

Full wwPDB X-ray Structure Validation Report (i)

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
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)	:	2.36

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 3.70 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578(3.90-3.50)

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	C	uality of chain		
1	А	553	36%	50%	5%	9%
1	В	553	36%	50%	5%	9%
1	С	553	3%	49%	5%	9%
1	D	553	3%	50%	5%	9%
1	Е	553	36%	50%	5%	9%



Mol	Chain	Length		Quality of chain		
1	F	553	3%	50%	5%	9%
1	G	553	4%	50%	5%	9%
1	Н	553	37%	50%	5%	9%
1	Ι	553	37%	49%	5%	9%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34884 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		At	oms			ZeroOcc	AltConf	Trace
1	Λ	505	Total	С	Ν	0	\mathbf{S}	0	0	0
1	Л	505	3849	2423	658	757	11	0	0	0
1	В	505	Total	С	Ν	Ο	\mathbf{S}	0	Ο	0
1	D	505	3849	2423	658	757	11	0	0	0
1	С	505	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
T	U	505	3849	2423	658	757	11	0	0	0
1	Л	505	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	D	505	3849	2423	658	757	11	0	0	0
1	E	505	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	Ľ	000	3849	2423	658	757	11	0	0	0
1	F	505	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	1	505	3849	2423	658	757	11	0	0	0
1	G	505	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	<u> </u>	505	3849	2423	658	757	11	0	0	0
1	н	505	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	11	500	3849	2423	658	757	11	0	0	0
1	т	505	Total	\mathbf{C}	N	0	S	0	0	0
	1	000	3849	2423	658	757	11		0	0

• Molecule 1 is a protein called Chaperonin.

• Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	Λ	1	Total	С	Ν	Ο	Р	7	0	
	Л	1	27	10	5	10	2	1	0	
2	В	1	Total	С	Ν	Ο	Р	7	0	
2	D	T	27	10	5	10	2	1	0	
2	С	1	Total	С	Ν	Ο	Р	7	0	
2	U	T	27	10	5	10	2	1	0	
2	П	1	Total	С	Ν	Ο	Р	7	0	
2	D	T	27	10	5	10	2	1	0	
2	F	1	Total	С	Ν	Ο	Р	7	0	
2	Ľ	T	27	10	5	10	2	1	0	
2	F	1	Total	\mathbf{C}	Ν	Ο	Р	7	0	
2	Ľ	1	27	10	5	10	2	1	0	
2	G	1	Total	\mathbf{C}	Ν	Ο	Р	7	0	
2	ŭ	1	27	10	5	10	2	1	0	
2	Ш 1	1	Total	Ċ	N	Ō	Р	7	0	
	11	1	27	10	5	10	2	1	0	
2	T	1	Total	С	Ν	Ο	Р	7	0	
	1	1	27	10	5	10	2	1		



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: Chaperonin













(211 (212

P505 A506 L507 V508 K509 M510

Chain F:

168 169

A515 A516 A516 T517

• Molecule 1: Chaperonin

36%



4520 1521 1522 V508 K509 M510

451

• Molecule 1: Chaperonin

Chain G:

Y432 A433 P434 Q435 Q435 G437 G437 G438

36%

DWIDE

50%

5% 9%

0493 P494

3501 V502 1503 1503 6504 P505 A506 L507





Q435 Q435 G437 G438 G444 A446 A466 A466







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	223.67Å 283.04Å 160.75Å	Deperitor
a, b, c, α , β , γ	90.00° 133.90° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	48.39 - 3.70	Depositor
Resolution (A)	48.39 - 3.70	EDS
% Data completeness	99.5(48.39-3.70)	Depositor
(in resolution range)	99.5 (48.39 - 3.70)	EDS
R _{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.25 (at 3.67 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0088, CNS 2.1	Depositor
B B.	0.277 , 0.283	Depositor
It, Itfree	0.275 , 0.280	DCC
R_{free} test set	3825 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	98.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 72.7	EDS
L-test for $twinning^2$	$< L > = 0.38, < L^2 > = 0.21$	Xtriage
	0.080 for h+2*l,k,-h-l	
Estimated twinning fraction	0.099 for -h-2*l,-k,l	Xtriage
	0.089 for h,-k,-h-l	
F_o, F_c correlation	0.89	EDS
Total number of atoms	34884	wwPDB-VP
Average B, all atoms $(Å^2)$	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.33% 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)

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

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

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/3886	0.67	3/5245~(0.1%)	
1	В	0.46	0/3886	0.67	3/5245~(0.1%)	
1	С	0.46	0/3886	0.67	3/5245~(0.1%)	
1	D	0.46	0/3886	0.67	3/5245~(0.1%)	
1	Е	0.46	0/3886	0.67	3/5245~(0.1%)	
1	F	0.46	0/3886	0.67	3/5245~(0.1%)	
1	G	0.46	0/3886	0.67	3/5245~(0.1%)	
1	Н	0.46	0/3886	0.67	3/5245~(0.1%)	
1	Ι	0.46	0/3886	0.67	3/5245~(0.1%)	
All	All	0.46	0/34974	0.67	27/47205~(0.1%)	

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	257	LYS	C-N-CD	-7.18	104.80	120.60
1	В	257	LYS	C-N-CD	-7.18	104.81	120.60
1	F	257	LYS	C-N-CD	-7.18	104.81	120.60
1	Н	257	LYS	C-N-CD	-7.17	104.81	120.60
1	А	257	LYS	C-N-CD	-7.17	104.83	120.60
1	D	257	LYS	C-N-CD	-7.16	104.85	120.60
1	Ι	257	LYS	C-N-CD	-7.16	104.86	120.60
1	С	257	LYS	C-N-CD	-7.15	104.86	120.60
1	G	257	LYS	C-N-CD	-7.15	104.87	120.60
1	D	263	GLU	N-CA-C	-6.08	94.59	111.00
1	G	263	GLU	N-CA-C	-6.06	94.63	111.00
1	А	263	GLU	N-CA-C	-6.06	94.64	111.00
1	F	263	GLU	N-CA-C	-6.06	94.64	111.00
1	В	263	GLU	N-CA-C	-6.06	94.64	111.00
1	С	263	GLU	N-CA-C	-6.06	94.64	111.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	263	GLU	N-CA-C	-6.06	94.64	111.00
1	Ι	263	GLU	N-CA-C	-6.06	94.65	111.00
1	Н	263	GLU	N-CA-C	-6.04	94.69	111.00
1	С	257	LYS	N-CA-C	-5.29	96.71	111.00
1	Е	257	LYS	N-CA-C	-5.29	96.71	111.00
1	А	257	LYS	N-CA-C	-5.29	96.72	111.00
1	D	257	LYS	N-CA-C	-5.29	96.72	111.00
1	G	257	LYS	N-CA-C	-5.29	96.72	111.00
1	Ι	257	LYS	N-CA-C	-5.29	96.73	111.00
1	F	257	LYS	N-CA-C	-5.28	96.74	111.00
1	В	257	LYS	N-CA-C	-5.28	96.74	111.00
1	Н	257	LYS	N-CA-C	-5.27	96.76	111.00

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	3849	0	3995	360	2
1	В	3849	0	3995	358	11
1	С	3849	0	3995	346	5
1	D	3849	0	3995	363	6
1	Е	3849	0	3995	378	12
1	F	3849	0	3995	389	1
1	G	3849	0	3995	374	2
1	Н	3849	0	3995	348	11
1	Ι	3849	0	3995	351	3
2	А	27	0	12	1	0
2	В	27	0	12	1	0
2	С	27	0	12	1	0
2	D	27	0	12	1	0
2	Е	27	0	12	1	0
2	F	27	0	12	1	0
2	G	$\overline{27}$	0	12	1	0
2	H	27	0	12	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ι	27	0	12	1	0
All	All	34884	0	36063	3175	28

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 45.

All (3175) 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:260:LEU:HD12	1:D:261:ASP:N	1.43	1.34
1:A:260:LEU:HD12	1:A:261:ASP:N	1.43	1.33
1:G:260:LEU:HD12	1:G:261:ASP:N	1.43	1.32
1:E:260:LEU:HD12	1:E:261:ASP:N	1.43	1.32
1:H:260:LEU:HD12	1:H:261:ASP:N	1.43	1.32
1:F:260:LEU:HD12	1:F:261:ASP:N	1.43	1.32
1:B:260:LEU:HD12	1:B:261:ASP:N	1.43	1.30
1:C:260:LEU:HD12	1:C:261:ASP:N	1.43	1.30
1:I:260:LEU:HD12	1:I:261:ASP:N	1.43	1.30
1:B:256:GLU:O	1:B:258:PRO:HD3	1.38	1.22
1:G:256:GLU:O	1:G:258:PRO:HD3	1.38	1.22
1:F:256:GLU:O	1:F:258:PRO:HD3	1.38	1.21
1:D:256:GLU:O	1:D:258:PRO:HD3	1.38	1.20
1:E:256:GLU:O	1:E:258:PRO:HD3	1.38	1.20
1:I:256:GLU:O	1:I:258:PRO:HD3	1.38	1.19
1:A:256:GLU:O	1:A:258:PRO:HD3	1.38	1.19
1:H:256:GLU:O	1:H:258:PRO:HD3	1.38	1.19
1:B:60:VAL:HG22	1:B:66:ILE:HG22	1.23	1.17
1:I:60:VAL:HG22	1:I:66:ILE:HG22	1.23	1.17
1:C:256:GLU:O	1:C:258:PRO:HD3	1.39	1.17
1:F:185:VAL:HG13	1:F:402:LEU:HD23	1.32	1.12
1:I:185:VAL:HG13	1:I:402:LEU:HD23	1.32	1.12
1:H:60:VAL:HG22	1:H:66:ILE:HG22	1.23	1.12
1:G:60:VAL:HG22	1:G:66:ILE:HG22	1.23	1.11
1:C:60:VAL:HG22	1:C:66:ILE:HG22	1.23	1.10
1:F:60:VAL:HG22	1:F:66:ILE:HG22	1.23	1.10
1:A:60:VAL:HG22	1:A:66:ILE:HG22	1.23	1.10
1:D:60:VAL:HG22	1:D:66:ILE:HG22	1.23	1.10
1:E:185:VAL:HG13	$1:\overline{E:402:LEU:HD23}$	1.32	1.10
1:E:60:VAL:HG22	1:E:66:ILE:HG22	1.23	1.10
1:G:185:VAL:HG13	$1:\overline{G:402:LEU:HD23}$	1.31	1.08
1:B:185:VAL:HG13	1:B:402:LEU:HD23	1.31	1.08



