecule 1 is a protein called HerA.



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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: HerA



V395











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	279.03Å 279.03 Å 105.68 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	10.00 - 3.00	Depositor
Resolution (A)	10.00 - 3.00	EDS
% Data completeness	99.8 (10.00-3.00)	Depositor
(in resolution range)	99.8 (10.00-3.00)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.23 (at 2.99 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D D.	0.225 , 0.246	Depositor
Π, Π_{free}	0.225 , 0.246	DCC
R_{free} test set	4632 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	85.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39, 59.7	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27153	wwPDB-VP
Average B, all atoms $(Å^2)$	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bo	ond lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.52	1/4621~(0.0%)	0.66	1/6273~(0.0%)	
1	В	0.48	1/4611~(0.0%)	0.67	1/6258~(0.0%)	
1	С	0.60	1/4621~(0.0%)	0.74	0/6273	
1	D	0.51	3/4621~(0.1%)	0.67	4/6273~(0.1%)	
1	Ε	0.53	4/4621~(0.1%)	0.63	4/6273~(0.1%)	
1	F	0.43	1/4621~(0.0%)	0.61	1/6273~(0.0%)	
All	All	0.51	11/27716~(0.0%)	0.66	11/37623~(0.0%)	

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	Е	88	PRO	N-CA	13.32	1.70	1.47
1	D	267	PRO	N-CA	13.24	1.69	1.47
1	Ε	104	PRO	N-CA	12.89	1.69	1.47
1	А	257	GLU	C-N	8.79	1.50	1.34
1	С	354	THR	C-N	8.69	1.50	1.34
1	В	278	VAL	C-N	8.56	1.50	1.34
1	D	354	THR	C-N	8.35	1.50	1.34
1	F	148	PRO	N-CD	-7.25	1.37	1.47
1	Ε	87	LEU	C-N	5.98	1.45	1.34
1	D	266	ALA	C-N	5.88	1.45	1.34
1	Ε	103	ASP	C-N	5.68	1.45	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	Е	104	PRO	N-CA-C	-8.04	91.21	112.10
1	Е	88	PRO	CA-N-CD	-7.66	100.77	111.50
1	D	267	PRO	CA-N-CD	-7.36	101.20	111.50
1	Е	104	PRO	CA-N-CD	-6.98	101.73	111.50
1	D	349	PHE	CB-CA-C	-6.48	97.44	110.40
1	F	148	PRO	N-CA-CB	-6.18	95.80	102.60
1	D	77	SER	N-CA-CB	5.65	118.98	110.50



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	104	PRO	N-CA-C	-5.22	98.54	112.10
1	Е	104	PRO	N-CD-CG	5.16	110.94	103.20
1	А	62	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	354	THR	C-N-CD	-5.01	109.57	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4527	0	4526	175	0
1	В	4518	0	4517	133	1
1	С	4527	0	4526	125	1
1	D	4527	0	4526	165	0
1	Е	4527	0	4526	203	0
1	F	4527	0	4526	204	0
All	All	27153	0	27147	914	1

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 17.

All (914) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:D:267:PRO:N	1:D:267:PRO:CA	1.69	1.45
1:A:188:ARG:NH2	1:A:260:ARG:HD3	1.25	1.43
1:A:188:ARG:NH2	1:A:260:ARG:CD	1.80	1.41
1:E:88:PRO:N	1:E:88:PRO:CA	1.69	1.38
1:F:69:ARG:HH21	1:A:23:ASP:CG	1.24	1.38
1:E:104:PRO:N	1:E:104:PRO:CA	1.69	1.33
1:E:235:GLU:OE2	1:E:248:ARG:HB2	1.24	1.28
1:E:145:ASP:OD1	1:E:242:LYS:HD3	1.22	1.27
1:E:145:ASP:OD1	1:E:242:LYS:CD	1.84	1.25
1:A:188:ARG:HH21	1:A:260:ARG:NE	1.36	1.24



	io ao pagoni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:188:ARG:NH2	1:A:260:ARG:NE	1.86	1.22
1:D:76:GLU:OE1	1:E:19:LEU:HD21	1.10	1.21
1:B:235:GLU:O	1:B:239:VAL:HG23	1.35	1.21
1:F:146:GLY:O	1:F:251:LEU:HD21	1.35	1.21
1:E:81:ASP:CB	1:E:87:LEU:HD11	1.73	1.18
1:E:81:ASP:HB3	1:E:87:LEU:HD11	1.25	1.16
1:E:57:VAL:HA	1:E:104:PRO:HG3	1.27	1.16
1:F:69:ARG:NH2	1:A:23:ASP:OD2	1.78	1.15
1:F:69:ARG:NH2	1:A:23:ASP:CG	1.97	1.15
1:F:226:LYS:CB	1:F:601:VAL:HG12	1.79	1.12
1:D:213:ILE:HD13	1:D:445:LEU:HD11	1.30	1.11
1:E:84:ALA:HB3	1:E:86:LEU:CD2	1.79	1.11
1:E:138:PHE:HB3	1:E:191:VAL:HG21	1.32	1.11
1:D:357:GLU:HG3	1:D:358:ASN:N	1.65	1.10
1:B:311:ALA:HB2	1:B:499:SER:HB3	1.26	1.10
1:F:124:LEU:HD21	1:F:147:GLN:HG3	1.24	1.08
1:C:595:ALA:CB	1:C:601:VAL:HG23	1.82	1.08
1:F:226:LYS:HB3	1:F:601:VAL:HG12	1.35	1.08
1:D:76:GLU:OE1	1:E:19:LEU:CD2	2.02	1.08
1:A:188:ARG:NH2	1:A:260:ARG:CZ	2.17	1.08
1:F:124:LEU:CD2	1:F:147:GLN:HG3	1.84	1.07
1:E:51:LYS:HE2	1:E:106:ASN:OD1	1.54	1.07
1:A:315:LEU:H	1:A:315:LEU:HD12	1.21	1.06
1:F:235:GLU:OE1	1:F:248:ARG:HB2	1.55	1.05
1:D:357:GLU:CG	1:D:358:ASN:H	1.65	1.05
1:E:84:ALA:HB3	1:E:86:LEU:HD21	1.38	1.04
1:D:311:ALA:HB2	1:D:499:SER:HB3	1.37	1.04
1:E:143:LEU:HD12	1:E:143:LEU:H	1.24	1.02
1:D:213:ILE:CD1	1:D:445:LEU:HD11	1.89	1.02
1:F:226:LYS:HG3	1:F:601:VAL:HG11	1.38	1.01
1:E:57:VAL:HG13	1:E:104:PRO:HG2	1.38	1.01
1:E:86:LEU:HD22	1:E:86:LEU:H	1.22	1.01
1:A:188:ARG:HH21	1:A:260:ARG:CD	1.56	1.00
1:A:210:ARG:HD2	1:A:480:ASP:OD1	1.61	1.00
1:E:155:PHE:HA	1:E:161:GLY:HA3	1.43	0.99
1:C:595:ALA:HB1	1:C:601:VAL:HG23	1.41	0.99
1:E:311:ALA:HB2	1:E:499:SER:HB3	1.46	0.97
1:D:357:GLU:HG3	1:D:358:ASN:H	0.81	0.97
1:E:57:VAL:HA	1:E:104:PRO:CG	1.94	0.97
1:B:41:LEU:O	1:B:63:VAL:O	1.83	0.96
1:C:595:ALA:CB	1:C:601:VAL:CG2	2.44	0.95



	io ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:87:LEU:HD12	1:E:87:LEU:H	1.31	0.95
1:F:383:LEU:HD12	1:F:404:LEU:HD22	1.49	0.94
1:A:188:ARG:HH22	1:A:260:ARG:CD	1.59	0.94
1:F:143:LEU:HD11	1:F:147:GLN:HE21	1.29	0.93
1:D:176:THR:OG1	1:D:217:LYS:NZ	2.02	0.93
1:A:311:ALA:HB2	1:A:499:SER:HB3	1.51	0.93
1:F:23:ASP:OD2	1:E:69:ARG:NH2	2.01	0.93
1:E:165:ASN:OD1	1:E:523:GLN:NE2	2.02	0.92
1:E:145:ASP:OD1	1:E:242:LYS:CE	2.17	0.92
1:E:26:PRO:O	1:E:99:VAL:HG21	1.69	0.91
1:C:311:ALA:HB2	1:C:499:SER:HB3	1.51	0.91
1:F:235:GLU:OE1	1:F:248:ARG:CB	2.18	0.91
1:E:84:ALA:CB	1:E:86:LEU:HD21	2.00	0.91
1:F:226:LYS:HG3	1:F:601:VAL:CG1	2.01	0.90
1:F:226:LYS:CB	1:F:601:VAL:CG1	2.50	0.90
1:F:149:LEU:HD12	1:F:150:PRO:HD2	1.51	0.90
1:E:81:ASP:CB	1:E:87:LEU:CD1	2.51	0.88
1:E:51:LYS:CE	1:E:106:ASN:OD1	2.22	0.88
1:E:81:ASP:HB2	1:E:87:LEU:HD11	1.53	0.88
1:C:396:VAL:HG21	1:C:404:LEU:HD11	1.54	0.88
1:D:269:ARG:HA	1:D:280:GLN:HG2	1.56	0.87
1:A:155:PHE:HA	1:A:161:GLY:HA3	1.55	0.87
1:E:41:LEU:O	1:E:63:VAL:O	1.93	0.86
1:A:311:ALA:CB	1:A:499:SER:HB3	2.05	0.86
1:F:23:ASP:CG	1:E:69:ARG:HH21	1.79	0.86
1:A:249:TYR:OH	1:A:591:PHE:O	1.94	0.86
1:B:69:ARG:NH2	1:C:23:ASP:OD2	2.07	0.86
1:F:92:SER:OG	1:E:76:GLU:OE2	1.92	0.86
1:E:42:ASP:OD2	1:E:565:ARG:NH1	2.09	0.86
1:B:26:PRO:O	1:B:99:VAL:HG21	1.75	0.85
1:E:104:PRO:N	1:E:104:PRO:C	2.30	0.85
1:D:213:ILE:CD1	1:D:445:LEU:CD1	2.54	0.85
1:A:188:ARG:HH22	1:A:260:ARG:HD3	1.11	0.85
1:A:231:MET:O	1:A:231:MET:HE2	1.77	0.84
1:B:235:GLU:O	1:B:239:VAL:CG2	2.23	0.84
1:A:57:VAL:HA	1:A:104:PRO:HG2	1.60	0.82
1:D:234:LYS:HE2	1:D:234:LYS:HA	1.60	0.82
1:D:176:THR:CB	1:D:217:LYS:NZ	2.43	0.81
1:D:234:LYS:HA	1:D:234:LYS:CE	2.10	0.81
1:A:167:SER:HG	1:A:555:TYR:HH	1.23	0.81
1:A:158:GLY:HA2	1:A:161:GLY:O	1.79	0.81