	hi a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:185:VAL:HG13	1:D:402:LEU:HD23	1.31	1.08
1:A:185:VAL:HG13	1:A:402:LEU:HD23	1.32	1.07
1:H:185:VAL:HG13	1:H:402:LEU:HD23	1.31	1.06
1:C:185:VAL:HG13	1:C:402:LEU:HD23	1.31	1.06
1:F:529:VAL:HG12	1:G:58:MET:HB3	1.15	1.06
1:E:522:LEU:HD11	1:F:68:ILE:HD12	1.37	1.04
1:I:260:LEU:HD12	1:I:261:ASP:H	1.23	1.02
1:E:260:LEU:HD12	1:E:261:ASP:H	1.23	1.01
1:A:260:LEU:HD12	1:A:261:ASP:H	1.23	1.01
1:D:529:VAL:HG12	1:E:58:MET:HB3	1.40	1.01
1:F:260:LEU:HD12	1:F:261:ASP:H	1.23	1.01
1:E:522:LEU:HD11	1:F:68:ILE:CD1	1.89	1.00
1:I:245:LYS:N	1:I:296:ASN:HD22	1.61	0.99
1:D:245:LYS:N	1:D:296:ASN:HD22	1.61	0.99
1:G:245:LYS:N	1:G:296:ASN:HD22	1.61	0.99
1:H:245:LYS:N	1:H:296:ASN:HD22	1.61	0.98
1:B:245:LYS:N	1:B:296:ASN:HD22	1.61	0.98
1:E:245:LYS:N	1:E:296:ASN:HD22	1.61	0.97
1:C:245:LYS:N	1:C:296:ASN:HD22	1.61	0.96
1:B:421:VAL:O	1:B:425:ILE:HG12	1.66	0.96
1:F:245:LYS:N	1:F:296:ASN:HD22	1.61	0.96
1:D:421:VAL:O	1:D:425:ILE:HG12	1.66	0.96
1:F:529:VAL:HG12	1:G:58:MET:CB	1.94	0.96
1:I:421:VAL:O	1:I:425:ILE:HG12	1.66	0.96
1:C:421:VAL:O	1:C:425:ILE:HG12	1.66	0.96
1:H:421:VAL:O	1:H:425:ILE:HG12	1.66	0.96
1:A:245:LYS:N	1:A:296:ASN:HD22	1.61	0.95
1:F:421:VAL:O	1:F:425:ILE:HG12	1.66	0.95
1:E:423:ILE:HD12	1:E:424:GLU:N	1.82	0.95
1:A:423:ILE:HD12	1:A:424:GLU:N	1.82	0.95
1:F:423:ILE:HD12	1:F:424:GLU:N	1.82	0.95
1:G:423:ILE:HD12	1:G:424:GLU:N	1.82	0.95
1:I:423:ILE:HD12	1:I:424:GLU:N	1.82	0.95
1:B:423:ILE:HD12	1:B:424:GLU:N	1.82	0.95
1:H:423:ILE:HD12	1:H:424:GLU:N	1.82	0.95
1:C:423:ILE:HD12	1:C:424:GLU:N	1.82	0.94
1:E:66:ILE:HD13	1:E:66:ILE:H	1.32	0.94
1:G:421:VAL:O	1:G:425:ILE:HG12	1.66	0.94
1:D:423:ILE:HD12	1:D:424:GLU:N	1.82	0.94
1:I:66:ILE:HD13	1:I:66:ILE:H	1.32	0.94
1:E:421:VAL:O	1:E:425:ILE:HG12	1.66	0.94



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:260:LEU:HD12	1:H:261:ASP:H	1.23	0.94
1:A:66:ILE:HD13	1:A:66:ILE:H	1.32	0.94
1:C:260:LEU:HD12	1:C:261:ASP:H	1.23	0.94
1:G:260:LEU:HD12	1:G:261:ASP:H	1.23	0.94
1:A:421:VAL:O	1:A:425:ILE:HG12	1.66	0.93
1:D:66:ILE:HD13	1:D:66:ILE:H	1.32	0.93
1:B:66:ILE:HD13	1:B:66:ILE:H	1.32	0.93
1:C:66:ILE:H	1:C:66:ILE:HD13	1.32	0.93
1:H:66:ILE:H	1:H:66:ILE:HD13	1.32	0.92
1:B:260:LEU:HD12	1:B:261:ASP:H	1.23	0.91
1:D:400:ASP:O	1:D:404:THR:HG22	1.71	0.91
1:C:212:LYS:HE2	1:C:212:LYS:HA	1.53	0.91
1:E:212:LYS:HA	1:E:212:LYS:HE2	1.53	0.91
1:G:256:GLU:O	1:G:258:PRO:CD	2.19	0.91
1:I:212:LYS:HE2	1:I:212:LYS:HA	1.53	0.91
1:D:256:GLU:O	1:D:258:PRO:CD	2.19	0.90
1:G:400:ASP:O	1:G:404:THR:HG22	1.71	0.90
1:A:400:ASP:O	1:A:404:THR:HG22	1.71	0.90
1:D:260:LEU:HD12	1:D:261:ASP:H	1.23	0.90
1:G:212:LYS:HE2	1:G:212:LYS:HA	1.53	0.90
1:A:256:GLU:O	1:A:258:PRO:CD	2.19	0.90
1:G:66:ILE:HD13	1:G:66:ILE:H	1.32	0.90
1:E:256:GLU:O	1:E:258:PRO:CD	2.19	0.90
1:E:258:PRO:HG2	1:E:279:GLU:OE2	1.72	0.90
1:F:66:ILE:H	1:F:66:ILE:HD13	1.32	0.90
1:H:256:GLU:O	1:H:258:PRO:CD	2.19	0.90
1:B:400:ASP:O	1:B:404:THR:HG22	1.71	0.89
1:C:258:PRO:HG2	1:C:279:GLU:OE2	1.72	0.89
1:F:258:PRO:HG2	1:F:279:GLU:OE2	1.72	0.89
1:B:212:LYS:HA	1:B:212:LYS:HE2	1.53	0.89
1:F:400:ASP:O	1:F:404:THR:HG22	1.71	0.89
1:A:258:PRO:HG2	1:A:279:GLU:OE2	1.72	0.89
1:B:258:PRO:HG2	1:B:279:GLU:OE2	1.72	0.89
1:C:256:GLU:O	1:C:258:PRO:CD	2.19	0.89
1:I:400:ASP:O	1:I:404:THR:HG22	1.71	0.89
1:D:258:PRO:HG2	1:D:279:GLU:OE2	1.72	0.89
1:G:258:PRO:HG2	1:G:279:GLU:OE2	1.72	0.89
1:F:260:LEU:CD1	1:F:261:ASP:N	2.35	0.89
1:A:212:LYS:HE2	1:A:212:LYS:HA	1.53	0.89
1:E:88:LEU:HD11	1:F:389:ARG:HH12	1.37	0.89
1:F:256:GLU:O	1:F:258:PRO:CD	2.19	0.89



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:212:LYS:HE2	1:H:212:LYS:HA	1.53	0.89
1:H:260:LEU:CD1	1:H:261:ASP:N	2.35	0.89
1:D:212:LYS:HE2	1:D:212:LYS:HA	1.53	0.88
1:I:258:PRO:HG2	1:I:279:GLU:OE2	1.72	0.88
1:H:400:ASP:O	1:H:404:THR:HG22	1.71	0.88
1:E:400:ASP:O	1:E:404:THR:HG22	1.71	0.88
1:B:256:GLU:O	1:B:258:PRO:CD	2.19	0.88
1:C:400:ASP:O	1:C:404:THR:HG22	1.71	0.88
1:F:88:LEU:HD11	1:G:389:ARG:HH12	1.36	0.88
1:F:212:LYS:HE2	1:F:212:LYS:HA	1.53	0.88
1:H:258:PRO:HG2	1:H:279:GLU:OE2	1.72	0.88
1:I:256:GLU:O	1:I:258:PRO:CD	2.19	0.87
1:A:58:MET:HB3	1:I:529:VAL:HG12	1.57	0.87
1:G:260:LEU:CD1	1:G:261:ASP:N	2.35	0.87
1:A:217:ILE:HG12	1:A:385:GLY:HA2	1.57	0.87
1:B:260:LEU:CD1	1:B:261:ASP:N	2.35	0.87
1:D:269:PRO:HA	1:D:272:MET:HG2	1.57	0.87
1:F:217:ILE:HG12	1:F:385:GLY:HA2	1.57	0.87
1:B:269:PRO:HA	1:B:272:MET:HG2	1.57	0.86
1:A:530:VAL:O	1:B:59:LEU:HD23	1.75	0.86
1:G:217:ILE:HG12	1:G:385:GLY:HA2	1.57	0.86
1:A:269:PRO:HA	1:A:272:MET:HG2	1.57	0.86
1:D:217:ILE:HG12	1:D:385:GLY:HA2	1.57	0.86
1:B:217:ILE:HG12	1:B:385:GLY:HA2	1.57	0.86
1:E:269:PRO:HA	1:E:272:MET:HG2	1.57	0.86
1:C:260:LEU:CD1	1:C:261:ASP:N	2.35	0.86
1:C:269:PRO:HA	1:C:272:MET:HG2	1.57	0.86
1:H:269:PRO:HA	1:H:272:MET:HG2	1.57	0.85
1:I:217:ILE:HG12	1:I:385:GLY:HA2	1.57	0.85
1:C:217:ILE:HG12	1:C:385:GLY:HA2	1.57	0.85
1:F:269:PRO:HA	1:F:272:MET:HG2	1.57	0.85
1:I:361:LYS:HB3	1:I:366:LYS:HG2	1.59	0.85
1:D:361:LYS:HB3	1:D:366:LYS:HG2	1.59	0.85
1:I:269:PRO:HA	1:I:272:MET:HG2	1.57	0.85
1:E:260:LEU:CD1	1:E:261:ASP:N	2.35	0.85
1:E:217:ILE:HG12	1:E:385:GLY:HA2	1.57	0.84
1:F:361:LYS:HB3	1:F:366:LYS:HG2	1.59	0.84
1:G:269:PRO:HA	1:G:272:MET:HG2	1.57	0.84
1:A:260:LEU:CD1	1:A:261:ASP:N	2.35	0.84
1:C:76:LEU:HD23	1:C:90:VAL:HG12	1.60	0.84
1:C:361:LYS:HB3	1:C:366:LYS:HG2	1.59	0.84