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:311:ALA:CB	1:E:499:SER:HB3	2.10	0.80
1:B:165:ASN:HD21	1:B:523:GLN:HE22	1.27	0.80
1:E:81:ASP:HB3	1:E:87:LEU:CD1	2.10	0.80
1:F:41:LEU:HD13	1:F:66:VAL:HG22	1.64	0.80
1:B:188:ARG:NH1	1:B:260:ARG:HG2	1.96	0.80
1:E:235:GLU:OE2	1:E:248:ARG:CB	2.20	0.80
1:F:146:GLY:O	1:F:251:LEU:CD2	2.26	0.80
1:E:81:ASP:HB2	1:E:87:LEU:CD1	2.12	0.79
1:D:219:GLU:HA	1:D:222:LEU:HD23	1.64	0.79
1:F:330:ARG:NH2	1:E:380:GLU:OE2	2.14	0.79
1:C:412:ARG:HG2	1:C:412:ARG:HH11	1.48	0.79
1:E:145:ASP:CG	1:E:242:LYS:HD3	2.02	0.78
1:F:69:ARG:NH2	1:A:23:ASP:OD1	2.16	0.78
1:F:268:PRO:CG	1:F:292:VAL:HG12	2.13	0.78
1:A:210:ARG:HH11	1:A:210:ARG:HG2	1.48	0.78
1:C:174:THR:OG1	1:C:589:TYR:OH	2.02	0.78
1:E:86:LEU:CD2	1:E:86:LEU:H	1.97	0.78
1:C:50:ARG:NH1	1:C:54:GLY:O	2.17	0.78
1:D:167:SER:HG	1:D:555:TYR:HH	1.31	0.78
1:A:450:ILE:HG23	1:A:458:GLN:HG2	1.66	0.77
1:B:69:ARG:HH21	1:C:23:ASP:CG	1.88	0.77
1:E:338:LYS:HE3	1:E:428:PRO:HG3	1.67	0.77
1:D:311:ALA:CB	1:D:499:SER:HB3	2.15	0.77
1:A:188:ARG:NH2	1:A:260:ARG:NH1	2.33	0.77
1:A:481:THR:CG2	1:A:483:PHE:CE2	2.67	0.77
1:E:84:ALA:CB	1:E:86:LEU:CD2	2.60	0.77
1:F:281:THR:OG1	1:F:284:ARG:O	2.02	0.76
1:A:42:ASP:OD2	1:A:565:ARG:NH1	2.17	0.76
1:A:281:THR:HG21	1:A:288:VAL:HG21	1.68	0.76
1:C:174:THR:CG2	1:C:572:GLY:H	1.97	0.76
1:E:87:LEU:HD12	1:E:87:LEU:N	2.01	0.76
1:B:24:VAL:CG1	1:B:110:PRO:HD2	2.16	0.76
1:C:396:VAL:CG2	1:C:404:LEU:HD11	2.15	0.76
1:A:143:LEU:O	1:A:143:LEU:HD12	1.85	0.76
1:F:226:LYS:CG	1:F:601:VAL:CG1	2.63	0.76
1:B:24:VAL:HG12	1:B:110:PRO:HD2	1.68	0.75
1:F:17:MET:CE	1:E:83:VAL:HG21	2.16	0.75
1:F:294:THR:HG23	1:F:297:GLU:H	1.52	0.75
1:E:33:VAL:HB	1:E:93:TYR:CD2	2.22	0.75
1:A:210:ARG:HG2	1:A:210:ARG:NH1	2.01	0.75
1:E:155:PHE:HA	1:E:161:GLY:CA	2.17	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:124:LEU:HD21	1:F:147:GLN:CG	2.13	0.74
1:F:143:LEU:O	1:F:143:LEU:HD12	1.87	0.74
1:C:145:ASP:OD2	1:C:145:ASP:N	2.21	0.73
1:D:70:HIS:HB3	1:D:73:VAL:HG23	1.70	0.73
1:C:595:ALA:HB2	1:C:601:VAL:CG2	2.17	0.73
1:B:27:THR:O	1:B:99:VAL:HG23	1.88	0.73
1:F:268:PRO:HG3	1:F:292:VAL:HG12	1.69	0.73
1:D:19:LEU:HD13	1:D:32:ALA:HB2	1.71	0.73
1:E:86:LEU:HD22	1:E:86:LEU:N	2.01	0.73
1:F:226:LYS:CG	1:F:601:VAL:HG11	2.19	0.73
1:D:70:HIS:HB3	1:D:73:VAL:CG2	2.18	0.73
1:D:76:GLU:HB3	1:E:21:THR:HG21	1.71	0.72
1:F:384:LEU:HD12	1:F:405:ARG:HE	1.52	0.72
1:F:356:PRO:HA	1:F:359:LEU:HD13	1.70	0.72
1:A:373:GLU:N	1:A:373:GLU:OE1	2.23	0.72
1:A:228:ASN:ND2	1:A:592:PRO:O	2.15	0.72
1:A:235:GLU:OE1	1:A:248:ARG:HD2	1.89	0.72
1:A:315:LEU:HD12	1:A:315:LEU:N	2.02	0.71
1:A:525:THR:HG22	1:A:527:SER:H	1.55	0.71
1:F:38:SER:HB3	1:A:52:PRO:HD2	1.73	0.71
1:C:135:GLU:OE2	1:C:154:ARG:NH2	2.24	0.71
1:C:603:ASP:N	1:C:603:ASP:OD1	2.23	0.71
1:B:135:GLU:OE2	1:B:154:ARG:NH2	2.22	0.70
1:B:188:ARG:HH12	1:B:260:ARG:HD3	1.56	0.70
1:F:42:ASP:OD1	1:F:565:ARG:NH1	2.24	0.70
1:B:401:PRO:HB2	1:C:397:LEU:HB3	1.72	0.70
1:E:143:LEU:HD12	1:E:143:LEU:N	2.00	0.70
1:A:549:GLU:OE1	1:A:552:ARG:NH1	2.23	0.70
1:A:553:PRO:HA	1:A:556:ARG:HD3	1.73	0.70
1:E:553:PRO:HA	1:E:556:ARG:HD3	1.72	0.69
1:A:19:LEU:HD13	1:A:32:ALA:HB2	1.74	0.69
1:A:228:ASN:HB3	1:A:231:MET:HB3	1.73	0.69
1:A:478:ARG:HG3	1:A:478:ARG:O	1.92	0.69
1:B:386:GLU:HB3	1:B:391:GLY:HA2	1.73	0.69
1:D:77:SER:OG	1:E:71:GLU:HG3	1.91	0.69
1:A:143:LEU:HD12	1:A:143:LEU:C	2.13	0.69
1:D:154:ARG:NH1	1:D:159:GLU:OE1	2.26	0.69
1:D:213:ILE:HD13	1:D:445:LEU:CD1	2.14	0.69
1:C:155:PHE:HA	1:C:161:GLY:HA3	1.74	0.68
1:E:57:VAL:CG1	1:E:104:PRO:HG2	2.18	0.68
1:A:210:ARG:CD	1:A:480:ASP:OD1	2.40	0.68



	i agein	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:396:VAL:O	1:C:396:VAL:HG13	1.93	0.68
1:F:340:THR:OG1	1:F:426:LEU:O	2.09	0.68
1:B:42:ASP:OD1	1:B:565:ARG:NH1	2.26	0.68
1:B:553:PRO:O	1:B:556:ARG:HG2	1.93	0.68
1:D:553:PRO:HA	1:D:556:ARG:HD3	1.76	0.68
1:E:155:PHE:CA	1:E:161:GLY:HA3	2.22	0.68
1:E:323:ASN:HD21	1:E:397:LEU:HG	1.58	0.68
1:C:373:GLU:OE1	1:C:373:GLU:N	2.22	0.68
1:A:155:PHE:CA	1:A:161:GLY:HA3	2.23	0.67
1:B:291:PHE:HB2	1:B:436:PRO:HG3	1.76	0.67
1:A:315:LEU:H	1:A:315:LEU:CD1	1.99	0.67
1:D:291:PHE:HB2	1:D:436:PRO:HG3	1.76	0.67
1:F:401:PRO:HB2	1:A:397:LEU:HB3	1.76	0.67
1:F:17:MET:HE1	1:E:83:VAL:HG21	1.77	0.67
1:E:281:THR:HG21	1:E:288:VAL:HG11	1.76	0.67
1:D:235:GLU:OE2	1:D:248:ARG:HD2	1.96	0.66
1:C:42:ASP:OD2	1:C:565:ARG:NH1	2.28	0.66
1:D:42:ASP:OD2	1:D:565:ARG:NH1	2.28	0.66
1:B:553:PRO:HA	1:B:556:ARG:HD3	1.77	0.66
1:D:176:THR:CB	1:D:217:LYS:HZ1	2.08	0.66
1:A:481:THR:HG22	1:A:483:PHE:CE2	2.31	0.66
1:C:19:LEU:HD13	1:C:32:ALA:HB2	1.78	0.66
1:F:111:GLN:HG2	1:E:68:LYS:NZ	2.11	0.66
1:F:226:LYS:HB2	1:F:601:VAL:CG1	2.26	0.66
1:A:60:TYR:HE2	1:A:103:ASP:HB2	1.61	0.66
1:A:188:ARG:HH22	1:A:260:ARG:NH1	1.94	0.66
1:C:57:VAL:HA	1:C:104:PRO:HG2	1.78	0.65
1:F:231:MET:HE3	1:F:249:TYR:CE2	2.31	0.65
1:B:69:ARG:HE	1:C:23:ASP:CG	1.99	0.65
1:B:57:VAL:HA	1:B:104:PRO:HG2	1.78	0.65
1:F:146:GLY:C	1:F:251:LEU:HD21	2.16	0.65
1:A:213:ILE:HD11	1:A:221:LEU:HG	1.79	0.65
1:A:155:PHE:HA	1:A:161:GLY:CA	2.25	0.65
1:A:235:GLU:OE1	1:A:248:ARG:HB2	1.97	0.65
1:D:235:GLU:OE1	1:D:235:GLU:HA	1.95	0.65
1:C:76:GLU:HG3	1:D:19:LEU:HD21	1.79	0.64
1:C:353:GLU:OE1	1:C:353:GLU:HA	1.95	0.64
1:D:294:THR:HG22	1:D:297:GLU:H	1.62	0.64
1:F:226:LYS:CG	1:F:601:VAL:HG12	2.26	0.64
1:F:330:ARG:HD3	1:E:353:GLU:HG3	1.80	0.64
1:E:478:ARG:O	1:E:478:ARG:HG3	1.96	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:346:ASP:OD2	1:C:382:LYS:NZ	2.23	0.64
1:B:19:LEU:HD21	1:A:76:GLU:HG3	1.79	0.64
1:F:264:LEU:HD23	1:F:447:VAL:HB	1.79	0.64
1:A:230:ARG:NH1	1:A:599:ASP:O	2.31	0.64
1:A:481:THR:HG21	1:A:483:PHE:CE2	2.33	0.64
1:C:412:ARG:HG2	1:C:412:ARG:NH1	2.12	0.64
1:F:231:MET:CE	1:F:249:TYR:CE2	2.80	0.64
1:F:294:THR:OG1	1:F:340:THR:HB	1.97	0.63
1:A:343:ILE:HD13	1:A:368:ASN:HB2	1.79	0.63
1:F:268:PRO:HG2	1:F:292:VAL:HG12	1.80	0.63
1:E:51:LYS:NZ	1:E:106:ASN:OD1	2.30	0.63
1:D:267:PRO:N	1:D:267:PRO:C	2.48	0.63
1:E:267:PRO:HG2	1:E:280:GLN:HG3	1.79	0.63
1:D:234:LYS:HA	1:D:234:LYS:NZ	2.13	0.63
1:F:231:MET:CE	1:F:249:TYR:CD2	2.82	0.63
1:D:235:GLU:OE2	1:D:248:ARG:CD	2.46	0.63
1:E:553:PRO:O	1:E:556:ARG:HG2	1.98	0.63
1:C:244:LEU:HD13	1:C:245:SER:H	1.64	0.63
1:D:235:GLU:OE1	1:D:591:PHE:HD2	1.81	0.63
1:D:267:PRO:HB3	1:D:453:LEU:HD21	1.81	0.63
1:F:382:LYS:NZ	1:F:392:ASP:OD1	2.32	0.63
1:E:156:ILE:HD13	1:E:164:ILE:HD11	1.81	0.63
1:E:164:ILE:HG12	1:E:539:ILE:HB	1.81	0.63
1:D:553:PRO:O	1:D:556:ARG:HG2	1.99	0.62
1:C:174:THR:OG1	1:C:174:THR:O	2.16	0.62
1:B:376:ILE:HD13	1:B:411:LEU:HB3	1.81	0.62
1:F:23:ASP:CG	1:E:69:ARG:HE	2.03	0.62
1:C:549:GLU:OE1	1:C:552:ARG:NH1	2.33	0.62
1:C:595:ALA:HB2	1:C:601:VAL:HG22	1.79	0.62
1:E:19:LEU:HD13	1:E:32:ALA:HB2	1.81	0.62
1:B:66:VAL:HG13	1:C:109:PRO:HG3	1.81	0.62
1:B:79:VAL:HG12	1:C:17:MET:CE	2.29	0.62
1:B:107:PHE:CB	1:A:41:LEU:HB2	2.29	0.62
1:F:71:GLU:HB3	1:E:75:PHE:CD1	2.34	0.62
1:D:525:THR:HG22	1:D:527:SER:H	1.65	0.62
1:D:226:LYS:HG3	1:D:601:VAL:CG1	2.30	0.61
1:E:139:PRO:HB3	1:E:252:LEU:HD22	1.82	0.61
1:E:111:GLN:HG3	1:E:112:PRO:HD2	1.81	0.61
1:D:268:PRO:HB2	1:D:277:ILE:HG23	1.83	0.61
1:E:291:PHE:HB2	1:E:436:PRO:HG3	1.82	0.61
1:F:123:GLU:OE1	1:F:123:GLU:HA	2.00	0.61