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:361:LYS:HB3	1:H:366:LYS:HG2	1.59	0.84
1:H:76:LEU:HD23	1:H:90:VAL:HG12	1.60	0.84
1:B:361:LYS:HB3	1:B:366:LYS:HG2	1.59	0.84
1:F:529:VAL:CG1	1:G:58:MET:HB3	2.04	0.84
1:H:217:ILE:HG12	1:H:385:GLY:HA2	1.57	0.84
1:D:260:LEU:CD1	1:D:261:ASP:N	2.35	0.83
1:B:76:LEU:HD23	1:B:90:VAL:HG12	1.60	0.83
1:E:361:LYS:HB3	1:E:366:LYS:HG2	1.59	0.83
1:D:76:LEU:HD23	1:D:90:VAL:HG12	1.60	0.83
1:E:76:LEU:HD23	1:E:90:VAL:HG12	1.60	0.83
1:I:76:LEU:HD23	1:I:90:VAL:HG12	1.60	0.83
1:A:361:LYS:HB3	1:A:366:LYS:HG2	1.59	0.83
1:G:76:LEU:HD23	1:G:90:VAL:HG12	1.60	0.82
1:D:245:LYS:H	1:D:296:ASN:HD22	1.28	0.82
1:F:76:LEU:HD23	1:F:90:VAL:HG12	1.60	0.82
1:A:76:LEU:HD23	1:A:90:VAL:HG12	1.60	0.82
1:I:260:LEU:CD1	1:I:261:ASP:N	2.35	0.81
1:C:245:LYS:H	1:C:296:ASN:HD22	1.28	0.81
1:F:530:VAL:O	1:G:59:LEU:HD23	1.80	0.81
1:G:361:LYS:HB3	1:G:366:LYS:HG2	1.59	0.81
1:F:88:LEU:CD1	1:G:389:ARG:HH12	1.93	0.81
1:C:290:ILE:O	1:C:293:THR:HG22	1.82	0.80
1:A:290:ILE:O	1:A:293:THR:HG22	1.82	0.80
1:H:60:VAL:HG22	1:H:66:ILE:CG2	2.10	0.80
1:B:245:LYS:H	1:B:296:ASN:HD22	1.28	0.80
1:H:260:LEU:CD1	1:H:261:ASP:OD1	2.30	0.80
1:A:260:LEU:CD1	1:A:261:ASP:OD1	2.30	0.80
1:D:290:ILE:O	1:D:293:THR:HG22	1.82	0.80
1:I:245:LYS:H	1:I:296:ASN:HD22	1.28	0.80
1:E:260:LEU:CD1	1:E:261:ASP:OD1	2.30	0.80
1:G:60:VAL:HG22	1:G:66:ILE:CG2	2.10	0.80
1:G:245:LYS:H	1:G:296:ASN:HD22	1.28	0.80
1:G:290:ILE:O	1:G:293:THR:HG22	1.81	0.80
1:B:290:ILE:O	1:B:293:THR:HG22	1.82	0.80
1:C:260:LEU:CD1	1:C:261:ASP:OD1	2.30	0.80
1:H:290:ILE:O	1:H:293:THR:HG22	1.82	0.80
1:C:351:LEU:HD23	1:C:351:LEU:H	1.48	0.79
1:A:245:LYS:H	1:A:296:ASN:HD22	1.28	0.79
1:B:260:LEU:CD1	1:B:261:ASP:OD1	2.30	0.79
1:F:245:LYS:H	1:F:296:ASN:HD22	1.28	0.79
1:I:260:LEU:CD1	1:I:261:ASP:OD1	2.30	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:529:VAL:HG12	1:B:58:MET:HB3	1.63	0.79
1:G:351:LEU:HD23	1:G:351:LEU:H	1.47	0.79
1:D:260:LEU:CD1	1:D:261:ASP:OD1	2.30	0.79
1:E:60:VAL:HG22	1:E:66:ILE:CG2	2.10	0.79
1:F:351:LEU:H	1:F:351:LEU:HD23	1.48	0.79
1:G:260:LEU:CD1	1:G:261:ASP:OD1	2.30	0.79
1:I:290:ILE:O	1:I:293:THR:HG22	1.82	0.79
1:F:290:ILE:O	1:F:293:THR:HG22	1.81	0.79
1:E:290:ILE:O	1:E:293:THR:HG22	1.82	0.79
1:B:351:LEU:HD23	1:B:351:LEU:H	1.48	0.79
1:H:351:LEU:HD23	1:H:351:LEU:H	1.48	0.79
1:E:351:LEU:HD23	1:E:351:LEU:H	1.48	0.79
1:F:260:LEU:CD1	1:F:261:ASP:OD1	2.30	0.79
1:D:60:VAL:HG22	1:D:66:ILE:CG2	2.10	0.78
1:E:245:LYS:H	1:E:296:ASN:HD22	1.28	0.78
1:I:351:LEU:HD23	1:I:351:LEU:H	1.48	0.78
1:G:141:VAL:HG21	1:G:432:TYR:CD1	2.19	0.78
1:H:60:VAL:CG2	1:H:66:ILE:HG22	2.12	0.78
1:A:129:THR:HG21	1:B:462:ALA:O	1.83	0.78
1:F:91:GLN:HE21	1:G:387:LEU:HD21	1.49	0.78
1:F:290:ILE:HG21	1:F:298:ILE:HD12	1.66	0.78
1:I:141:VAL:HG21	1:I:432:TYR:CD1	2.19	0.78
1:A:60:VAL:HG22	1:A:66:ILE:CG2	2.10	0.78
1:A:351:LEU:HD23	1:A:351:LEU:H	1.47	0.78
1:B:141:VAL:HG21	1:B:432:TYR:CD1	2.19	0.78
1:I:290:ILE:HG21	1:I:298:ILE:HD12	1.66	0.78
1:D:60:VAL:CG2	1:D:66:ILE:HG22	2.12	0.77
1:E:290:ILE:HG21	1:E:298:ILE:HD12	1.66	0.77
1:G:290:ILE:HG21	1:G:298:ILE:HD12	1.66	0.77
1:D:141:VAL:HG21	1:D:432:TYR:CD1	2.19	0.77
1:D:351:LEU:HD23	1:D:351:LEU:H	1.47	0.77
1:F:141:VAL:HG21	1:F:432:TYR:CD1	2.19	0.77
1:H:141:VAL:HG21	1:H:432:TYR:CD1	2.19	0.77
1:A:290:ILE:HG21	1:A:298:ILE:HD12	1.66	0.77
1:D:433:ALA:O	1:D:436:VAL:HG22	1.85	0.77
1:F:91:GLN:NE2	1:G:387:LEU:HD21	2.00	0.77
1:I:60:VAL:HG22	1:I:66:ILE:CG2	2.10	0.77
1:C:141:VAL:HG21	1:C:432:TYR:CD1	2.19	0.76
1:E:433:ALA:O	1:E:436:VAL:HG22	1.85	0.76
1:A:60:VAL:CG2	1:A:66:ILE:HG22	2.12	0.76
1:D:290:ILE:HG21	1:D:298:ILE:HD12	1.66	0.76



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:60:VAL:HG22	1:F:66:ILE:CG2	2.10	0.76
1:A:141:VAL:HG21	1:A:432:TYR:CD1	2.19	0.76
1:C:60:VAL:HG22	1:C:66:ILE:CG2	2.10	0.76
1:E:141:VAL:HG21	1:E:432:TYR:CD1	2.19	0.76
1:B:220:THR:HG22	1:B:384:ARG:N	2.01	0.76
1:C:60:VAL:CG2	1:C:66:ILE:HG22	2.12	0.76
1:F:60:VAL:CG2	1:F:66:ILE:HG22	2.12	0.76
1:B:433:ALA:O	1:B:436:VAL:HG22	1.85	0.76
1:D:88:LEU:HD11	1:E:389:ARG:HH12	1.50	0.76
1:G:433:ALA:O	1:G:436:VAL:HG22	1.85	0.76
1:H:290:ILE:HG21	1:H:298:ILE:HD12	1.66	0.76
1:H:433:ALA:O	1:H:436:VAL:HG22	1.85	0.76
1:B:290:ILE:HG21	1:B:298:ILE:HD12	1.66	0.76
1:H:220:THR:HG22	1:H:384:ARG:N	2.01	0.76
1:C:290:ILE:HG21	1:C:298:ILE:HD12	1.66	0.76
1:D:220:THR:HG22	1:D:384:ARG:N	2.01	0.76
1:A:433:ALA:O	1:A:436:VAL:HG22	1.85	0.76
1:H:254:GLU:HA	1:H:305:ASP:HB2	1.68	0.76
1:I:433:ALA:O	1:I:436:VAL:HG22	1.85	0.76
1:H:89:LEU:HD21	1:H:108:VAL:HG23	1.68	0.76
1:E:89:LEU:HD21	1:E:108:VAL:HG23	1.68	0.75
1:G:254:GLU:HA	1:G:305:ASP:HB2	1.68	0.75
1:I:220:THR:HG22	1:I:384:ARG:N	2.01	0.75
1:E:141:VAL:HG21	1:E:432:TYR:CE1	2.21	0.75
1:H:245:LYS:H	1:H:296:ASN:HD22	1.28	0.75
1:C:220:THR:HG22	1:C:384:ARG:N	2.01	0.75
1:C:433:ALA:O	1:C:436:VAL:HG22	1.85	0.75
1:D:141:VAL:HG21	1:D:432:TYR:CE1	2.21	0.75
1:F:433:ALA:O	1:F:436:VAL:HG22	1.85	0.75
1:E:220:THR:HG22	1:E:384:ARG:N	2.01	0.75
1:E:254:GLU:HA	1:E:305:ASP:HB2	1.68	0.75
1:E:526:ILE:HD12	1:F:58:MET:HB2	1.68	0.75
1:F:527:ASP:HB2	1:G:55:MET:HB3	1.69	0.75
1:A:141:VAL:HG21	1:A:432:TYR:CE1	2.21	0.75
1:C:424:GLU:OE2	1:C:477:HIS:CD2	2.40	0.75
1:G:424:GLU:OE2	1:G:477:HIS:CD2	2.40	0.75
1:H:141:VAL:HG21	1:H:432:TYR:CE1	2.21	0.75
1:I:141:VAL:HG21	1:I:432:TYR:CE1	2.21	0.75
1:I:432:TYR:CE2	1:I:436:VAL:HG12	2.22	0.75
1:D:89:LEU:HD21	1:D:108:VAL:HG23	1.68	0.75
1:H:424:GLU:OE2	1:H:477:HIS:CD2	2.40	0.75