	le us page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:148:PRO:HB3	1:A:252:LEU:HD23	1.83	0.61
1:E:188:ARG:NH1	1:E:260:ARG:HG2	2.15	0.61
1:F:103:ASP:HB3	1:F:104:PRO:HD3	1.83	0.60
1:E:145:ASP:OD1	1:E:242:LYS:HE2	2.01	0.60
1:E:153:PHE:HD2	1:E:195:THR:HG21	1.66	0.60
1:E:549:GLU:OE1	1:E:552:ARG:NH1	2.32	0.60
1:B:79:VAL:HG21	1:C:19:LEU:HD12	1.82	0.60
1:D:268:PRO:CB	1:D:277:ILE:HG23	2.31	0.60
1:B:79:VAL:HG12	1:C:17:MET:HE2	1.83	0.60
1:A:235:GLU:OE1	1:A:248:ARG:CD	2.49	0.60
1:C:417:TYR:HH	1:D:474:GLU:CD	2.05	0.60
1:F:474:GLU:OE1	1:F:511:ARG:NH2	2.34	0.60
1:D:41:LEU:HB2	1:E:107:PHE:HB3	1.83	0.60
1:E:166:ILE:HG22	1:E:175:LYS:HG2	1.84	0.60
1:B:335:GLN:NE2	1:B:343:ILE:O	2.35	0.60
1:F:153:PHE:HD2	1:F:195:THR:HG21	1.66	0.60
1:A:120:ALA:O	1:A:124:LEU:N	2.25	0.60
1:A:174:THR:OG1	1:A:589:TYR:OH	2.19	0.60
1:B:68:LYS:NZ	1:C:111:GLN:HG2	2.17	0.60
1:D:153:PHE:HD2	1:D:195:THR:HG21	1.67	0.59
1:F:143:LEU:HD11	1:F:147:GLN:NE2	2.11	0.59
1:B:107:PHE:HB3	1:A:41:LEU:HB2	1.83	0.59
1:B:68:LYS:HZ2	1:C:111:GLN:HG2	1.66	0.59
1:D:103:ASP:HB3	1:D:104:PRO:HD3	1.85	0.59
1:B:188:ARG:HH12	1:B:260:ARG:HG2	1.66	0.59
1:F:381:TYR:HA	1:F:385:GLU:HG3	1.84	0.59
1:E:82:VAL:HG13	1:E:89:ALA:HB3	1.83	0.59
1:F:251:LEU:HD12	1:F:251:LEU:O	2.03	0.58
1:A:142:LEU:CD1	1:A:248:ARG:HG2	2.33	0.58
1:D:79:VAL:HG21	1:E:19:LEU:HD12	1.85	0.58
1:E:87:LEU:H	1:E:87:LEU:CD1	2.11	0.58
1:E:371:THR:HG23	1:E:374:GLN:H	1.67	0.58
1:E:103:ASP:HB3	1:E:104:PRO:HD3	1.85	0.58
1:B:165:ASN:ND2	1:B:523:GLN:HE22	1.99	0.58
1:E:225:ASP:OD2	1:E:225:ASP:N	2.30	0.58
1:F:64:ASP:OD1	1:F:96:ARG:HD2	2.04	0.58
1:A:188:ARG:HH22	1:A:260:ARG:HH11	1.50	0.58
1:A:219:GLU:HG2	1:A:222:LEU:HD12	1.86	0.58
1:B:166:ILE:HG22	1:B:175:LYS:HG2	1.86	0.58
1:E:281:THR:HG21	1:E:288:VAL:HG21	1.84	0.58
1:F:189:SER:O	1:F:194:ARG:NH2	2.36	0.58



	is as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:269:ARG:O	1:D:269:ARG:HG3	2.03	0.58
1:A:149:LEU:HD12	1:A:150:PRO:HD2	1.85	0.58
1:F:353:GLU:HG2	1:A:330:ARG:NH2	2.19	0.58
1:D:76:GLU:N	1:E:71:GLU:OE1	2.35	0.58
1:E:294:THR:HG22	1:E:297:GLU:H	1.68	0.58
1:B:398:LYS:HD3	1:A:401:PRO:HG2	1.86	0.57
1:D:120:ALA:O	1:D:124:LEU:N	2.29	0.57
1:C:478:ARG:O	1:C:478:ARG:HG2	2.03	0.57
1:E:294:THR:OG1	1:E:340:THR:HB	2.04	0.57
1:F:164:ILE:HG12	1:F:539:ILE:HB	1.85	0.57
1:F:356:PRO:O	1:F:359:LEU:HD13	2.04	0.57
1:A:419:SER:N	1:A:420:PRO:HD2	2.20	0.57
1:F:427:THR:H	1:F:430:GLN:HE22	1.52	0.57
1:D:234:LYS:HA	1:D:234:LYS:HZ3	1.68	0.57
1:D:235:GLU:OE2	1:D:248:ARG:HB2	2.04	0.57
1:C:396:VAL:HG23	1:C:404:LEU:HD21	1.87	0.57
1:A:311:ALA:HB2	1:A:499:SER:CB	2.30	0.57
1:B:24:VAL:HG11	1:B:110:PRO:O	2.04	0.57
1:C:174:THR:HG21	1:C:572:GLY:N	2.19	0.57
1:A:143:LEU:HD23	1:A:149:LEU:HB2	1.86	0.57
1:C:79:VAL:HG21	1:D:19:LEU:HD12	1.86	0.57
1:E:24:VAL:HG11	1:E:110:PRO:O	2.05	0.57
1:E:525:THR:HG22	1:E:527:SER:H	1.69	0.57
1:B:371:THR:OG1	1:B:373:GLU:OE1	2.23	0.56
1:C:174:THR:CG2	1:C:572:GLY:N	2.66	0.56
1:F:111:GLN:HG2	1:E:68:LYS:HZ3	1.68	0.56
1:F:217:LYS:HG3	1:F:221:LEU:HD11	1.86	0.56
1:F:279:PRO:HD3	1:F:290:PRO:HG3	1.87	0.56
1:D:349:PHE:N	1:D:349:PHE:CD2	2.72	0.56
1:B:19:LEU:HD12	1:A:79:VAL:HG21	1.87	0.56
1:C:349:PHE:CD2	1:C:349:PHE:N	2.73	0.56
1:F:83:VAL:HG21	1:A:17:MET:SD	2.46	0.56
1:D:392:ASP:OD1	1:D:394:LYS:HE3	2.03	0.56
1:E:323:ASN:ND2	1:E:397:LEU:HG	2.20	0.56
1:F:349:PHE:HB2	1:F:352:SER:HB3	1.86	0.56
1:F:556:ARG:HB3	1:E:548:ALA:HB2	1.86	0.56
1:D:338:LYS:HE3	1:D:428:PRO:HG2	1.88	0.56
1:E:81:ASP:O	1:E:86:LEU:HD23	2.05	0.56
1:F:23:ASP:OD1	1:E:69:ARG:NE	2.37	0.56
1:F:427:THR:H	1:F:430:GLN:NE2	2.04	0.56
1:D:357:GLU:CG	1:D:358:ASN:N	2.37	0.56



	is as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:188:ARG:HH12	1:B:260:ARG:CD	2.19	0.56
1:F:235:GLU:OE1	1:F:248:ARG:HB3	2.05	0.56
1:D:223:PHE:CE1	1:D:284:ARG:HB2	2.41	0.56
1:E:263:GLN:HE21	1:E:265:LEU:HD21	1.70	0.56
1:A:396:VAL:HG22	1:A:396:VAL:O	2.03	0.56
1:D:188:ARG:NH1	1:D:260:ARG:HG2	2.20	0.56
1:F:221:LEU:HD12	1:F:221:LEU:N	2.20	0.56
1:E:62:LEU:C	1:E:62:LEU:HD23	2.26	0.56
1:A:174:THR:HG1	1:A:589:TYR:HH	1.52	0.56
1:D:174:THR:HG21	1:D:572:GLY:H	1.70	0.55
1:B:269:ARG:HA	1:B:280:GLN:HG2	1.88	0.55
1:F:78:ASP:O	1:F:82:VAL:HG23	2.06	0.55
1:D:281:THR:HG21	1:D:288:VAL:HG21	1.89	0.55
1:C:546:ASP:HB3	1:C:549:GLU:HG2	1.88	0.55
1:F:231:MET:HE3	1:F:249:TYR:CD2	2.41	0.55
1:D:453:LEU:HB3	1:D:457:ALA:HB3	1.89	0.55
1:E:142:LEU:CD1	1:E:248:ARG:HG2	2.37	0.55
1:E:414:VAL:HG22	1:E:418:LEU:HD13	1.87	0.55
1:B:51:LYS:HG2	1:B:52:PRO:HD2	1.88	0.55
1:E:143:LEU:O	1:E:143:LEU:HD13	2.07	0.55
1:B:264:LEU:HD23	1:B:447:VAL:HB	1.89	0.55
1:F:71:GLU:HB3	1:E:75:PHE:HD1	1.71	0.55
1:F:346:ASP:OD1	1:F:346:ASP:N	2.36	0.55
1:B:320:VAL:HG22	1:B:399:GLN:HG2	1.88	0.55
1:B:219:GLU:HG2	1:B:222:LEU:HD22	1.89	0.55
1:C:551:GLU:H	1:C:551:GLU:CD	2.10	0.55
1:D:76:GLU:HB2	1:E:19:LEU:HD11	1.89	0.55
1:A:473:LYS:HG3	1:A:517:ILE:HD11	1.89	0.55
1:B:223:PHE:CE1	1:B:284:ARG:HB2	2.42	0.54
1:C:57:VAL:HG13	1:C:104:PRO:HD2	1.89	0.54
1:C:315:LEU:HG	1:C:317:LEU:HD13	1.89	0.54
1:F:268:PRO:HD3	1:F:291:PHE:O	2.07	0.54
1:B:69:ARG:NE	1:C:23:ASP:OD1	2.40	0.54
1:B:155:PHE:CD1	1:B:161:GLY:HA3	2.43	0.54
1:C:149:LEU:HD22	1:C:587:VAL:HG21	1.89	0.54
1:C:79:VAL:HG12	1:D:17:MET:HE3	1.90	0.54
1:F:384:LEU:CD1	1:F:405:ARG:HE	2.20	0.54
1:C:51:LYS:HG2	1:C:52:PRO:HD2	1.90	0.54
1:A:369:LEU:HD22	1:A:375:LEU:HA	1.90	0.54
1:F:149:LEU:HD12	1:F:150:PRO:CD	2.32	0.54
1:D:401:PRO:HB2	1:E:397:LEU:HB3	1.89	0.54



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:550:ALA:HB1	1:D:563:ARG:HD2	1.90	0.54
1:E:356:PRO:HA	1:E:359:LEU:HD12	1.89	0.54
1:E:416:LYS:HE2	1:E:417:TYR:CE1	2.43	0.54
1:D:342:LEU:O	1:D:369:LEU:HD12	2.06	0.54
1:A:359:LEU:HD12	1:A:360:ASP:H	1.72	0.54
1:F:219:GLU:OE2	1:F:222:LEU:HD21	2.08	0.54
1:D:176:THR:HB	1:D:217:LYS:NZ	2.21	0.54
1:A:211:ALA:HB3	1:A:445:LEU:HD12	1.90	0.54
1:A:553:PRO:O	1:A:556:ARG:HG2	2.08	0.54
1:B:26:PRO:HG2	1:A:41:LEU:HD22	1.91	0.53
1:B:453:LEU:HB3	1:B:457:ALA:HB3	1.90	0.53
1:D:213:ILE:CD1	1:D:445:LEU:HD12	2.39	0.53
1:E:57:VAL:HA	1:E:104:PRO:HG2	1.88	0.53
1:B:219:GLU:OE1	1:B:283:GLN:HB2	2.07	0.53
1:B:353:GLU:OE2	1:B:353:GLU:N	2.42	0.53
1:C:137:ALA:O	1:C:194:ARG:NH1	2.42	0.53
1:C:163:HIS:HB3	1:C:519:LEU:O	2.08	0.53
1:D:70:HIS:CG	1:D:73:VAL:HG21	2.44	0.53
1:F:231:MET:HE3	1:F:256:ALA:HB1	1.90	0.53
1:B:70:HIS:HB3	1:B:73:VAL:HG23	1.91	0.53
1:B:155:PHE:HD1	1:B:161:GLY:HA3	1.73	0.53
1:C:525:THR:HG21	1:C:549:GLU:OE1	2.08	0.53
1:F:175:LYS:HD2	1:F:522:ALA:HB1	1.90	0.53
1:D:549:GLU:OE1	1:D:552:ARG:NH1	2.41	0.53
1:B:157:ASN:O	1:B:478:ARG:NH1	2.40	0.53
1:F:57:VAL:HG13	1:F:104:PRO:HD2	1.90	0.53
1:D:68:LYS:HA	1:D:92:SER:O	2.08	0.53
1:F:320:VAL:HG22	1:F:399:GLN:HG2	1.91	0.53
1:A:294:THR:HG22	1:A:297:GLU:HB2	1.91	0.53
1:B:311:ALA:CB	1:B:499:SER:HB3	2.18	0.53
1:C:103:ASP:HB3	1:C:104:PRO:HD3	1.90	0.53
1:C:417:TYR:OH	1:D:474:GLU:CD	2.47	0.53
1:D:226:LYS:HG3	1:D:601:VAL:HG11	1.91	0.53
1:D:416:LYS:HE2	1:D:417:TYR:CE1	2.44	0.53
1:A:550:ALA:HB1	1:A:563:ARG:HD2	1.91	0.53
1:C:434:TYR:N	1:C:434:TYR:HD1	2.07	0.53
1:F:343:ILE:HD13	1:F:368:ASN:HB2	1.90	0.53
1:D:371:THR:HG23	1:D:374:GLN:H	1.74	0.53
1:B:268:PRO:HG3	1:B:292:VAL:HG12	1.91	0.52
1:C:162:GLY:H	1:C:538:ALA:HB2	1.74	0.52
1:E:244:LEU:H	1:E:244:LEU:HD22	1.74	0.52



	io ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:323:ASN:HD21	1:A:397:LEU:HB2	1.73	0.52
1:E:406:ALA:O	1:E:410:ARG:HG3	2.08	0.52
1:E:544:ARG:NE	1:E:569:LEU:O	2.41	0.52
1:D:174:THR:CG2	1:D:572:GLY:H	2.21	0.52
1:F:57:VAL:HG22	1:F:104:PRO:HG2	1.92	0.52
1:D:166:ILE:HG22	1:D:175:LYS:HG2	1.90	0.52
1:E:277:ILE:HD11	1:E:434:TYR:CD2	2.44	0.52
1:F:510:GLU:HG3	1:F:511:ARG:HG3	1.90	0.52
1:F:153:PHE:HE1	1:F:186:ILE:HD13	1.72	0.52
1:E:143:LEU:HD12	1:E:147:GLN:O	2.09	0.52
1:B:105:GLU:OE2	1:A:570:GLN:HB2	2.10	0.52
1:F:154:ARG:NH1	1:F:159:GLU:OE1	2.42	0.52
1:A:142:LEU:HD12	1:A:248:ARG:HG2	1.92	0.52
1:D:86:LEU:N	1:D:86:LEU:CD2	2.73	0.52
1:D:176:THR:HG21	1:D:217:LYS:HZ2	1.74	0.52
1:D:296:ARG:NH1	1:D:337:GLY:O	2.40	0.52
1:E:231:MET:HE2	1:E:232:VAL:HG22	1.92	0.52
1:E:294:THR:CG2	1:E:297:GLU:H	2.23	0.52
1:E:454:SER:O	1:E:458:GLN:HG3	2.10	0.52
1:B:19:LEU:HD13	1:B:32:ALA:HB2	1.91	0.52
1:F:231:MET:HE2	1:F:249:TYR:CE2	2.45	0.52
1:E:450:ILE:HG23	1:E:458:GLN:HG2	1.92	0.52
1:B:162:GLY:H	1:B:538:ALA:HB2	1.75	0.51
1:D:149:LEU:HD21	1:D:576:VAL:HG21	1.92	0.51
1:E:320:VAL:HG22	1:E:399:GLN:HG2	1.92	0.51
1:A:70:HIS:HB3	1:A:73:VAL:HG23	1.91	0.51
1:F:79:VAL:HG21	1:A:19:LEU:HD12	1.92	0.51
1:F:142:LEU:HD11	1:F:248:ARG:HG2	1.91	0.51
1:E:143:LEU:N	1:E:143:LEU:CD1	2.73	0.51
1:D:234:LYS:NZ	1:D:234:LYS:CA	2.72	0.51
1:D:454:SER:O	1:D:458:GLN:HG3	2.11	0.51
1:B:282:ASP:OD1	1:B:283:GLN:N	2.41	0.51
1:C:257:GLU:HB2	1:C:258:PRO:HD2	1.93	0.51
1:F:261:ASP:HB2	1:F:444:GLN:H	1.74	0.51
1:F:269:ARG:N	1:F:278:VAL:O	2.42	0.51
1:F:217:LYS:HG3	1:F:221:LEU:CD1	2.40	0.51
1:E:33:VAL:HG11	1:E:93:TYR:CE2	2.45	0.51
1:C:149:LEU:HD12	1:C:150:PRO:HD2	1.92	0.51
1:F:231:MET:CE	1:F:256:ALA:HB1	2.41	0.51
1:A:291:PHE:HB2	1:A:436:PRO:HG3	1.92	0.51
1:B:188:ARG:NH1	1:B:260:ARG:CG	2.70	0.51



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:219:GLU:OE1	1:F:219:GLU:HA	2.11	0.51
1:E:453:LEU:HB3	1:E:457:ALA:HB3	1.93	0.51
1:B:412:ARG:O	1:B:415:GLN:HG2	2.11	0.51
1:D:79:VAL:O	1:D:83:VAL:HG23	2.11	0.51
1:E:307:VAL:HG13	1:E:414:VAL:HG11	1.92	0.51
1:D:142:LEU:CD1	1:D:248:ARG:HG2	2.41	0.51
1:E:33:VAL:CB	1:E:93:TYR:CD2	2.93	0.51
1:E:73:VAL:HG22	1:E:82:VAL:HG21	1.92	0.51
1:E:88:PRO:N	1:E:88:PRO:C	2.59	0.51
1:E:155:PHE:CD1	1:E:161:GLY:HA3	2.46	0.51
1:A:128:LEU:HD13	1:A:150:PRO:HD2	1.93	0.51
1:B:343:ILE:HG12	1:B:368:ASN:HB2	1.92	0.50
1:C:223:PHE:O	1:C:595:ALA:HB3	2.10	0.50
1:F:194:ARG:O	1:F:197:GLN:HG3	2.11	0.50
1:D:319:PHE:O	1:D:323:ASN:HB2	2.10	0.50
1:E:45:VAL:HG21	1:E:97:VAL:HG21	1.93	0.50
1:B:86:LEU:N	1:B:86:LEU:CD1	2.73	0.50
1:B:560:GLN:HA	1:B:563:ARG:HG3	1.92	0.50
1:E:550:ALA:HB1	1:E:563:ARG:HD2	1.93	0.50
1:C:76:GLU:HA	1:D:21:THR:HG21	1.93	0.50
1:C:189:SER:HB2	1:C:191:VAL:HG12	1.93	0.50
1:D:156:ILE:HD13	1:D:164:ILE:HD11	1.93	0.50
1:D:383:LEU:HD22	1:D:404:LEU:HD22	1.93	0.50
1:E:88:PRO:O	1:E:88:PRO:HG2	2.11	0.50
1:E:155:PHE:CD1	1:E:579:PRO:HG2	2.46	0.50
1:E:566:ALA:HA	1:E:569:LEU:HD13	1.93	0.50
1:D:412:ARG:O	1:D:415:GLN:HG2	2.11	0.50
1:D:414:VAL:HG22	1:D:418:LEU:HD13	1.93	0.50
1:A:174:THR:CG2	1:A:572:GLY:H	2.25	0.50
1:B:163:HIS:CD2	1:B:163:HIS:N	2.79	0.50
1:B:216:VAL:O	1:B:216:VAL:HG22	2.11	0.50
1:C:248:ARG:HB3	1:C:590:PRO:HG3	1.93	0.50
1:C:434:TYR:N	1:C:434:TYR:CD1	2.79	0.50
1:A:324:ILE:CD1	1:A:324:ILE:N	2.74	0.50
1:A:371:THR:HG22	1:A:374:GLN:HG3	1.94	0.50
1:B:473:LYS:NZ	1:B:480:ASP:O	2.33	0.50
1:F:384:LEU:N	1:F:384:LEU:HD22	2.27	0.50
1:F:41:LEU:HD22	1:A:26:PRO:HG2	1.94	0.49
1:F:267:PRO:HG2	1:F:280:GLN:HB3	1.93	0.49
1:F:398:LYS:HD3	1:E:401:PRO:HG2	1.94	0.49
1:A:174:THR:HG21	1:A:572:GLY:H	1.77	0.49