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:254:GLU:HA	1:I:305:ASP:HB2	1.68	0.75
1:A:254:GLU:HA	1:A:305:ASP:HB2	1.68	0.75
1:B:141:VAL:HG21	1:B:432:TYR:CE1	2.21	0.75
1:B:424:GLU:OE2	1:B:477:HIS:CD2	2.40	0.75
1:D:424:GLU:OE2	1:D:477:HIS:CD2	2.40	0.75
1:G:141:VAL:HG21	1:G:432:TYR:CE1	2.21	0.75
1:B:81:LEU:H	1:B:81:LEU:HD12	1.52	0.75
1:E:248:LEU:HD11	1:E:331:LEU:HD22	1.69	0.75
1:A:424:GLU:OE2	1:A:477:HIS:CD2	2.40	0.74
1:D:432:TYR:CE2	1:D:436:VAL:HG12	2.22	0.74
1:E:81:LEU:H	1:E:81:LEU:HD12	1.52	0.74
1:E:424:GLU:OE2	1:E:477:HIS:CD2	2.40	0.74
1:F:141:VAL:HG21	1:F:432:TYR:CE1	2.21	0.74
1:A:220:THR:HG22	1:A:384:ARG:N	2.01	0.74
1:B:89:LEU:HD21	1:B:108:VAL:HG23	1.68	0.74
1:C:141:VAL:HG21	1:C:432:TYR:CE1	2.21	0.74
1:G:220:THR:HG22	1:G:384:ARG:N	2.01	0.74
1:C:248:LEU:HD11	1:C:331:LEU:HD22	1.69	0.74
1:C:432:TYR:CE2	1:C:436:VAL:HG12	2.22	0.74
1:F:424:GLU:OE2	1:F:477:HIS:CD2	2.40	0.74
1:I:424:GLU:OE2	1:I:477:HIS:CD2	2.40	0.74
1:E:432:TYR:CE2	1:E:436:VAL:HG12	2.22	0.74
1:H:81:LEU:HD12	1:H:81:LEU:H	1.52	0.74
1:A:248:LEU:HD11	1:A:331:LEU:HD22	1.69	0.74
1:A:280:GLU:HG2	1:A:284:LYS:HE3	1.69	0.74
1:D:81:LEU:H	1:D:81:LEU:HD12	1.52	0.74
1:F:220:THR:HG22	1:F:384:ARG:N	2.01	0.74
1:A:299:ILE:H	1:A:299:ILE:HD13	1.53	0.74
1:F:280:GLU:HG2	1:F:284:LYS:HE3	1.69	0.74
1:F:432:TYR:CE2	1:F:436:VAL:HG12	2.22	0.74
1:A:89:LEU:HD21	1:A:108:VAL:HG23	1.68	0.74
1:B:60:VAL:HG22	1:B:66:ILE:CG2	2.10	0.74
1:B:254:GLU:HA	1:B:305:ASP:HB2	1.68	0.74
1:F:530:VAL:O	1:G:59:LEU:CD2	2.35	0.74
1:G:89:LEU:HD21	1:G:108:VAL:HG23	1.68	0.74
1:F:89:LEU:HD21	1:F:108:VAL:HG23	1.68	0.74
1:G:299:ILE:H	1:G:299:ILE:HD13	1.53	0.74
1:B:248:LEU:HD11	1:B:331:LEU:HD22	1.69	0.74
1:F:299:ILE:H	1:F:299:ILE:HD13	1.53	0.74
1:I:280:GLU:HG2	1:I:284:LYS:HE3	1.69	0.74
1:C:254:GLU:HA	1:C:305:ASP:HB2	1.68	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:424:GLU:OE2	1:G:477:HIS:HD2	1.71	0.73
1:H:432:TYR:CE2	1:H:436:VAL:HG12	2.22	0.73
1:I:424:GLU:OE2	1:I:477:HIS:HD2	1.71	0.73
1:A:432:TYR:CE2	1:A:436:VAL:HG12	2.22	0.73
1:E:525:ARG:CG	1:F:56:ASP:OD2	2.36	0.73
1:G:248:LEU:HD11	1:G:331:LEU:HD22	1.69	0.73
1:G:280:GLU:HG2	1:G:284:LYS:HE3	1.69	0.73
1:A:401:ALA:O	1:A:405:VAL:HG23	1.89	0.73
1:B:432:TYR:CE2	1:B:436:VAL:HG12	2.22	0.73
1:D:209:ILE:HB	1:D:399:ARG:HH22	1.53	0.73
1:D:280:GLU:HG2	1:D:284:LYS:HE3	1.69	0.73
1:G:81:LEU:H	1:G:81:LEU:HD12	1.52	0.73
1:E:60:VAL:CG2	1:E:66:ILE:HG22	2.12	0.73
1:F:153:VAL:HG23	1:F:160:LEU:HD23	1.70	0.73
1:C:81:LEU:HD12	1:C:81:LEU:H	1.53	0.73
1:C:424:GLU:OE2	1:C:477:HIS:HD2	1.71	0.73
1:D:299:ILE:H	1:D:299:ILE:HD13	1.53	0.73
1:E:424:GLU:OE2	1:E:477:HIS:HD2	1.71	0.73
1:F:424:GLU:OE2	1:F:477:HIS:HD2	1.71	0.73
1:G:432:TYR:CE2	1:G:436:VAL:HG12	2.22	0.73
1:I:401:ALA:O	1:I:405:VAL:HG23	1.88	0.73
1:C:264:ILE:HG13	1:C:265:ARG:N	2.02	0.73
1:D:248:LEU:HD11	1:D:331:LEU:HD22	1.69	0.73
1:E:153:VAL:HG23	1:E:160:LEU:HD23	1.70	0.73
1:F:254:GLU:HA	1:F:305:ASP:HB2	1.68	0.73
1:I:248:LEU:HD11	1:I:331:LEU:HD22	1.69	0.73
1:B:424:GLU:OE2	1:B:477:HIS:HD2	1.71	0.73
1:C:280:GLU:HG2	1:C:284:LYS:HE3	1.69	0.73
1:D:424:GLU:OE2	1:D:477:HIS:HD2	1.72	0.73
1:E:209:ILE:HB	1:E:399:ARG:HH22	1.53	0.73
1:E:280:GLU:HG2	1:E:284:LYS:HE3	1.69	0.73
1:F:209:ILE:HB	1:F:399:ARG:HH22	1.53	0.73
1:G:401:ALA:O	1:G:405:VAL:HG23	1.88	0.73
1:H:401:ALA:O	1:H:405:VAL:HG23	1.88	0.73
1:C:153:VAL:HG23	1:C:160:LEU:HD23	1.70	0.73
1:D:254:GLU:HA	1:D:305:ASP:HB2	1.68	0.73
1:F:452:GLU:O	1:F:455:VAL:HG22	1.89	0.73
1:I:81:LEU:H	1:I:81:LEU:HD12	1.52	0.73
1:A:81:LEU:H	1:A:81:LEU:HD12	1.52	0.73
1:B:452:GLU:O	1:B:455:VAL:HG22	1.89	0.73
1:G:209:ILE:HB	1:G:399:ARG:HH22	1.54	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:89:LEU:HD21	1:I:108:VAL:HG23	1.68	0.73
1:C:299:ILE:HD13	1:C:299:ILE:H	1.53	0.72
1:D:401:ALA:O	1:D:405:VAL:HG23	1.89	0.72
1:H:209:ILE:HB	1:H:399:ARG:HH22	1.54	0.72
1:I:299:ILE:H	1:I:299:ILE:HD13	1.53	0.72
1:C:89:LEU:HD21	1:C:108:VAL:HG23	1.68	0.72
1:G:153:VAL:HG23	1:G:160:LEU:HD23	1.70	0.72
1:B:280:GLU:HG2	1:B:284:LYS:HE3	1.69	0.72
1:C:209:ILE:HB	1:C:399:ARG:HH22	1.53	0.72
1:E:299:ILE:HD13	1:E:299:ILE:H	1.53	0.72
1:E:527:ASP:HB3	1:F:57:LYS:HZ2	1.53	0.72
1:H:415:ILE:HD12	1:H:506:ALA:HA	1.72	0.72
1:C:415:ILE:HD12	1:C:506:ALA:HA	1.72	0.72
1:H:452:GLU:O	1:H:455:VAL:HG22	1.89	0.72
1:I:452:GLU:O	1:I:455:VAL:HG22	1.89	0.72
1:A:424:GLU:OE2	1:A:477:HIS:HD2	1.72	0.72
1:A:452:GLU:O	1:A:455:VAL:HG22	1.89	0.72
1:F:81:LEU:H	1:F:81:LEU:HD12	1.52	0.72
1:F:401:ALA:O	1:F:405:VAL:HG23	1.88	0.72
1:A:153:VAL:HG23	1:A:160:LEU:HD23	1.70	0.72
1:B:153:VAL:HG23	1:B:160:LEU:HD23	1.70	0.72
1:H:248:LEU:HD11	1:H:331:LEU:HD22	1.69	0.72
1:H:299:ILE:HD13	1:H:299:ILE:H	1.53	0.72
1:B:209:ILE:HB	1:B:399:ARG:HH22	1.54	0.72
1:F:248:LEU:HD11	1:F:331:LEU:HD22	1.69	0.72
1:F:531:SER:HB2	1:G:60:VAL:O	1.90	0.72
1:C:401:ALA:O	1:C:405:VAL:HG23	1.88	0.72
1:H:38:ALA:O	1:H:41:ALA:HB3	1.90	0.72
1:H:153:VAL:HG23	1:H:160:LEU:HD23	1.70	0.72
1:H:280:GLU:HG2	1:H:284:LYS:HE3	1.69	0.72
1:I:60:VAL:CG2	1:I:66:ILE:HG22	2.12	0.72
1:I:209:ILE:HB	1:I:399:ARG:HH22	1.54	0.72
1:C:38:ALA:O	1:C:41:ALA:HB3	1.90	0.72
1:D:415:ILE:HD12	1:D:506:ALA:HA	1.72	0.72
1:E:401:ALA:O	1:E:405:VAL:HG23	1.89	0.72
1:F:415:ILE:HD12	1:F:506:ALA:HA	1.72	0.71
1:H:264:ILE:HG13	1:H:265:ARG:N	2.03	0.71
1:B:401:ALA:O	1:B:405:VAL:HG23	1.88	0.71
1:G:415:ILE:HD12	1:G:506:ALA:HA	1.72	0.71
1:A:38:ALA:O	1:A:41:ALA:HB3	1.90	0.71
1:B:38:ALA:O	1:B:41:ALA:HB3	1.90	0.71



	, and pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:153:VAL:HG23	1:D:160:LEU:HD23	1.70	0.71
1:I:153:VAL:HG23	1:I:160:LEU:HD23	1.70	0.71
1:B:299:ILE:HD13	1:B:299:ILE:H	1.53	0.71
1:A:209:ILE:HB	1:A:399:ARG:HH22	1.54	0.71
1:B:415:ILE:HD12	1:B:506:ALA:HA	1.72	0.71
1:D:452:GLU:O	1:D:455:VAL:HG22	1.89	0.71
1:E:38:ALA:O	1:E:41:ALA:HB3	1.90	0.71
1:G:38:ALA:O	1:G:41:ALA:HB3	1.90	0.71
1:D:38:ALA:O	1:D:41:ALA:HB3	1.90	0.71
1:E:529:VAL:HG12	1:F:58:MET:HB3	1.72	0.71
1:I:38:ALA:O	1:I:41:ALA:HB3	1.90	0.71
1:D:264:ILE:HG13	1:D:265:ARG:N	2.02	0.71
1:E:415:ILE:HD12	1:E:506:ALA:HA	1.72	0.71
1:G:60:VAL:CG2	1:G:66:ILE:HG22	2.12	0.71
1:G:452:GLU:O	1:G:455:VAL:HG22	1.89	0.71
1:I:415:ILE:HD12	1:I:506:ALA:HA	1.72	0.71
1:C:452:GLU:O	1:C:455:VAL:HG22	1.89	0.71
1:E:452:GLU:O	1:E:455:VAL:HG22	1.89	0.71
1:F:264:ILE:HG13	1:F:265:ARG:N	2.03	0.71
1:D:529:VAL:HG12	1:E:58:MET:CB	2.19	0.71
1:F:469:LEU:HB3	1:F:487:ILE:HD13	1.73	0.70
1:B:60:VAL:CG2	1:B:66:ILE:HG22	2.12	0.70
1:F:38:ALA:O	1:F:41:ALA:HB3	1.90	0.70
1:B:264:ILE:HG13	1:B:265:ARG:N	2.03	0.70
1:D:259:GLU:C	1:D:259:GLU:OE1	2.30	0.70
1:G:469:LEU:HB3	1:G:487:ILE:HD13	1.73	0.70
1:A:415:ILE:HD12	1:A:506:ALA:HA	1.72	0.70
1:B:259:GLU:C	1:B:259:GLU:OE1	2.30	0.70
1:C:469:LEU:HB3	1:C:487:ILE:HD13	1.73	0.70
1:H:259:GLU:C	1:H:259:GLU:OE1	2.30	0.70
1:A:259:GLU:OE1	1:A:259:GLU:C	2.30	0.70
1:E:264:ILE:HG13	1:E:265:ARG:N	2.02	0.70
1:F:259:GLU:OE1	1:F:259:GLU:C	2.30	0.70
1:H:424:GLU:OE2	1:H:477:HIS:HD2	1.71	0.70
1:A:425:ILE:O	1:A:429:LEU:HB2	1.92	0.70
1:C:259:GLU:C	1:C:259:GLU:OE1	2.30	0.70
1:E:259:GLU:C	1:E:259:GLU:OE1	2.30	0.70
1:I:107:ALA:O	1:I:111:SER:HB2	1.92	0.70
1:A:469:LEU:HB3	1:A:487:ILE:HD13	1.73	0.70
1:B:425:ILE:O	1:B:429:LEU:HB2	1.92	0.70
1:D:398:LEU:O	1:D:402:LEU:HG	1.92	0.70



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:107:ALA:O	1:F:111:SER:HB2	1.92	0.69
1:G:83:HIS:CG	1:G:84:PRO:HD2	2.27	0.69
1:H:469:LEU:HB3	1:H:487:ILE:HD13	1.73	0.69
1:H:475:SER:O	1:H:478:GLU:HG2	1.92	0.69
1:A:264:ILE:HG13	1:A:265:ARG:N	2.03	0.69
1:B:83:HIS:CG	1:B:84:PRO:HD2	2.27	0.69
1:B:398:LEU:O	1:B:402:LEU:HG	1.92	0.69
1:E:264:ILE:HG13	1:E:265:ARG:O	1.92	0.69
1:E:469:LEU:HB3	1:E:487:ILE:HD13	1.73	0.69
1:F:83:HIS:CG	1:F:84:PRO:HD2	2.27	0.69
1:B:475:SER:O	1:B:478:GLU:HG2	1.93	0.69
1:F:398:LEU:O	1:F:402:LEU:HG	1.92	0.69
1:H:107:ALA:O	1:H:111:SER:HB2	1.92	0.69
1:B:107:ALA:O	1:B:111:SER:HB2	1.92	0.69
1:D:475:SER:O	1:D:478:GLU:HG2	1.92	0.69
1:G:220:THR:CG2	1:G:384:ARG:H	2.05	0.69
1:I:259:GLU:OE1	1:I:259:GLU:C	2.30	0.69
1:A:475:SER:O	1:A:478:GLU:HG2	1.92	0.69
1:C:475:SER:O	1:C:478:GLU:HG2	1.92	0.69
1:D:425:ILE:O	1:D:429:LEU:HB2	1.92	0.69
1:E:220:THR:CG2	1:E:384:ARG:H	2.05	0.69
1:E:470:LEU:O	1:E:474:ARG:HG2	1.93	0.69
1:F:475:SER:O	1:F:478:GLU:HG2	1.92	0.69
1:G:66:ILE:H	1:G:66:ILE:CD1	2.06	0.69
1:H:83:HIS:CG	1:H:84:PRO:HD2	2.27	0.69
1:B:220:THR:CG2	1:B:384:ARG:H	2.05	0.69
1:D:83:HIS:CG	1:D:84:PRO:HD2	2.27	0.69
1:D:470:LEU:O	1:D:474:ARG:HG2	1.93	0.69
1:H:398:LEU:O	1:H:402:LEU:HG	1.92	0.69
1:H:425:ILE:O	1:H:429:LEU:HB2	1.92	0.69
1:B:264:ILE:HG13	1:B:265:ARG:O	1.92	0.69
1:C:220:THR:CG2	1:C:384:ARG:H	2.05	0.69
1:C:398:LEU:O	1:C:402:LEU:HG	1.92	0.69
1:C:425:ILE:O	1:C:429:LEU:HB2	1.92	0.69
1:E:398:LEU:O	1:E:402:LEU:HG	1.92	0.69
1:E:425:ILE:O	1:E:429:LEU:HB2	1.92	0.69
1:F:470:LEU:O	1:F:474:ARG:HG2	1.93	0.69
1:G:259:GLU:C	1:G:259:GLU:OE1	2.30	0.69
1:I:398:LEU:O	1:I:402:LEU:HG	1.92	0.69
1:A:107:ALA:O	1:A:111:SER:HB2	1.92	0.69
1:A:398:LEU:O	1:A:402:LEU:HG	1.92	0.69



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:469:LEU:HB3	1:B:487:ILE:HD13	1.73	0.69
1:C:83:HIS:CG	1:C:84:PRO:HD2	2.27	0.69
1:C:107:ALA:O	1:C:111:SER:HB2	1.91	0.69
1:D:107:ALA:O	1:D:111:SER:HB2	1.92	0.69
1:D:264:ILE:HG13	1:D:265:ARG:O	1.92	0.69
1:D:469:LEU:HB3	1:D:487:ILE:HD13	1.73	0.69
1:E:107:ALA:O	1:E:111:SER:HB2	1.92	0.69
1:E:475:SER:O	1:E:478:GLU:HG2	1.92	0.69
1:G:264:ILE:HG13	1:G:265:ARG:O	1.92	0.69
1:G:470:LEU:O	1:G:474:ARG:HG2	1.93	0.69
1:G:475:SER:O	1:G:478:GLU:HG2	1.92	0.69
1:H:220:THR:CG2	1:H:384:ARG:H	2.05	0.69
1:I:220:THR:CG2	1:I:384:ARG:H	2.05	0.69
1:I:470:LEU:O	1:I:474:ARG:HG2	1.93	0.69
1:A:220:THR:CG2	1:A:384:ARG:H	2.05	0.69
1:E:83:HIS:CG	1:E:84:PRO:HD2	2.27	0.69
1:F:66:ILE:H	1:F:66:ILE:CD1	2.06	0.69
1:F:220:THR:CG2	1:F:384:ARG:H	2.05	0.69
1:G:264:ILE:HG13	1:G:265:ARG:N	2.02	0.69
1:I:475:SER:O	1:I:478:GLU:HG2	1.92	0.69
1:F:184:ILE:HD12	1:F:222:LEU:HD22	1.75	0.69
1:G:425:ILE:O	1:G:429:LEU:HB2	1.92	0.69
1:H:184:ILE:HD12	1:H:222:LEU:HD22	1.75	0.69
1:E:184:ILE:HD12	1:E:222:LEU:HD22	1.75	0.68
1:I:264:ILE:HG13	1:I:265:ARG:N	2.02	0.68
1:I:469:LEU:HB3	1:I:487:ILE:HD13	1.73	0.68
1:A:144:GLN:O	1:A:148:GLU:HG2	1.94	0.68
1:C:144:GLN:O	1:C:148:GLU:HG2	1.94	0.68
1:C:264:ILE:HG13	1:C:265:ARG:O	1.92	0.68
1:G:184:ILE:HD12	1:G:222:LEU:HD22	1.75	0.68
1:I:83:HIS:CG	1:I:84:PRO:HD2	2.28	0.68
1:I:184:ILE:HD12	1:I:222:LEU:HD22	1.75	0.68
1:A:83:HIS:CG	1:A:84:PRO:HD2	2.27	0.68
1:B:144:GLN:O	1:B:148:GLU:HG2	1.94	0.68
1:D:184:ILE:HD12	1:D:222:LEU:HD22	1.75	0.68
1:G:107:ALA:O	1:G:111:SER:HB2	1.92	0.68
1:I:425:ILE:O	1:I:429:LEU:HB2	1.92	0.68
1:A:184:ILE:HD12	1:A:222:LEU:HD22	1.75	0.68
1:A:264:ILE:HG13	1:A:265:ARG:O	1.92	0.68
1:B:184:ILE:HD12	1:B:222:LEU:HD22	1.75	0.68
1:B:470:LEU:O	1:B:474:ARG:HG2	1.93	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:470:LEU:O	1:A:474:ARG:HG2	1.93	0.68
1:D:91:GLN:NE2	1:E:387:LEU:HD21	2.09	0.68
1:D:144:GLN:O	1:D:148:GLU:HG2	1.94	0.68
1:E:162:ARG:NH1	1:E:162:ARG:HB2	2.09	0.68
1:F:264:ILE:HG13	1:F:265:ARG:O	1.92	0.68
1:F:425:ILE:O	1:F:429:LEU:HB2	1.92	0.68
1:A:66:ILE:H	1:A:66:ILE:CD1	2.06	0.68
1:C:470:LEU:O	1:C:474:ARG:HG2	1.93	0.68
1:D:217:ILE:HD11	1:D:390:LEU:HD21	1.76	0.68
1:D:220:THR:CG2	1:D:384:ARG:H	2.05	0.68
1:G:144:GLN:O	1:G:148:GLU:HG2	1.94	0.68
1:H:470:LEU:O	1:H:474:ARG:HG2	1.93	0.68
1:I:264:ILE:HG13	1:I:265:ARG:O	1.93	0.68
1:A:162:ARG:NH1	1:A:162:ARG:HB2	2.09	0.68
1:H:264:ILE:HG13	1:H:265:ARG:O	1.92	0.68
1:C:184:ILE:HD12	1:C:222:LEU:HD22	1.75	0.68
1:F:76:LEU:HD23	1:F:90:VAL:CG1	2.24	0.68
1:G:248:LEU:HD13	1:G:299:ILE:HD11	1.76	0.68
1:G:398:LEU:O	1:G:402:LEU:HG	1.92	0.68
1:I:144:GLN:O	1:I:148:GLU:HG2	1.94	0.68
1:E:255:VAL:HA	1:E:283:ILE:HD11	1.76	0.68
1:B:255:VAL:HA	1:B:283:ILE:HD11	1.76	0.68
1:C:529:VAL:HG12	1:D:58:MET:HB3	1.74	0.68
1:A:248:LEU:HD13	1:A:299:ILE:HD11	1.76	0.67
1:G:245:LYS:N	1:G:296:ASN:ND2	2.41	0.67
1:H:255:VAL:HA	1:H:283:ILE:HD11	1.76	0.67
1:I:217:ILE:HD11	1:I:390:LEU:HD21	1.76	0.67
1:A:208:GLN:HB3	1:A:380:SER:OG	1.94	0.67
1:C:162:ARG:NH1	1:C:162:ARG:HB2	2.09	0.67
1:F:144:GLN:O	1:F:148:GLU:HG2	1.94	0.67
1:I:208:GLN:HB3	1:I:380:SER:OG	1.94	0.67
1:C:76:LEU:HD23	1:C:90:VAL:CG1	2.24	0.67
1:E:144:GLN:O	1:E:148:GLU:HG2	1.94	0.67
1:E:208:GLN:HB3	1:E:380:SER:OG	1.94	0.67
1:G:208:GLN:HB3	1:G:380:SER:OG	1.94	0.67
1:H:76:LEU:HD23	1:H:90:VAL:CG1	2.24	0.67
1:I:162:ARG:HB2	1:I:162:ARG:NH1	2.09	0.67
1:B:76:LEU:HD23	1:B:90:VAL:CG1	2.24	0.67
1:E:76:LEU:HD23	1:E:90:VAL:CG1	2.24	0.67
1:B:208:GLN:HB3	1:B:380:SER:OG	1.94	0.67
1:E:525:ARG:HG3	1:F:56:ASP:HB2	1.76	0.67