	1	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:386:GLU:HG3	1:F:387:ARG:HG3	1.93	0.49
1:F:525:THR:HG22	1:F:527:SER:H	1.77	0.49
1:F:223:PHE:CZ	1:F:284:ARG:HB2	2.47	0.49
1:E:423:ARG:HG3	1:E:425:ASP:H	1.77	0.49
1:B:473:LYS:NZ	1:B:478:ARG:O	2.44	0.49
1:D:396:VAL:HB	1:D:404:LEU:HD11	1.95	0.49
1:C:64:ASP:OD1	1:C:96:ARG:HD2	2.13	0.49
1:F:157:ASN:O	1:F:478:ARG:NH1	2.45	0.49
1:F:473:LYS:HG3	1:F:517:ILE:HD11	1.95	0.49
1:D:214:PHE:HB3	1:D:450:ILE:HD12	1.95	0.49
1:D:566:ALA:HA	1:D:569:LEU:HD13	1.93	0.49
1:E:45:VAL:HG21	1:E:97:VAL:CG2	2.42	0.49
1:B:269:ARG:HG3	1:B:270:ALA:H	1.78	0.49
1:F:17:MET:HE3	1:E:83:VAL:HG21	1.91	0.49
1:F:57:VAL:HA	1:F:104:PRO:HG2	1.95	0.49
1:F:215:ASN:HB3	1:F:449:ASP:HA	1.95	0.49
1:D:155:PHE:CD1	1:D:579:PRO:HG2	2.47	0.49
1:D:174:THR:OG1	1:D:589:TYR:OH	2.25	0.49
1:D:295:ILE:HG12	1:D:422:ILE:HG22	1.94	0.49
1:A:320:VAL:HG22	1:A:399:GLN:HG2	1.94	0.49
1:B:530:GLU:OE2	1:B:532:ARG:HD3	2.13	0.49
1:C:352:SER:O	1:C:354:THR:HG23	2.13	0.49
1:C:566:ALA:HA	1:C:569:LEU:HD13	1.94	0.49
1:F:124:LEU:CD2	1:F:147:GLN:CG	2.74	0.49
1:F:368:ASN:OD1	1:F:370:GLN:HG3	2.13	0.49
1:D:244:LEU:H	1:D:244:LEU:HD22	1.78	0.49
1:B:19:LEU:CD1	1:B:32:ALA:HB2	2.43	0.48
1:B:188:ARG:HH12	1:B:260:ARG:CG	2.26	0.48
1:A:196:ALA:HB2	1:A:207:ALA:CB	2.43	0.48
1:B:349:PHE:N	1:B:349:PHE:CD2	2.80	0.48
1:A:189:SER:HB3	1:A:254:LEU:HD21	1.96	0.48
1:A:427:THR:HB	1:A:428:PRO:HD2	1.94	0.48
1:C:315:LEU:HD12	1:C:316:ASN:H	1.77	0.48
1:E:382:LYS:NZ	1:E:386:GLU:OE1	2.37	0.48
1:B:269:ARG:HB2	1:B:278:VAL:O	2.13	0.48
1:D:423:ARG:HG3	1:D:425:ASP:H	1.78	0.48
1:A:279:PRO:HG3	1:A:290:PRO:HD3	1.96	0.48
1:C:553:PRO:HA	1:C:556:ARG:HG2	1.95	0.48
1:F:40:GLY:N	1:F:43:ASP:OD2	2.42	0.48
1:F:546:ASP:HB3	1:F:549:GLU:HG2	1.96	0.48
1:A:163:HIS:CD2	1:A:163:HIS:N	2.80	0.48



	1 · · · · · · · · · · · · · · · · · · ·	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:23:ASP:OD1	1:B:23:ASP:N	2.47	0.48
1:F:213:ILE:HG12	1:F:485:VAL:HB	1.94	0.48
1:F:277:ILE:H	1:F:277:ILE:HD12	1.79	0.48
1:F:566:ALA:HA	1:F:569:LEU:HD13	1.94	0.48
1:F:266:ALA:HB1	1:F:267:PRO:HD2	1.95	0.48
1:D:548:ALA:HB2	1:E:556:ARG:HB2	1.95	0.48
1:E:215:ASN:HA	1:E:221:LEU:HD23	1.96	0.48
1:A:15:ILE:HG12	1:A:117:ARG:HA	1.96	0.48
1:A:490:ASN:OD1	1:A:490:ASN:N	2.47	0.48
1:C:595:ALA:HB2	1:C:601:VAL:HG23	1.80	0.48
1:F:51:LYS:HG2	1:F:52:PRO:HD2	1.95	0.48
1:A:158:GLY:CA	1:A:161:GLY:O	2.57	0.48
1:B:149:LEU:HD13	1:B:585:VAL:HG21	1.95	0.47
1:F:383:LEU:CD1	1:F:404:LEU:HD22	2.31	0.47
1:E:268:PRO:HG3	1:E:292:VAL:HG12	1.95	0.47
1:A:167:SER:OG	1:A:555:TYR:OH	2.14	0.47
1:A:263:GLN:HB2	1:A:443:ILE:HD12	1.95	0.47
1:B:210:ARG:NH1	1:B:443:ILE:O	2.46	0.47
1:F:430:GLN:HB2	1:F:434:TYR:CE2	2.48	0.47
1:D:344:VAL:HG22	1:D:369:LEU:HD11	1.96	0.47
1:E:215:ASN:HB3	1:E:449:ASP:HA	1.95	0.47
1:D:86:LEU:N	1:D:86:LEU:HD22	2.29	0.47
1:D:234:LYS:HZ3	1:D:234:LYS:CA	2.26	0.47
1:B:103:ASP:HB3	1:B:104:PRO:HD3	1.95	0.47
1:C:76:GLU:OE2	1:D:94:ALA:HB2	2.13	0.47
1:F:580:ASP:HA	1:E:172:VAL:HG11	1.97	0.47
1:A:277:ILE:HD13	1:A:292:VAL:HG11	1.96	0.47
1:A:213:ILE:HG23	1:A:447:VAL:HG22	1.97	0.47
1:B:82:VAL:HG13	1:B:89:ALA:HB3	1.97	0.47
1:B:210:ARG:NH2	1:B:440:ARG:O	2.43	0.47
1:F:142:LEU:CD1	1:F:248:ARG:HG2	2.45	0.47
1:D:392:ASP:O	1:D:396:VAL:HG13	2.13	0.47
1:D:502:LYS:HE3	1:D:530:GLU:HB2	1.97	0.47
1:E:224:LEU:HD12	1:E:447:VAL:HG21	1.96	0.47
1:E:386:GLU:HG2	1:E:387:ARG:HG3	1.96	0.47
1:A:249:TYR:CE2	1:A:590:PRO:HB2	2.49	0.47
1:C:595:ALA:CB	1:C:601:VAL:HG22	2.36	0.47
1:F:17:MET:HE1	1:E:83:VAL:CG2	2.42	0.47
1:F:353:GLU:HG2	1:A:330:ARG:HH21	1.79	0.47
1:D:294:THR:OG1	1:D:340:THR:HB	2.15	0.47
1:D:490:ASN:OD1	1:D:490:ASN:N	2.48	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:515:LEU:HD12	1:D:515:LEU:HA	1.78	0.47
1:D:574:MET:O	1:D:587:VAL:HG12	2.14	0.47
1:B:71:GLU:HG2	1:B:92:SER:HB3	1.95	0.47
1:B:556:ARG:HB2	1:A:548:ALA:HB2	1.96	0.47
1:F:405:ARG:CZ	1:A:397:LEU:HD11	2.45	0.47
1:F:426:LEU:HB3	1:F:430:GLN:HE21	1.79	0.47
1:E:128:LEU:HD13	1:E:150:PRO:HD2	1.97	0.47
1:E:184:HIS:CE1	1:E:188:ARG:HG3	2.50	0.47
1:B:163:HIS:HB3	1:B:519:LEU:O	2.15	0.47
1:B:235:GLU:C	1:B:239:VAL:HG23	2.27	0.47
1:F:532:ARG:O	1:F:536:ASN:ND2	2.39	0.47
1:D:44:LEU:HD11	1:D:128:LEU:HD21	1.97	0.47
1:D:70:HIS:HB3	1:D:73:VAL:HG21	1.96	0.47
1:F:155:PHE:CD1	1:F:579:PRO:HG2	2.50	0.47
1:D:371:THR:HG22	1:D:374:GLN:CD	2.35	0.47
1:A:111:GLN:HG2	1:A:112:PRO:HD2	1.97	0.47
1:A:315:LEU:HB2	1:A:317:LEU:HD13	1.97	0.47
1:C:66:VAL:HG13	1:D:109:PRO:HD3	1.98	0.46
1:F:360:ASP:O	1:F:368:ASN:HB3	2.15	0.46
1:D:80:GLU:HA	1:E:17:MET:HE1	1.96	0.46
1:E:281:THR:CG2	1:E:288:VAL:HG21	2.45	0.46
1:E:373:GLU:OE1	1:E:373:GLU:N	2.45	0.46
1:A:196:ALA:HB2	1:A:207:ALA:HB1	1.97	0.46
1:C:174:THR:HG22	1:C:572:GLY:H	1.78	0.46
1:F:143:LEU:CD1	1:F:147:GLN:HE21	2.15	0.46
1:A:135:GLU:OE2	1:A:154:ARG:NH2	2.48	0.46
1:A:470:PHE:C	1:A:470:PHE:CD2	2.88	0.46
1:A:472:TYR:CZ	1:A:476:VAL:HG21	2.50	0.46
1:D:393:PRO:O	1:D:397:LEU:HD23	2.15	0.46
1:A:231:MET:HE1	1:A:235:GLU:HG2	1.98	0.46
1:E:248:ARG:HB3	1:E:590:PRO:HB3	1.97	0.46
1:C:155:PHE:HA	1:C:161:GLY:CA	2.44	0.46
1:C:157:ASN:O	1:C:478:ARG:NH1	2.46	0.46
1:F:149:LEU:HD21	1:F:576:VAL:HG21	1.97	0.46
1:D:213:ILE:HD11	1:D:445:LEU:CD1	2.40	0.46
1:D:270:ALA:HA	1:D:420:PRO:HB3	1.97	0.46
1:A:153:PHE:HD2	1:A:195:THR:HG21	1.79	0.46
1:F:223:PHE:CE1	1:F:284:ARG:HB2	2.51	0.46
1:A:68:LYS:HA	1:A:92:SER:O	2.15	0.46
1:B:175:LYS:HD2	1:B:522:ALA:HB1	1.97	0.46
1:F:156:ILE:HD13	1:F:164:ILE:HD11	1.97	0.46



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:485:VAL:HG22	1:F:520:ILE:HB	1.97	0.46
1:D:79:VAL:HG21	1:E:19:LEU:CD1	2.45	0.46
1:C:304:LEU:HB3	1:C:305:PRO:HD3	1.98	0.46
1:F:163:HIS:HB3	1:F:519:LEU:O	2.16	0.46
1:F:530:GLU:HG3	1:F:532:ARG:H	1.79	0.46
1:F:570:GLN:HG3	1:F:571:PRO:HD2	1.96	0.46
1:F:142:LEU:CD1	1:F:248:ARG:CG	2.94	0.46
1:F:210:ARG:NH1	1:F:444:GLN:HA	2.31	0.46
1:A:380:GLU:HG2	1:A:384:LEU:HD12	1.97	0.46
1:A:487:ASP:OD1	1:A:488:GLU:N	2.45	0.46
1:B:566:ALA:HA	1:B:569:LEU:HD13	1.98	0.46
1:F:142:LEU:HD11	1:F:248:ARG:CG	2.46	0.46
1:F:548:ALA:O	1:F:551:GLU:HG2	2.16	0.46
1:E:295:ILE:HG13	1:E:424:GLY:N	2.31	0.46
1:E:301:ARG:HH12	1:E:435:ARG:HH21	1.64	0.46
1:A:481:THR:HG21	1:A:483:PHE:CZ	2.51	0.46
1:A:566:ALA:HA	1:A:569:LEU:HD13	1.98	0.46
1:C:221:LEU:HD12	1:C:221:LEU:HA	1.69	0.45
1:F:320:VAL:HG21	1:F:403:THR:HG22	1.98	0.45
1:F:598:ARG:O	1:F:601:VAL:CG2	2.65	0.45
1:E:26:PRO:HG2	1:E:107:PHE:O	2.16	0.45
1:E:392:ASP:OD1	1:E:394:LYS:HE3	2.16	0.45
1:B:108:ILE:HG13	1:B:108:ILE:O	2.15	0.45
1:B:277:ILE:HD11	1:B:426:LEU:HD21	1.97	0.45
1:B:570:GLN:HG3	1:B:571:PRO:HD2	1.97	0.45
1:C:80:GLU:HA	1:D:17:MET:HE1	1.98	0.45
1:E:578:GLN:HG3	1:E:581:VAL:HG12	1.98	0.45
1:F:182:LEU:O	1:F:186:ILE:HG13	2.16	0.45
1:D:294:THR:CG2	1:D:297:GLU:H	2.27	0.45
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.73	0.45
1:E:301:ARG:NH1	1:E:435:ARG:HH21	2.13	0.45
1:B:107:PHE:HB2	1:A:41:LEU:CB	2.47	0.45
1:C:111:GLN:HE21	1:C:111:GLN:HB3	1.53	0.45
1:C:206:THR:N	1:C:480:ASP:HA	2.31	0.45
1:F:327:LYS:O	1:F:331:LEU:HB2	2.16	0.45
1:E:145:ASP:OD1	1:E:242:LYS:CG	2.60	0.45
1:C:162:GLY:HA2	1:C:513:ARG:HG2	1.99	0.45
1:C:304:LEU:N	1:C:305:PRO:CD	2.80	0.45
1:C:392:ASP:OD1	1:C:393:PRO:HD2	2.16	0.45
1:A:79:VAL:O	1:A:83:VAL:HG23	2.16	0.45
1:A:298:PHE:C	1:A:298:PHE:CD2	2.90	0.45



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:60:TYR:HE2	1:C:103:ASP:HB2	1.82	0.45
1:F:353:GLU:CG	1:A:330:ARG:HH21	2.30	0.45
1:F:353:GLU:OE1	1:F:353:GLU:HA	2.16	0.45
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.80	0.45
1:B:294:THR:HA	1:B:423:ARG:O	2.17	0.45
1:C:371:THR:HG23	1:C:374:GLN:H	1.82	0.45
1:C:396:VAL:O	1:C:396:VAL:CG1	2.61	0.45
1:C:472:TYR:CZ	1:C:476:VAL:HG21	2.52	0.45
1:D:277:ILE:HD13	1:D:292:VAL:HG11	1.98	0.45
1:E:281:THR:HB	1:E:284:ARG:O	2.17	0.45
1:D:168:GLY:O	1:D:524:GLN:HA	2.17	0.45
1:D:478:ARG:HE	1:D:478:ARG:HB2	1.46	0.45
1:F:23:ASP:CG	1:E:69:ARG:NH2	2.56	0.45
1:F:146:GLY:HA2	1:F:251:LEU:HD21	1.99	0.45
1:F:348:GLN:H	1:F:348:GLN:HG2	1.69	0.45
1:D:165:ASN:OD1	1:D:523:GLN:NE2	2.39	0.45
1:E:342:LEU:O	1:E:369:LEU:HD12	2.17	0.45
1:A:120:ALA:H	1:A:123:GLU:HB2	1.82	0.45
1:B:348:GLN:HG2	1:B:381:TYR:OH	2.18	0.44
1:F:47:VAL:HG12	1:F:59:PHE:HB2	1.99	0.44
1:F:165:ASN:OD1	1:F:523:GLN:NE2	2.31	0.44
1:E:473:LYS:HG3	1:E:517:ILE:HD11	1.99	0.44
1:B:237:LYS:HE2	1:B:237:LYS:HB2	1.65	0.44
1:F:487:ASP:OD1	1:F:488:GLU:N	2.48	0.44
1:F:221:LEU:N	1:F:221:LEU:CD1	2.79	0.44
1:D:158:GLY:HA2	1:D:161:GLY:O	2.17	0.44
1:D:331:LEU:HD21	1:D:344:VAL:HG12	1.99	0.44
1:E:176:THR:HG21	1:E:217:LYS:HE3	2.00	0.44
1:B:394:LYS:HB2	1:B:394:LYS:HE3	1.71	0.44
1:C:349:PHE:HB3	1:C:352:SER:HB2	1.98	0.44
1:F:453:LEU:HB3	1:F:457:ALA:HB3	1.98	0.44
1:D:174:THR:HG21	1:D:572:GLY:CA	2.47	0.44
1:D:331:LEU:HD12	1:D:331:LEU:HA	1.67	0.44
1:A:231:MET:HE2	1:A:231:MET:C	2.36	0.44
1:F:472:TYR:O	1:F:476:VAL:HG12	2.18	0.44
1:D:265:LEU:HA	1:D:289:THR:O	2.18	0.44
1:B:155:PHE:HA	1:B:161:GLY:HA3	2.00	0.44
1:B:546:ASP:HB3	1:B:549:GLU:HG2	1.99	0.44
1:C:131:ASP:OD1	1:C:131:ASP:N	2.50	0.44
1:D:304:LEU:HD22	1:D:324:ILE:HG22	2.00	0.44
1:E:57:VAL:CA	1:E:104:PRO:CG	2.82	0.44



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:277:ILE:HD12	1:A:434:TYR:CD2	2.52	0.44
1:C:405:ARG:HG3	1:C:405:ARG:HH11	1.83	0.44
1:D:64:ASP:OD1	1:D:96:ARG:HD2	2.17	0.44
1:E:31:PHE:CE2	1:E:95:ALA:HB3	2.52	0.44
1:A:310:ASP:O	1:A:314:SER:OG	2.36	0.44
1:F:379:LEU:HD23	1:F:395:TRP:HZ3	1.82	0.44
1:D:70:HIS:CB	1:D:73:VAL:HG21	2.48	0.44
1:E:23:ASP:OD1	1:E:23:ASP:N	2.50	0.44
1:E:515:LEU:HA	1:E:515:LEU:HD12	1.67	0.44
1:A:288:VAL:O	1:A:288:VAL:HG13	2.18	0.44
1:B:469:VAL:O	1:B:473:LYS:HG2	2.18	0.43
1:C:139:PRO:HB3	1:C:252:LEU:HD22	2.00	0.43
1:C:372:PHE:CE2	1:C:376:ILE:HD11	2.53	0.43
1:D:570:GLN:HB2	1:E:105:GLU:OE2	2.18	0.43
1:D:320:VAL:HG22	1:D:399:GLN:HG2	2.00	0.43
1:D:386:GLU:HG2	1:D:387:ARG:HG3	2.00	0.43
1:A:213:ILE:CG2	1:A:447:VAL:HG22	2.48	0.43
1:B:423:ARG:NH1	1:B:425:ASP:OD1	2.51	0.43
1:C:490:ASN:OD1	1:C:490:ASN:N	2.47	0.43
1:F:231:MET:HE2	1:F:249:TYR:CD2	2.52	0.43
1:F:396:VAL:HB	1:F:404:LEU:HD11	1.99	0.43
1:E:87:LEU:HB3	1:E:88:PRO:HD2	1.99	0.43
1:A:143:LEU:C	1:A:143:LEU:CD1	2.85	0.43
1:A:235:GLU:OE2	1:A:591:PHE:HD2	2.01	0.43
1:B:247:ASP:OD1	1:B:248:ARG:N	2.51	0.43
1:C:41:LEU:O	1:C:63:VAL:O	2.36	0.43
1:C:155:PHE:CD1	1:C:579:PRO:HG2	2.53	0.43
1:C:168:GLY:N	1:C:175:LYS:HD3	2.34	0.43
1:C:223:PHE:HB3	1:C:601:VAL:HG21	2.01	0.43
1:C:244:LEU:HA	1:C:244:LEU:HD22	1.63	0.43
1:A:163:HIS:HB3	1:A:519:LEU:O	2.18	0.43
1:C:76:GLU:HG3	1:D:19:LEU:HD11	2.01	0.43
1:A:168:GLY:O	1:A:524:GLN:HA	2.18	0.43
1:B:361:PHE:CE2	1:B:367:VAL:HG22	2.54	0.43
1:D:450:ILE:HG23	1:D:458:GLN:HG2	2.00	0.43
1:C:545:LEU:HD23	1:C:545:LEU:HA	1.79	0.43
1:F:145:ASP:HB2	1:F:147:GLN:NE2	2.34	0.43
1:D:532:ARG:O	1:D:536:ASN:ND2	2.41	0.43
1:E:42:ASP:CG	1:E:565:ARG:NH1	2.71	0.43
1:A:23:ASP:OD1	1:A:23:ASP:N	2.51	0.43
1:B:104:PRO:HD2	1:B:104:PRO:O	2.19	0.43



	i agein	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:26:PRO:HG2	1:E:41:LEU:HD22	2.01	0.43
1:D:174:THR:HG21	1:D:572:GLY:HA2	2.00	0.43
1:D:174:THR:HG21	1:D:572:GLY:N	2.31	0.43
1:A:255:PRO:HB2	1:A:257:GLU:HG2	1.99	0.43
1:B:107:PHE:CB	1:A:41:LEU:CB	2.97	0.43
1:B:168:GLY:O	1:B:524:GLN:HA	2.19	0.43
1:F:119:ALA:HB1	1:F:124:LEU:HA	2.01	0.43
1:E:100:THR:HB	1:E:582:PRO:HG2	2.01	0.43
1:A:174:THR:HG21	1:A:572:GLY:HA2	2.00	0.43
1:B:188:ARG:NH1	1:B:260:ARG:CD	2.81	0.43
1:C:23:ASP:OD1	1:C:23:ASP:N	2.52	0.43
1:F:405:ARG:NH1	1:A:397:LEU:HD11	2.33	0.43
1:D:84:ALA:HB3	1:D:86:LEU:HD23	2.01	0.43
1:D:235:GLU:O	1:D:238:VAL:N	2.50	0.43
1:B:355:PRO:HA	1:B:356:PRO:HD3	1.91	0.42
1:F:146:GLY:CA	1:F:251:LEU:HD21	2.48	0.42
1:F:156:ILE:O	1:F:518:ILE:HG12	2.19	0.42
1:F:427:THR:OG1	1:F:430:GLN:OE1	2.37	0.42
1:A:294:THR:HG22	1:A:297:GLU:HG2	2.00	0.42
1:A:331:LEU:HD21	1:A:344:VAL:HG12	2.01	0.42
1:A:383:LEU:HA	1:A:383:LEU:HD12	1.81	0.42
1:F:573:THR:CG2	1:F:586:LEU:HD11	2.49	0.42
1:D:184:HIS:CE1	1:D:188:ARG:HG3	2.54	0.42
1:E:277:ILE:HG22	1:E:423:ARG:HH22	1.83	0.42
1:E:311:ALA:HB2	1:E:499:SER:CB	2.33	0.42
1:E:427:THR:HB	1:E:428:PRO:HD2	2.01	0.42
1:E:546:ASP:HB3	1:E:549:GLU:HG2	2.01	0.42
1:F:52:PRO:HD2	1:E:38:SER:HB3	2.01	0.42
1:F:188:ARG:HB3	1:F:255:PRO:HD2	2.01	0.42
1:A:585:VAL:O	1:A:587:VAL:HG23	2.18	0.42
1:B:346:ASP:OD1	1:B:346:ASP:N	2.52	0.42
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.75	0.42
1:F:294:THR:HA	1:F:423:ARG:O	2.19	0.42
1:F:556:ARG:HB3	1:E:548:ALA:CB	2.50	0.42
1:F:560:GLN:O	1:F:563:ARG:HG3	2.19	0.42
1:E:135:GLU:OE2	1:E:154:ARG:NH2	2.52	0.42
1:A:281:THR:CG2	1:A:288:VAL:HG21	2.44	0.42
1:B:470:PHE:CZ	1:B:507:ASP:HB3	2.55	0.42
1:C:247:ASP:OD1	1:C:247:ASP:N	2.48	0.42
1:F:239:VAL:O	1:F:243:GLY:N	2.52	0.42
1:F:415:GLN:HG3	1:F:416:LYS:N	2.35	0.42