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:162:ARG:HB2	1:F:162:ARG:NH1	2.09	0.67
1:G:162:ARG:NH1	1:G:162:ARG:HB2	2.09	0.67
1:G:232:VAL:HG13	1:G:359:GLU:OE2	1.95	0.67
1:H:144:GLN:O	1:H:148:GLU:HG2	1.94	0.67
1:I:255:VAL:HA	1:I:283:ILE:HD11	1.76	0.67
1:I:269:PRO:HA	1:I:272:MET:CG	2.25	0.67
1:B:305:ASP:O	1:B:309:GLN:HG3	1.95	0.67
1:C:208:GLN:HB3	1:C:380:SER:OG	1.94	0.67
1:D:66:ILE:H	1:D:66:ILE:CD1	2.06	0.67
1:E:305:ASP:O	1:E:309:GLN:HG3	1.95	0.67
1:F:208:GLN:HB3	1:F:380:SER:OG	1.94	0.67
1:H:471:MET:SD	1:H:474:ARG:HD3	2.35	0.67
1:A:76:LEU:HD23	1:A:90:VAL:CG1	2.24	0.67
1:D:76:LEU:HD23	1:D:90:VAL:CG1	2.24	0.67
1:D:162:ARG:NH1	1:D:162:ARG:HB2	2.09	0.67
1:F:217:ILE:HD11	1:F:390:LEU:HD21	1.76	0.67
1:H:248:LEU:HD13	1:H:299:ILE:HD11	1.76	0.67
1:I:66:ILE:H	1:I:66:ILE:CD1	2.06	0.67
1:B:162:ARG:NH1	1:B:162:ARG:HB2	2.09	0.67
1:C:471:MET:SD	1:C:474:ARG:HD3	2.35	0.67
1:D:208:GLN:HB3	1:D:380:SER:OG	1.94	0.67
1:D:248:LEU:HD13	1:D:299:ILE:HD11	1.76	0.67
1:E:248:LEU:HD13	1:E:299:ILE:HD11	1.76	0.67
1:E:269:PRO:HA	1:E:272:MET:CG	2.25	0.67
1:G:305:ASP:O	1:G:309:GLN:HG3	1.95	0.67
1:I:305:ASP:O	1:I:309:GLN:HG3	1.95	0.67
1:C:305:ASP:O	1:C:309:GLN:HG3	1.95	0.67
1:D:232:VAL:HG13	1:D:359:GLU:OE2	1.95	0.67
1:E:232:VAL:HG13	1:E:359:GLU:OE2	1.95	0.67
1:H:305:ASP:O	1:H:309:GLN:HG3	1.95	0.67
1:I:471:MET:SD	1:I:474:ARG:HD3	2.35	0.67
1:A:232:VAL:HG13	1:A:359:GLU:OE2	1.95	0.67
1:B:217:ILE:HD11	1:B:390:LEU:HD21	1.76	0.67
1:B:471:MET:SD	1:B:474:ARG:HD3	2.35	0.67
1:D:255:VAL:HA	1:D:283:ILE:HD11	1.76	0.67
1:D:525:ARG:HG2	1:D:525:ARG:HH11	1.60	0.67
1:G:217:ILE:HD11	1:G:390:LEU:HD21	1.76	0.67
1:G:471:MET:SD	1:G:474:ARG:HD3	2.35	0.67
1:H:162:ARG:NH1	1:H:162:ARG:HB2	2.09	0.67
1:H:217:ILE:HD11	1:H:390:LEU:HD21	1.76	0.67
1:A:479:ASN:HB2	1:A:482:ASN:OD1	1.96	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:269:PRO:HA	1:B:272:MET:CG	2.25	0.66
1:E:66:ILE:H	1:E:66:ILE:CD1	2.06	0.66
1:F:232:VAL:HG13	1:F:359:GLU:OE2	1.95	0.66
1:F:255:VAL:HA	1:F:283:ILE:HD11	1.76	0.66
1:F:471:MET:SD	1:F:474:ARG:HD3	2.35	0.66
1:I:232:VAL:HG13	1:I:359:GLU:OE2	1.95	0.66
1:B:232:VAL:HG13	1:B:359:GLU:OE2	1.95	0.66
1:B:331:LEU:O	1:B:331:LEU:HD23	1.96	0.66
1:C:479:ASN:HB2	1:C:482:ASN:OD1	1.96	0.66
1:H:331:LEU:O	1:H:331:LEU:HD23	1.96	0.66
1:A:525:ARG:HH11	1:A:525:ARG:HG2	1.61	0.66
1:D:479:ASN:HB2	1:D:482:ASN:OD1	1.96	0.66
1:E:217:ILE:HD11	1:E:390:LEU:HD21	1.76	0.66
1:E:331:LEU:O	1:E:331:LEU:HD23	1.96	0.66
1:F:305:ASP:O	1:F:309:GLN:HG3	1.95	0.66
1:A:471:MET:SD	1:A:474:ARG:HD3	2.35	0.66
1:B:248:LEU:HD13	1:B:299:ILE:HD11	1.76	0.66
1:F:479:ASN:HB2	1:F:482:ASN:OD1	1.96	0.66
1:H:232:VAL:HG13	1:H:359:GLU:OE2	1.95	0.66
1:A:269:PRO:HA	1:A:272:MET:CG	2.25	0.66
1:C:255:VAL:HA	1:C:283:ILE:HD11	1.76	0.66
1:E:471:MET:SD	1:E:474:ARG:HD3	2.35	0.66
1:H:423:ILE:HG21	1:H:473:LEU:HD12	1.78	0.66
1:A:245:LYS:N	1:A:296:ASN:ND2	2.41	0.66
1:A:305:ASP:O	1:A:309:GLN:HG3	1.95	0.66
1:C:232:VAL:HG13	1:C:359:GLU:OE2	1.95	0.66
1:F:423:ILE:HG21	1:F:473:LEU:HD12	1.78	0.66
1:G:415:ILE:HG13	1:G:421:VAL:HG21	1.78	0.66
1:H:208:GLN:HB3	1:H:380:SER:OG	1.94	0.66
1:I:76:LEU:HD23	1:I:90:VAL:CG1	2.24	0.66
1:B:88:LEU:HD22	1:C:58:MET:HE1	1.78	0.66
1:B:415:ILE:HG13	1:B:421:VAL:HG21	1.78	0.66
1:D:471:MET:SD	1:D:474:ARG:HD3	2.35	0.66
1:E:525:ARG:HG2	1:F:56:ASP:OD2	1.95	0.66
1:E:526:ILE:HA	1:F:56:ASP:O	1.96	0.66
1:F:231:GLU:HG3	1:F:366:LYS:HZ2	1.60	0.66
1:G:76:LEU:HD23	1:G:90:VAL:CG1	2.24	0.66
1:G:210:VAL:HG23	1:G:382:LEU:CD1	2.26	0.66
1:I:210:VAL:HG23	1:I:382:LEU:CD1	2.26	0.66
1:I:525:ARG:HH11	1:I:525:ARG:HG2	1.60	0.66
1:A:217:ILE:HD11	1:A:390:LEU:HD21	1.76	0.66



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:255:VAL:HA	1:A:283:ILE:HD11	1.76	0.66
1:C:248:LEU:HD13	1:C:299:ILE:HD11	1.76	0.66
1:H:220:THR:HG22	1:H:384:ARG:H	1.61	0.66
1:H:269:PRO:HA	1:H:272:MET:CG	2.25	0.66
1:I:331:LEU:HD23	1:I:331:LEU:O	1.96	0.66
1:I:415:ILE:HG13	1:I:421:VAL:HG21	1.78	0.66
1:B:220:THR:HG22	1:B:384:ARG:H	1.61	0.66
1:B:479:ASN:HB2	1:B:482:ASN:OD1	1.96	0.66
1:F:127:HIS:CD2	1:F:129:THR:HB	2.31	0.66
1:G:479:ASN:HB2	1:G:482:ASN:OD1	1.96	0.66
1:C:210:VAL:HG23	1:C:382:LEU:CD1	2.26	0.66
1:E:415:ILE:HG13	1:E:421:VAL:HG21	1.78	0.66
1:C:423:ILE:HG21	1:C:473:LEU:HD12	1.78	0.65
1:D:210:VAL:HG23	1:D:382:LEU:CD1	2.26	0.65
1:E:46:LEU:HD12	1:E:46:LEU:N	2.12	0.65
1:E:245:LYS:N	1:E:296:ASN:ND2	2.41	0.65
1:E:525:ARG:HG2	1:E:525:ARG:HH11	1.61	0.65
1:F:269:PRO:HA	1:F:272:MET:CG	2.25	0.65
1:G:525:ARG:HG2	1:G:525:ARG:HH11	1.60	0.65
1:H:127:HIS:CD2	1:H:129:THR:HB	2.31	0.65
1:H:210:VAL:HG23	1:H:382:LEU:CD1	2.26	0.65
1:I:423:ILE:HG21	1:I:473:LEU:HD12	1.78	0.65
1:A:415:ILE:HG13	1:A:421:VAL:HG21	1.78	0.65
1:B:127:HIS:CD2	1:B:129:THR:HB	2.31	0.65
1:B:128:PRO:O	1:B:132:ILE:HG12	1.96	0.65
1:C:127:HIS:CD2	1:C:129:THR:HB	2.31	0.65
1:C:217:ILE:HD11	1:C:390:LEU:HD21	1.76	0.65
1:D:127:HIS:CD2	1:D:129:THR:HB	2.31	0.65
1:D:269:PRO:HA	1:D:272:MET:CG	2.25	0.65
1:D:305:ASP:O	1:D:309:GLN:HG3	1.95	0.65
1:D:331:LEU:O	1:D:331:LEU:HD23	1.96	0.65
1:D:473:LEU:O	1:D:476:THR:HG22	1.97	0.65
1:F:248:LEU:HD13	1:F:299:ILE:HD11	1.76	0.65
1:H:415:ILE:HG13	1:H:421:VAL:HG21	1.78	0.65
1:I:127:HIS:CD2	1:I:129:THR:HB	2.31	0.65
1:A:220:THR:HG22	1:A:384:ARG:H	1.61	0.65
1:A:455:VAL:O	1:A:459:ILE:HG12	1.97	0.65
1:D:423:ILE:HG21	1:D:473:LEU:HD12	1.78	0.65
1:D:455:VAL:O	1:D:459:ILE:HG12	1.96	0.65
1:E:479:ASN:HB2	1:E:482:ASN:OD1	1.96	0.65
1:F:473:LEU:O	1:F:476:THR:HG22	1.97	0.65