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:474:GLU:HG2	1:D:515:LEU:HD21	2.00	0.42
1:A:174:THR:HG21	1:A:572:GLY:CA	2.50	0.42
1:A:188:ARG:NH1	1:A:257:GLU:OE1	2.53	0.42
1:C:151:LEU:HD23	1:C:151:LEU:HA	1.82	0.42
1:C:280:GLN:HG2	1:C:280:GLN:O	2.20	0.42
1:E:210:ARG:NH1	1:E:439:LEU:HA	2.34	0.42
1:A:64:ASP:OD1	1:A:96:ARG:HD2	2.19	0.42
1:A:419:SER:N	1:A:420:PRO:CD	2.83	0.42
1:B:165:ASN:HD21	1:B:523:GLN:NE2	2.07	0.42
1:F:381:TYR:HA	1:F:385:GLU:CG	2.49	0.42
1:D:247:ASP:OD1	1:D:247:ASP:N	2.53	0.42
1:E:191:VAL:HG23	1:E:194:ARG:NH2	2.34	0.42
1:E:550:ALA:HB1	1:E:563:ARG:CD	2.50	0.42
1:A:544:ARG:NE	1:A:569:LEU:O	2.52	0.42
1:B:387:ARG:O	1:B:390:GLU:HG2	2.18	0.42
1:B:515:LEU:HD12	1:B:515:LEU:HA	1.85	0.42
1:C:277:ILE:HB	1:C:434:TYR:HE2	1.85	0.42
1:D:41:LEU:HB2	1:E:107:PHE:CB	2.48	0.42
1:E:354:THR:HA	1:E:355:PRO:HD3	1.85	0.42
1:B:188:ARG:NH1	1:B:260:ARG:HD3	2.27	0.42
1:C:320:VAL:HG22	1:C:399:GLN:HG2	2.02	0.42
1:C:453:LEU:HB3	1:C:457:ALA:HB3	2.02	0.42
1:F:71:GLU:HB3	1:E:75:PHE:CE1	2.55	0.42
1:F:381:TYR:CE2	1:F:386:GLU:OE2	2.73	0.42
1:D:231:MET:CE	1:D:256:ALA:HB1	2.49	0.42
1:D:315:LEU:HD21	1:E:319:PHE:HE1	1.85	0.42
1:A:294:THR:HG22	1:A:297:GLU:CB	2.50	0.42
1:B:24:VAL:O	1:A:67:ARG:HA	2.20	0.42
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.92	0.42
1:B:277:ILE:HD11	1:B:426:LEU:CD2	2.49	0.42
1:F:23:ASP:OD1	1:E:69:ARG:NH2	2.53	0.42
1:E:57:VAL:CB	1:E:104:PRO:HG2	2.50	0.42
1:E:142:LEU:HD12	1:E:248:ARG:HG2	2.01	0.42
1:A:371:THR:HG22	1:A:374:GLN:CG	2.50	0.42
1:B:45:VAL:HG21	1:B:97:VAL:CG2	2.49	0.41
1:B:327:LYS:HE3	1:B:394:LYS:O	2.20	0.41
1:B:530:GLU:HG3	1:B:532:ARG:H	1.84	0.41
1:C:262:VAL:HG22	1:C:445:LEU:HB3	2.00	0.41
1:C:473:LYS:CG	1:C:517:ILE:HD11	2.50	0.41
1:F:67:ARG:HA	1:A:24:VAL:O	2.19	0.41
1:D:224:LEU:HD12	1:D:447:VAL:HG21	2.01	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:145:ASP:OD2	1:E:145:ASP:N	2.53	0.41
1:E:223:PHE:CE1	1:E:284:ARG:HB2	2.55	0.41
1:B:327:LYS:NZ	1:B:394:LYS:HB3	2.35	0.41
1:F:24:VAL:HG12	1:F:110:PRO:HD2	2.03	0.41
1:A:481:THR:HG22	1:A:481:THR:O	2.19	0.41
1:C:473:LYS:HG3	1:C:517:ILE:HD11	2.01	0.41
1:E:15:ILE:HG12	1:E:117:ARG:HA	2.02	0.41
1:D:76:GLU:CB	1:E:21:THR:HG21	2.47	0.41
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.84	0.41
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.79	0.41
1:F:68:LYS:HA	1:F:92:SER:O	2.21	0.41
1:F:269:ARG:HB2	1:F:278:VAL:HB	2.01	0.41
1:D:176:THR:HB	1:D:217:LYS:HZ3	1.84	0.41
1:D:497:GLY:O	1:D:502:LYS:NZ	2.37	0.41
1:D:550:ALA:HB1	1:D:563:ARG:CD	2.49	0.41
1:E:295:ILE:HG12	1:E:422:ILE:HG22	2.01	0.41
1:E:382:LYS:HE3	1:E:382:LYS:HB3	1.82	0.41
1:E:428:PRO:HG2	1:E:429:GLU:OE2	2.21	0.41
1:C:495:ARG:HA	1:C:530:GLU:HA	2.02	0.41
1:F:474:GLU:OE2	1:E:417:TYR:OH	2.38	0.41
1:D:128:LEU:HD13	1:D:150:PRO:HD2	2.03	0.41
1:D:142:LEU:HD11	1:D:248:ARG:HG2	2.01	0.41
1:E:187:PHE:HD1	1:E:192:MET:CE	2.33	0.41
1:A:215:ASN:HD21	1:A:219:GLU:HA	1.86	0.41
1:C:143:LEU:HB2	1:C:147:GLN:O	2.21	0.41
1:C:502:LYS:HE3	1:C:530:GLU:HB2	2.02	0.41
1:F:71:GLU:HA	1:F:71:GLU:OE2	2.21	0.41
1:F:323:ASN:O	1:F:327:LYS:HG2	2.20	0.41
1:D:149:LEU:HD21	1:D:576:VAL:CG2	2.51	0.41
1:D:354:THR:HA	1:D:355:PRO:HD2	1.83	0.41
1:A:17:MET:HE3	1:A:17:MET:HB2	1.87	0.41
1:C:19:LEU:CD1	1:C:32:ALA:HB2	2.49	0.41
1:C:310:ASP:HB3	1:C:410:ARG:NH2	2.35	0.41
1:C:405:ARG:HG3	1:C:405:ARG:NH1	2.35	0.41
1:F:547:LEU:HD11	1:A:582:PRO:O	2.21	0.41
1:A:246:ALA:HB3	1:A:251:LEU:CD1	2.51	0.41
1:B:157:ASN:O	1:B:478:ARG:NH2	2.50	0.41
1:B:220:ASP:N	1:B:220:ASP:OD1	2.54	0.41
1:F:476:VAL:HG21	1:F:479:GLN:HE21	1.86	0.41
1:D:187:PHE:HB3	1:D:188:ARG:NH2	2.36	0.41
1:A:227:PRO:HG2	1:A:602:ASP:HB3	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:546:ASP:HB3	1:A:549:GLU:HG2	2.03	0.41
1:E:265:LEU:HA	1:E:289:THR:O	2.21	0.41
1:A:131:ASP:OD1	1:A:131:ASP:N	2.54	0.41
1.B.142.LEU.HG	1·B·252·LEU·HD11	2.03	0.40
1:B:581:VAL:HA	1:B:582:PRO:HD3	1.86	0.40
1:C:596:THR:OG1	1:C:600:GLU:OE1	2.33	0.40
1:F:57:VAL:HA	1:F:104:PRO:CG	2.51	0.40
1:F:164:ILE:HD12	1:F:520:ILE:HD12	2.03	0.40
1:F:381:TYR:CZ	1:F:386:GLU:OE2	2.74	0.40
1:A:78:ASP:O	1:A:82:VAL:HG23	2.21	0.40
1:A:175:LYS:HE3	1:A:175:LYS:HB2	1.79	0.40
1:A:292:VAL:HG21	1:A:426:LEU:CD1	2.51	0.40
1:A:299:CYS:SG	1:A:342:LEU:HD22	2.61	0.40
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.96	0.40
1:B:386:GLU:HG3	1:B:387:ARG:HG3	2.04	0.40
1:B:490:ASN:OD1	1:B:490:ASN:N	2.54	0.40
1:D:348:GLN:HG2	1:D:381:TYR:OH	2.21	0.40
1:E:66:VAL:O	1:E:66:VAL:HG13	2.19	0.40
1:E:369:LEU:HD12	1:E:369:LEU:H	1.86	0.40
1:B:45:VAL:HG21	1:B:97:VAL:HG21	2.03	0.40
1:B:61:GLY:HA3	1:B:97:VAL:HG13	2.03	0.40
1:C:277:ILE:HD12	1:C:434:TYR:CE2	2.56	0.40
1:F:26:PRO:HD3	1:E:66:VAL:HG13	2.04	0.40
1:F:47:VAL:HG23	1:F:115:HIS:O	2.22	0.40
1:F:278:VAL:HG12	1:F:279:PRO:HD2	2.03	0.40
1:F:315:LEU:N	1:F:315:LEU:HD12	2.36	0.40
1:F:476:VAL:HG21	1:F:479:GLN:NE2	2.35	0.40
1:D:155:PHE:HA	1:D:161:GLY:HA3	2.03	0.40
1:D:228:ASN:OD1	1:D:600:GLU:HB3	2.21	0.40
1:D:488:GLU:HB3	1:D:491:LYS:HD3	2.03	0.40
1:E:24:VAL:HG12	1:E:110:PRO:HD2	2.03	0.40
1:A:392:ASP:HA	1:A:393:PRO:HD3	1.96	0.40
1:A:470:PHE:CE1	1:A:507:ASP:HB3	2.56	0.40
1:C:163:HIS:CD2	1:C:163:HIS:N	2.88	0.40
1:F:111:GLN:HG2	1:E:68:LYS:HZ2	1.83	0.40
1:F:151:LEU:HD23	1:F:151:LEU:HA	1.96	0.40
1:F:239:VAL:O	1:F:243:GLY:CA	2.70	0.40
1:E:490:ASN:OD1	1:E:490:ASN:N	2.50	0.40
1:A:304:LEU:N	1:A:305:PRO:CD	2.84	0.40
1:B:29:PHE:CZ	1:B:47:VAL:HG11	2.56	0.40
1:F:265:LEU:HA	1:F:289:THR:O	2.22	0.40



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:LEU:HD22	1:E:324:ILE:HG22	2.04	0.40
1:A:331:LEU:HD12	1:A:331:LEU:HA	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASP:OD1	1:C:598:ARG:NH2[2_654]	2.11	0.09

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 X-ray entries followed by that with respect to entries of similar resolution.

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	579/618~(94%)	567~(98%)	12 (2%)	0	100	100
1	В	575/618~(93%)	556~(97%)	19 (3%)	0	100	100
1	С	579/618~(94%)	565~(98%)	14 (2%)	0	100	100
1	D	579/618~(94%)	561 (97%)	18 (3%)	0	100	100
1	Ε	579/618~(94%)	563~(97%)	16 (3%)	0	100	100
1	F	579/618~(94%)	559~(96%)	20~(4%)	0	100	100
All	All	3470/3708~(94%)	3371 (97%)	99~(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 sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	480/499~(96%)	444 (92%)	36 (8%)	13 43
1	В	480/499~(96%)	462 (96%)	18 (4%)	33 69
1	С	480/499~(96%)	454 (95%)	26 (5%)	22 57
1	D	480/499~(96%)	455 (95%)	25~(5%)	23 59
1	Ε	480/499~(96%)	460 (96%)	20 (4%)	30 66
1	F	480/499~(96%)	457 (95%)	23~(5%)	25 62
All	All	2880/2994~(96%)	2732 (95%)	148 (5%)	24 60

analysed, and the total number of residues.