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:255:VAL:HA	1:G:283:ILE:HD11	1.76	0.65
1:G:269:PRO:HA	1:G:272:MET:CG	2.25	0.65
1:I:248:LEU:HD13	1:I:299:ILE:HD11	1.76	0.65
1:C:128:PRO:O	1:C:132:ILE:HG12	1.96	0.65
1:G:46:LEU:HD12	1:G:46:LEU:N	2.12	0.65
1:H:46:LEU:N	1:H:46:LEU:HD12	2.12	0.65
1:H:169:LEU:HD12	1:H:170:SER:N	2.12	0.65
1:H:455:VAL:O	1:H:459:ILE:HG12	1.97	0.65
1:I:128:PRO:O	1:I:132:ILE:HG12	1.96	0.65
1:I:455:VAL:O	1:I:459:ILE:HG12	1.97	0.65
1:B:210:VAL:HG23	1:B:382:LEU:CD1	2.26	0.65
1:B:525:ARG:HG2	1:B:525:ARG:HH11	1.61	0.65
1:E:210:VAL:HG23	1:E:382:LEU:CD1	2.26	0.65
1:G:331:LEU:O	1:G:331:LEU:HD23	1.96	0.65
1:I:46:LEU:N	1:I:46:LEU:HD12	2.12	0.65
1:A:423:ILE:HG21	1:A:473:LEU:HD12	1.78	0.65
1:B:46:LEU:HD12	1:B:46:LEU:N	2.12	0.65
1:B:259:GLU:OE1	1:B:260:LEU:N	2.30	0.65
1:C:46:LEU:N	1:C:46:LEU:HD12	2.12	0.65
1:D:128:PRO:O	1:D:132:ILE:HG12	1.97	0.65
1:E:128:PRO:O	1:E:132:ILE:HG12	1.97	0.65
1:F:220:THR:HG22	1:F:384:ARG:H	1.61	0.65
1:I:169:LEU:HD12	1:I:170:SER:N	2.12	0.65
1:A:121:LEU:O	1:A:126:VAL:HG22	1.97	0.65
1:A:127:HIS:CD2	1:A:129:THR:HB	2.31	0.65
1:A:473:LEU:O	1:A:476:THR:HG22	1.97	0.65
1:B:231:GLU:HG3	1:B:366:LYS:HZ2	1.62	0.65
1:D:46:LEU:HD12	1:D:46:LEU:N	2.12	0.65
1:D:245:LYS:N	1:D:296:ASN:ND2	2.41	0.65
1:F:455:VAL:O	1:F:459:ILE:HG12	1.97	0.65
1:A:210:VAL:HG23	1:A:382:LEU:CD1	2.26	0.65
1:B:473:LEU:O	1:B:476:THR:HG22	1.97	0.65
1:C:66:ILE:H	1:C:66:ILE:CD1	2.06	0.65
1:C:455:VAL:O	1:C:459:ILE:HG12	1.96	0.65
1:D:88:LEU:CD1	1:E:389:ARG:HH12	2.09	0.65
1:D:91:GLN:HE21	1:E:387:LEU:HD21	1.62	0.65
1:F:331:LEU:HD23	1:F:331:LEU:O	1.96	0.65
1:F:415:ILE:HG13	1:F:421:VAL:HG21	1.78	0.65
1:G:455:VAL:O	1:G:459:ILE:HG12	1.97	0.65
1:H:128:PRO:O	1:H:132:ILE:HG12	1.96	0.65
1:H:479:ASN:HB2	1:H:482:ASN:OD1	1.96	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:121:LEU:O	1:I:126:VAL:HG22	1.97	0.65
1:I:473:LEU:O	1:I:476:THR:HG22	1.97	0.65
1:A:331:LEU:HD23	1:A:331:LEU:O	1.96	0.65
1:C:220:THR:HG22	1:C:384:ARG:H	1.61	0.65
1:C:331:LEU:HD23	1:C:331:LEU:O	1.96	0.65
1:E:121:LEU:O	1:E:126:VAL:HG22	1.97	0.65
1:E:423:ILE:HG21	1:E:473:LEU:HD12	1.78	0.65
1:F:210:VAL:HG23	1:F:382:LEU:CD1	2.26	0.65
1:G:423:ILE:HG21	1:G:473:LEU:HD12	1.78	0.65
1:A:128:PRO:O	1:A:132:ILE:HG12	1.96	0.65
1:D:121:LEU:O	1:D:126:VAL:HG22	1.97	0.65
1:E:127:HIS:CD2	1:E:129:THR:HB	2.31	0.65
1:G:169:LEU:HD12	1:G:170:SER:N	2.12	0.65
1:G:260:LEU:HD12	1:G:260:LEU:C	2.17	0.65
1:G:473:LEU:O	1:G:476:THR:HG22	1.97	0.65
1:B:121:LEU:O	1:B:126:VAL:HG22	1.97	0.64
1:B:455:VAL:O	1:B:459:ILE:HG12	1.97	0.64
1:C:415:ILE:HG13	1:C:421:VAL:HG21	1.78	0.64
1:C:473:LEU:O	1:C:476:THR:HG22	1.97	0.64
1:D:259:GLU:OE1	1:D:260:LEU:N	2.30	0.64
1:F:128:PRO:O	1:F:132:ILE:HG12	1.96	0.64
1:F:169:LEU:HD12	1:F:170:SER:N	2.12	0.64
1:H:121:LEU:O	1:H:126:VAL:HG22	1.97	0.64
1:I:479:ASN:HB2	1:I:482:ASN:OD1	1.96	0.64
1:A:149:LEU:O	1:A:149:LEU:HD23	1.98	0.64
1:A:169:LEU:HD12	1:A:170:SER:N	2.12	0.64
1:C:269:PRO:HA	1:C:272:MET:CG	2.25	0.64
1:D:169:LEU:HD12	1:D:170:SER:N	2.12	0.64
1:I:259:GLU:OE1	1:I:260:LEU:N	2.30	0.64
1:B:245:LYS:N	1:B:296:ASN:ND2	2.41	0.64
1:C:260:LEU:HD12	1:C:260:LEU:C	2.17	0.64
1:C:525:ARG:HG2	1:C:525:ARG:HH11	1.60	0.64
1:E:259:GLU:OE1	1:E:260:LEU:N	2.30	0.64
1:F:525:ARG:HG2	1:F:525:ARG:HH11	1.61	0.64
1:G:128:PRO:O	1:G:132:ILE:HG12	1.96	0.64
1:H:473:LEU:O	1:H:476:THR:HG22	1.97	0.64
1:A:46:LEU:HD12	1:A:46:LEU:N	2.12	0.64
1:B:149:LEU:HD23	1:B:149:LEU:O	1.98	0.64
1:E:169:LEU:HD12	1:E:170:SER:N	2.12	0.64
1:E:473:LEU:O	1:E:476:THR:HG22	1.97	0.64
1:F:46:LEU:N	1:F:46:LEU:HD12	2.12	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:525:ARG:HG2	1:H:525:ARG:HH11	1.61	0.64
1:A:259:GLU:OE1	1:A:260:LEU:N	2.30	0.64
1:B:423:ILE:HG21	1:B:473:LEU:HD12	1.78	0.64
1:C:121:LEU:O	1:C:126:VAL:HG22	1.97	0.64
1:C:169:LEU:HD12	1:C:170:SER:N	2.12	0.64
1:F:245:LYS:N	1:F:296:ASN:ND2	2.41	0.64
1:C:259:GLU:OE1	1:C:260:LEU:N	2.30	0.64
1:D:149:LEU:O	1:D:149:LEU:HD23	1.98	0.64
1:E:149:LEU:HD23	1:E:149:LEU:O	1.98	0.64
1:F:259:GLU:OE1	1:F:260:LEU:N	2.30	0.64
1:G:127:HIS:CD2	1:G:129:THR:HB	2.31	0.64
1:I:220:THR:HG22	1:I:384:ARG:H	1.61	0.64
1:A:231:GLU:HG3	1:A:366:LYS:HZ2	1.63	0.64
1:F:260:LEU:HD12	1:F:260:LEU:C	2.17	0.64
1:G:259:GLU:OE1	1:G:260:LEU:N	2.30	0.64
1:B:66:ILE:H	1:B:66:ILE:CD1	2.06	0.64
1:G:110:PHE:CE2	1:G:451:LEU:HG	2.33	0.64
1:H:66:ILE:H	1:H:66:ILE:CD1	2.06	0.64
1:B:169:LEU:HD12	1:B:170:SER:N	2.12	0.64
1:C:110:PHE:CE2	1:C:451:LEU:HG	2.33	0.64
1:G:220:THR:HG22	1:G:384:ARG:H	1.61	0.64
1:E:455:VAL:O	1:E:459:ILE:HG12	1.97	0.64
1:F:121:LEU:O	1:F:126:VAL:HG22	1.97	0.64
1:A:527:ASP:HB2	1:B:55:MET:HG3	1.80	0.63
1:G:155:ILE:HG21	1:G:200:TRP:CH2	2.34	0.63
1:D:284:LYS:HD3	1:D:311:TYR:HE2	1.64	0.63
1:D:415:ILE:HG13	1:D:421:VAL:HG21	1.78	0.63
1:E:527:ASP:HB3	1:F:57:LYS:NZ	2.13	0.63
1:G:149:LEU:HD23	1:G:149:LEU:O	1.98	0.63
1:C:149:LEU:O	1:C:149:LEU:HD23	1.98	0.63
1:C:245:LYS:N	1:C:296:ASN:ND2	2.41	0.63
1:C:284:LYS:HD3	1:C:311:TYR:HE2	1.64	0.63
1:F:110:PHE:CE2	1:F:451:LEU:HG	2.33	0.63
1:F:266:ILE:HG21	1:F:272:MET:SD	2.39	0.63
1:H:408:VAL:HG22	1:H:505:PRO:HG3	1.81	0.63
1:I:155:ILE:HG21	1:I:200:TRP:CH2	2.34	0.63
1:F:149:LEU:O	1:F:149:LEU:HD23	1.98	0.63
1:A:389:ARG:HH12	1:I:88:LEU:HD11	1.63	0.63
1:D:220:THR:HG22	1:D:384:ARG:H	1.61	0.63
1:H:259:GLU:OE1	1:H:260:LEU:N	2.30	0.63
1:I:110:PHE:CE2	1:I:451:LEU:HG	2.33	0.63



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:284:LYS:HD3	1:A:311:TYR:HE2	1.64	0.63
1:C:266:ILE:HG21	1:C:272:MET:SD	2.39	0.63
1:F:155:ILE:HG21	1:F:200:TRP:CH2	2.34	0.63
1:G:121:LEU:O	1:G:126:VAL:HG22	1.97	0.63
1:G:210:VAL:HG23	1:G:382:LEU:HD13	1.81	0.63
1:H:149:LEU:HD23	1:H:149:LEU:O	1.98	0.63
1:I:110:PHE:HE2	1:I:451:LEU:HG	1.64	0.63
1:I:149:LEU:O	1:I:149:LEU:HD23	1.98	0.63
1:B:110:PHE:CE2	1:B:451:LEU:HG	2.33	0.63
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.64	0.63
1:D:110:PHE:CE2	1:D:451:LEU:HG	2.33	0.63
1:E:110:PHE:CE2	1:E:451:LEU:HG	2.33	0.63
1:G:408:VAL:HG22	1:G:505:PRO:HG3	1.81	0.63
1:H:110:PHE:HE2	1:H:451:LEU:HG	1.64	0.63
1:I:266:ILE:HG21	1:I:272:MET:SD	2.39	0.63
1:B:266:ILE:HG21	1:B:272:MET:SD	2.39	0.63
1:E:110:PHE:HE2	1:E:451:LEU:HG	1.64	0.63
1:G:284:LYS:HD3	1:G:311:TYR:HE2	1.64	0.63
1:H:210:VAL:HG23	1:H:382:LEU:HD13	1.81	0.63
1:I:408:VAL:HG22	1:I:505:PRO:HG3	1.81	0.63
1:A:408:VAL:HG22	1:A:505:PRO:HG3	1.81	0.63
1:B:155:ILE:HG21	1:B:200:TRP:CH2	2.34	0.63
1:B:260:LEU:HD12	1:B:260:LEU:C	2.17	0.63
1:C:210:VAL:HG23	1:C:382:LEU:HD13	1.81	0.63
1:D:210:VAL:HG23	1:D:382:LEU:HD13	1.81	0.63
1:A:110:PHE:CE2	1:A:451:LEU:HG	2.33	0.62
1:D:155:ILE:HG21	1:D:200:TRP:CH2	2.34	0.62
1:E:155:ILE:HG21	1:E:200:TRP:CH2	2.34	0.62
1:E:266:ILE:HG21	1:E:272:MET:SD	2.39	0.62
1:G:266:ILE:HG21	1:G:272:MET:SD	2.39	0.62
1:C:155:ILE:HG21	1:C:200:TRP:CH2	2.34	0.62
1:D:110:PHE:HE2	1:D:451:LEU:HG	1.64	0.62
1:D:231:GLU:HG3	1:D:366:LYS:HZ2	1.64	0.62
1:D:408:VAL:HG22	1:D:505:PRO:HG3	1.81	0.62
1:F:129:THR:HG23	1:G:53:ARG:HH12	1.63	0.62
1:H:245:LYS:N	1:H:296:ASN:ND2	2.41	0.62
1:H:430:ARG:HG2	1:H:430:ARG:HH11	1.64	0.62
1:I:210:VAL:HG23	1:I:382:LEU:HD13	1.81	0.62
1:A:266:ILE:HG21	1:A:272:MET:SD	2.39	0.62
1:F:430:ARG:HG2	1:F:430:ARG:HH11	1.64	0.62
1:G:231:GLU:HG3	1:G:366:LYS:HZ2	1.64	0.62