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	23	ASP
1	В	41	LEU
1	В	86	LEU
1	В	221	LEU
1	В	224	LEU
1	В	236	ASP
1	В	275	THR
1	В	315	LEU
1	В	349	PHE
1	В	350	GLU
1	В	351	ASP
1	В	353	GLU
1	В	364	LEU
1	В	371	THR
1	В	489	LEU
1	В	561	SER
1	В	581	VAL
1	В	587	VAL
1	С	13	ASP
1	С	49	THR
1	С	111	GLN
1	С	114	ASP
1	С	145	ASP
1	С	174	THR
1	С	176	THR
1	С	213	ILE
1	С	221	LEU
1	С	244	LEU



Mol	Chain	Res	Type
1	С	247	ASP
1	С	275	THR
1	С	286	GLU
1	С	336	THR
1	С	349	PHE
1	С	353	GLU
1	С	354	THR
1	С	408	THR
1	С	434	TYR
1	С	481	THR
1	С	496	GLU
1	С	535	SER
1	С	551	GLU
1	С	561	SER
1	С	569	LEU
1	С	603	ASP
1	F	19	LEU
1	F	49	THR
1	F	73	VAL
1	F	172	VAL
1	F	219	GLU
1	F	220	ASP
1	F	225	ASP
1	F	235	GLU
1	F	236	ASP
1	F	251	LEU
1	F	277	ILE
1	F	283	GLN
1	F	316	ASN
1	F	346	ASP
1	F	348	GLN
1	F	357	GLU
1	F	364	LEU
1	F	454	SER
1	F	481	THR
1	F	561	SER
1	F	585	VAL
1	F	587	VAL
1	F	601	VAL
1	D	65	ASN
1	D	221	LEU
1	D	231	MET



Mol	Chain	Res	Type
1	D	234	LYS
1	D	235	GLU
1	D	236	ASP
1	D	244	LEU
1	D	247	ASP
1	D	275	THR
1	D	294	THR
1	D	317	LEU
1	D	323	ASN
1	D	349	PHE
1	D	353	GLU
1	D	364	LEU
1	D	396	VAL
1	D	501	ILE
1	D	517	ILE
1	D	560	GLN
1	D	561	SER
1	D	586	LEU
1	D	596	THR
1	D	600	GLU
1	D	601	VAL
1	D	603	ASP
1	Е	86	LEU
1	Е	87	LEU
1	Е	106	ASN
1	Е	143	LEU
1	Е	145	ASP
1	Е	213	ILE
1	Е	231	MET
1	Е	244	LEU
1	Е	247	ASP
1	Е	294	THR
1	E	317	LEU
1	E	364	LEU
1	E	383	LEU
1	E	396	VAL
1	E	414	VAL
1	Е	481	THR
1	E	517	ILE
1	Е	560	GLN
1	E	561	SER
1	Е	602	ASP



Mol	Chain	Res	Type
1	А	65	ASN
1	А	133	MET
1	А	147	GLN
1	А	163	HIS
1	А	188	ARG
1	А	206	THR
1	А	213	ILE
1	А	230	ARG
1	А	231	MET
1	А	232	VAL
1	А	234	LYS
1	А	235	GLU
1	А	247	ASP
1	А	251	LEU
1	А	275	THR
1	А	285	SER
1	А	294	THR
1	А	315	LEU
1	А	324	ILE
1	А	336	THR
1	А	348	GLN
1	А	349	PHE
1	А	352	SER
1	А	359	LEU
1	А	371	THR
1	А	383	LEU
1	А	386	GLU
1	А	388	GLU
1	А	396	VAL
1	А	408	THR
1	А	450	ILE
1	А	451	HIS
1	А	481	THR
1	А	501	ILE
1	А	560	GLN
1	А	561	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	479	GLN
1	В	523	GLN



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Mol	Chain	Res	Type
1	С	280	GLN
1	Е	323	ASN
1	А	323	ASN
1	А	348	GLN
1	А	479	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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	583/618~(94%)	0.03	33 (5%) 23 8	68, 88, 107, 118	0
1	В	581/618~(94%)	-0.15	26 (4%) 33 12	58, 72, 90, 100	0
1	С	583/618~(94%)	-0.19	20 (3%) 45 19	55, 67, 90, 102	0
1	D	583/618~(94%)	-0.10	27 (4%) 32 12	61, 76, 101, 110	0
1	Е	583/618~(94%)	0.09	37 (6%) 20 6	72, 91, 117, 127	0
1	F	583/618~(94%)	0.15	42 (7%) 15 4	74, 98, 121, 127	0
All	All	3496/3708~(94%)	-0.03	185 (5%) 26 10	55, 82, 112, 127	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	276	ALA	8.2
1	В	358	ASN	7.1
1	D	355	PRO	6.8
1	F	312	SER	6.7
1	D	313	ALA	6.1
1	С	273	ALA	6.0
1	F	275	THR	6.0
1	Е	313	ALA	6.0
1	F	351	ASP	5.9
1	А	272	ALA	5.8
1	D	197	GLN	5.7
1	В	351	ASP	5.6
1	D	351	ASP	5.5
1	F	357	GLU	5.4
1	F	314	SER	5.3
1	С	351	ASP	5.3
1	А	275	THR	5.2
1	В	275	THR	5.2
1	F	358	ASN	5.1



Mol	Chain	Res	Type	RSRZ
1	А	206	THR	5.1
1	А	313	ALA	5.1
1	Е	602	ASP	4.9
1	F	603	ASP	4.9
1	F	313	ALA	4.9
1	Е	275	THR	4.8
1	А	273	ALA	4.8
1	С	272	ALA	4.7
1	F	273	ALA	4.7
1	В	197	GLN	4.7
1	С	275	THR	4.7
1	F	206	THR	4.7
1	Е	197	GLN	4.6
1	Е	603	ASP	4.6
1	D	358	ASN	4.6
1	В	273	ALA	4.6
1	Е	358	ASN	4.6
1	Е	272	ALA	4.5
1	А	351	ASP	4.5
1	Е	351	ASP	4.4
1	Е	206	THR	4.4
1	А	270	ALA	4.4
1	А	603	ASP	4.4
1	С	355	PRO	4.3
1	F	272	ALA	4.3
1	А	352	SER	4.2
1	D	273	ALA	4.2
1	D	350	GLU	4.0
1	А	602	ASP	4.0
1	Е	353	GLU	4.0
1	С	358	ASN	3.9
1	Е	271	GLY	3.9
1	Е	355	PRO	3.9
1	А	314	SER	3.8
1	В	603	ASP	3.8
1	F	81	ASP	3.8
1	А	285	SER	3.8
1	А	353	GLU	3.8
1	С	353	GLU	3.8
1	А	312	SER	3.8
1	С	314	SER	3.7
1	Е	276	ALA	3.6



Mol	Chain	Res	Type	RSRZ
1	А	310	ASP	3.6
1	А	355	PRO	3.6
1	С	197	GLN	3.6
1	F	244	LEU	3.6
1	F	240	ARG	3.5
1	А	350	GLU	3.5
1	F	311	ALA	3.5
1	D	206	THR	3.5
1	F	310	ASP	3.4
1	F	355	PRO	3.4
1	С	274	GLY	3.4
1	С	312	SER	3.4
1	В	355	PRO	3.4
1	А	358	ASN	3.4
1	D	310	ASP	3.4
1	А	197	GLN	3.4
1	Е	597	ARG	3.4
1	F	276	ALA	3.4
1	E	84	ALA	3.4
1	В	312	SER	3.4
1	Е	273	ALA	3.4
1	Е	352	SER	3.4
1	F	316	ASN	3.3
1	F	353	GLU	3.3
1	D	354	THR	3.3
1	D	603	ASP	3.3
1	В	285	SER	3.3
1	D	275	THR	3.3
1	С	271	GLY	3.3
1	F	350	GLU	3.3
1	F	352	SER	3.3
1	F	197	GLN	3.2
1	В	276	ALA	3.2
1	С	313	ALA	3.2
1	F	274	GLY	3.2
1	A	271	GLY	3.2
1	В	602	ASP	3.2
1	F	360	ASP	3.1
1	D	312	SER	3.1
1	D	357	GLU	3.1
1	E	247	ASP	3.1
1	A	280	GLN	3.1



Mol	Chain	Res	Type	RSRZ
1	В	357	GLU	3.1
1	D	314	SER	3.1
1	D	602	ASP	3.0
1	В	314	SER	3.0
1	Е	85	GLY	3.0
1	А	441	ARG	3.0
1	Е	144	ALA	2.9
1	В	274	GLY	2.9
1	Е	312	SER	2.9
1	А	276	ALA	2.9
1	F	103	ASP	2.9
1	С	350	GLU	2.9
1	D	272	ALA	2.9
1	В	313	ALA	2.9
1	Е	357	GLU	2.9
1	А	236	ASP	2.8
1	А	196	ALA	2.8
1	Е	285	SER	2.8
1	F	271	GLY	2.8
1	Е	103	ASP	2.8
1	F	354	THR	2.8
1	Е	350	GLU	2.8
1	Е	356	PRO	2.7
1	А	316	ASN	2.7
1	А	336	THR	2.7
1	D	353	GLU	2.7
1	D	85	GLY	2.7
1	В	270	ALA	2.7
1	F	193	ASP	2.7
1	В	206	THR	2.6
1	F	260	ARG	2.6
1	F	336	THR	2.6
1	Е	81	ASP	2.6
1	А	145	ASP	2.6
1	В	433	GLY	2.6
1	Е	336	THR	2.6
1	А	357	GLU	2.6
1	Е	240	ARG	2.6
1	Е	310	ASP	2.6
1	Е	274	GLY	2.5
1	F	285	SER	2.5
1	D	363	GLU	2.5



Mol	Chain	Res	Type	RSRZ
1	А	471	GLU	2.5
1	А	144	ALA	2.5
1	С	206	THR	2.4
1	D	240	ARG	2.4
1	F	602	ASP	2.4
1	С	84	ALA	2.4
1	В	145	ASP	2.4
1	С	603	ASP	2.4
1	Е	233	GLU	2.4
1	Е	227	PRO	2.4
1	А	240	ARG	2.3
1	D	207	ALA	2.3
1	D	597	ARG	2.3
1	С	352	SER	2.3
1	F	471	GLU	2.3
1	В	337	GLY	2.3
1	F	196	ALA	2.3
1	В	207	ALA	2.3
1	В	193	ASP	2.2
1	В	310	ASP	2.2
1	А	260	ARG	2.2
1	D	88	PRO	2.2
1	F	477	GLY	2.2
1	F	241	ALA	2.2
1	F	236	ASP	2.2
1	Ε	316	ASN	2.2
1	В	350	GLU	2.2
1	F	363	GLU	2.2
1	Ε	239	VAL	2.2
1	В	353	GLU	2.1
1	D	84	ALA	2.1
1	F	229	ALA	2.1
1	F	245	SER	2.1
1	D	352	SER	2.1
1	С	429	GLU	2.1
1	Е	389	GLY	2.1
1	В	354	THR	2.0
1	D	35	HIS	2.0
1	F	88	PRO	2.0
1	Е	80	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