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:110:PHE:CE2	1:H:451:LEU:HG	2.33	0.62
1:I:284:LYS:HD3	1:I:311:TYR:HE2	1.64	0.62
1:I:430:ARG:HG2	1:I:430:ARG:HH11	1.64	0.62
1:B:210:VAL:HG23	1:B:382:LEU:HD13	1.81	0.62
1:B:260:LEU:HD12	1:B:261:ASP:CA	2.29	0.62
1:B:260:LEU:HD11	1:B:261:ASP:OD1	2.00	0.62
1:B:408:VAL:HG22	1:B:505:PRO:HG3	1.81	0.62
1:D:260:LEU:HD11	1:D:261:ASP:OD1	2.00	0.62
1:D:266:ILE:HG21	1:D:272:MET:SD	2.39	0.62
1:A:230:LYS:NZ	1:A:321:ARG:NH1	2.48	0.62
1:H:266:ILE:HG21	1:H:272:MET:SD	2.39	0.62
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.64	0.62
1:D:531:SER:HB2	1:E:60:VAL:O	2.00	0.62
1:E:430:ARG:HH11	1:E:430:ARG:HG2	1.64	0.62
1:F:230:LYS:NZ	1:F:321:ARG:NH1	2.48	0.62
1:H:155:ILE:HG21	1:H:200:TRP:CH2	2.34	0.62
1:A:155:ILE:HG21	1:A:200:TRP:CH2	2.34	0.62
1:C:110:PHE:HE2	1:C:451:LEU:HG	1.64	0.62
1:C:231:GLU:HG3	1:C:366:LYS:HZ2	1.64	0.62
1:C:260:LEU:HD11	1:C:261:ASP:OD1	2.00	0.62
1:G:110:PHE:HE2	1:G:451:LEU:HG	1.64	0.62
1:G:230:LYS:NZ	1:G:321:ARG:NH1	2.48	0.62
1:H:231:GLU:HG3	1:H:366:LYS:HZ2	1.65	0.62
1:H:260:LEU:HD11	1:H:261:ASP:OD1	2.00	0.62
1:B:110:PHE:HE2	1:B:451:LEU:HG	1.64	0.62
1:E:220:THR:HG22	1:E:384:ARG:H	1.61	0.62
1:G:260:LEU:HD11	1:G:261:ASP:OD1	2.00	0.62
1:I:260:LEU:HD11	1:I:261:ASP:OD1	2.00	0.62
1:A:110:PHE:HE2	1:A:451:LEU:HG	1.64	0.62
1:G:297:VAL:HG23	1:G:318:LEU:O	2.00	0.62
1:A:238:PRO:HB2	1:A:241:LEU:HD21	1.82	0.62
1:C:230:LYS:NZ	1:C:321:ARG:NH1	2.48	0.62
1:D:230:LYS:NZ	1:D:321:ARG:NH1	2.48	0.62
1:E:284:LYS:HD3	1:E:311:TYR:HE2	1.64	0.62
1:F:210:VAL:HG23	1:F:382:LEU:HD13	1.81	0.62
1:B:297:VAL:HG23	1:B:318:LEU:O	2.00	0.61
1:C:260:LEU:HD12	1:C:261:ASP:CA	2.29	0.61
1:C:408:VAL:HG22	1:C:505:PRO:HG3	1.81	0.61
1:C:427:LYS:NZ	1:C:477:HIS:O	2.33	0.61
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.64	0.61
1:E:427:LYS:NZ	1:E:477:HIS:O	2.33	0.61


	to ac pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:408:VAL:HG22	1:F:505:PRO:HG3	1.81	0.61
1:H:284:LYS:HD3	1:H:311:TYR:HE2	1.64	0.61
1:D:430:ARG:HG2	1:D:430:ARG:HH11	1.64	0.61
1:G:105:LYS:O	1:G:109:ILE:HG12	2.00	0.61
1:G:238:PRO:HB2	1:G:241:LEU:HD21	1.82	0.61
1:I:231:GLU:HG3	1:I:366:LYS:HZ2	1.65	0.61
1:A:297:VAL:HG23	1:A:318:LEU:O	2.00	0.61
1:E:230:LYS:NZ	1:E:321:ARG:NH1	2.48	0.61
1:F:105:LYS:O	1:F:109:ILE:HG12	2.00	0.61
1:H:105:LYS:O	1:H:109:ILE:HG12	2.00	0.61
1:I:105:LYS:O	1:I:109:ILE:HG12	2.00	0.61
1:A:105:LYS:O	1:A:109:ILE:HG12	2.00	0.61
1:B:88:LEU:HD22	1:C:58:MET:CE	2.31	0.61
1:C:297:VAL:HG23	1:C:318:LEU:O	2.00	0.61
1:D:238:PRO:HB2	1:D:241:LEU:HD21	1.82	0.61
1:D:427:LYS:NZ	1:D:477:HIS:O	2.33	0.61
1:F:110:PHE:HE2	1:F:451:LEU:HG	1.64	0.61
1:F:284:LYS:HD3	1:F:311:TYR:HE2	1.64	0.61
1:H:230:LYS:NZ	1:H:321:ARG:NH1	2.48	0.61
1:I:230:LYS:NZ	1:I:321:ARG:NH1	2.48	0.61
1:D:297:VAL:HG23	1:D:318:LEU:O	2.00	0.61
1:E:260:LEU:HD11	1:E:261:ASP:OD1	2.00	0.61
1:E:408:VAL:HG22	1:E:505:PRO:HG3	1.81	0.61
1:G:427:LYS:NZ	1:G:477:HIS:O	2.33	0.61
1:A:530:VAL:O	1:B:59:LEU:CD2	2.48	0.61
1:B:284:LYS:HD3	1:B:311:TYR:HE2	1.64	0.61
1:H:297:VAL:HG23	1:H:318:LEU:O	2.00	0.61
1:B:230:LYS:NZ	1:B:321:ARG:NH1	2.48	0.61
1:D:260:LEU:HD12	1:D:261:ASP:CA	2.29	0.61
1:I:427:LYS:NZ	1:I:477:HIS:O	2.33	0.61
1:A:427:LYS:NZ	1:A:477:HIS:O	2.33	0.61
1:B:427:LYS:NZ	1:B:477:HIS:O	2.33	0.61
1:E:88:LEU:CD2	1:F:58:MET:CE	2.79	0.61
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.64	0.61
1:I:238:PRO:HB2	1:I:241:LEU:HD21	1.82	0.61
1:E:105:LYS:O	1:E:109:ILE:HG12	2.00	0.61
1:F:297:VAL:HG23	1:F:318:LEU:O	2.00	0.61
1:I:245:LYS:N	1:I:296:ASN:ND2	2.41	0.61
1:I:260:LEU:HD12	1:I:260:LEU:C	2.17	0.60
1:I:297:VAL:HG23	1:I:318:LEU:O	2.00	0.60
1:A:260:LEU:HD11	1:A:261:ASP:OD1	2.00	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:207:ILE:HA	1:A:379:ILE:O	2.02	0.60
1:H:427:LYS:NZ	1:H:477:HIS:O	2.33	0.60
1:I:260:LEU:HD12	1:I:261:ASP:CA	2.29	0.60
1:D:105:LYS:O	1:D:109:ILE:HG12	2.00	0.60
1:E:502:VAL:O	1:E:502:VAL:HG12	2.02	0.60
1:G:260:LEU:HD12	1:G:261:ASP:CA	2.29	0.60
1:I:207:ILE:HA	1:I:379:ILE:O	2.02	0.60
1:B:358:GLU:HG3	1:B:360:ARG:HH22	1.67	0.60
1:C:238:PRO:HB2	1:C:241:LEU:HD21	1.82	0.60
1:C:415:ILE:HG23	1:C:506:ALA:HB2	1.84	0.60
1:E:210:VAL:HG23	1:E:382:LEU:HD13	1.81	0.60
1:H:238:PRO:HB2	1:H:241:LEU:HD21	1.82	0.60
1:C:105:LYS:O	1:C:109:ILE:HG12	2.00	0.60
1:F:427:LYS:NZ	1:F:477:HIS:O	2.33	0.60
1:G:502:VAL:O	1:G:502:VAL:HG12	2.02	0.60
1:A:415:ILE:HG23	1:A:506:ALA:HB2	1.84	0.60
1:B:238:PRO:HB2	1:B:241:LEU:HD21	1.82	0.60
1:D:119:GLU:HA	1:D:122:LEU:HD23	1.84	0.60
1:D:207:ILE:HA	1:D:379:ILE:O	2.02	0.60
1:G:529:VAL:HG12	1:H:58:MET:HB3	1.84	0.60
1:B:105:LYS:O	1:B:109:ILE:HG12	2.00	0.60
1:E:231:GLU:HG3	1:E:366:LYS:HZ2	1.66	0.60
1:E:238:PRO:HB2	1:E:241:LEU:HD21	1.82	0.60
1:E:260:LEU:HD12	1:E:260:LEU:C	2.17	0.60
1:G:415:ILE:HG23	1:G:506:ALA:HB2	1.84	0.60
1:A:119:GLU:HA	1:A:122:LEU:HD23	1.84	0.60
1:A:210:VAL:HG23	1:A:382:LEU:HD13	1.81	0.60
1:A:502:VAL:O	1:A:502:VAL:HG12	2.02	0.60
1:B:161:LEU:HD12	1:B:161:LEU:N	2.17	0.60
1:F:238:PRO:HB2	1:F:241:LEU:HD21	1.82	0.60
1:F:260:LEU:HD11	1:F:261:ASP:OD1	2.00	0.60
1:G:119:GLU:HA	1:G:122:LEU:HD23	1.84	0.60
1:H:260:LEU:HD12	1:H:260:LEU:C	2.17	0.60
1:H:358:GLU:HG3	1:H:360:ARG:HH22	1.67	0.60
1:E:119:GLU:HA	1:E:122:LEU:HD23	1.84	0.60
1:G:207:ILE:HA	1:G:379:ILE:O	2.02	0.60
1:H:502:VAL:O	1:H:502:VAL:HG12	2.02	0.60
1:B:207:ILE:HA	1:B:379:ILE:O	2.02	0.59
1:B:432:TYR:O	1:B:435:GLN:HG2	2.02	0.59
1:B:502:VAL:O	1:B:502:VAL:HG12	2.02	0.59
1:C:432:TYR:O	1:C:435:GLN:HG2	2.02	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:358:GLU:HG3	1:I:360:ABG:HH22	1.67	0.59
1:I:415:ILE:HG23	1:I:506:ALA:HB2	1.84	0.59
1:B:415:ILE:HG23	1:B:506:ALA:HB2	1.84	0.59
1:D:358:GLU:HG3	1:D:360:ARG:HH22	1.67	0.59
1:H:119:GLU:HA	1:H:122:LEU:HD23	1.84	0.59
1:B:119:GLU:HA	1:B:122:LEU:HD23	1.84	0.59
1:E:297:VAL:HG23	1:E:318:LEU:O	2.00	0.59
1:E:415:ILE:HG23	1:E:506:ALA:HB2	1.84	0.59
1:G:324:LYS:O	1:G:327:ASP:OD2	2.21	0.59
1:C:207:ILE:HA	1:C:379:ILE:O	2.02	0.59
1:E:324:LYS:O	1:E:327:ASP:OD2	2.21	0.59
1:F:119:GLU:HA	1:F:122:LEU:HD23	1.84	0.59
1:I:166:MET:HE1	1:I:179:GLU:HG2	1.85	0.59
1:A:161:LEU:HD12	1:A:161:LEU:N	2.17	0.59
1:C:161:LEU:N	1:C:161:LEU:HD12	2.17	0.59
1:C:502:VAL:HG12	1:C:502:VAL:O	2.02	0.59
1:E:161:LEU:N	1:E:161:LEU:HD12	2.17	0.59
1:F:161:LEU:HD12	1:F:161:LEU:N	2.17	0.59
1:F:358:GLU:HG3	1:F:360:ARG:HH22	1.67	0.59
1:H:324:LYS:O	1:H:327:ASP:OD2	2.21	0.59
1:H:415:ILE:HG23	1:H:506:ALA:HB2	1.84	0.59
1:I:502:VAL:O	1:I:502:VAL:HG12	2.02	0.59
1:E:207:ILE:HA	1:E:379:ILE:O	2.02	0.59
1:F:527:ASP:N	1:G:56:ASP:O	2.26	0.59
1:I:324:LYS:O	1:I:327:ASP:OD2	2.21	0.59
1:A:358:GLU:HG3	1:A:360:ARG:HH22	1.67	0.59
1:B:324:LYS:O	1:B:327:ASP:OD2	2.21	0.59
1:C:358:GLU:HG3	1:C:360:ARG:HH22	1.67	0.59
1:D:502:VAL:O	1:D:502:VAL:HG12	2.02	0.59
1:E:358:GLU:HG3	1:E:360:ARG:HH22	1.67	0.59
1:F:207:ILE:HA	1:F:379:ILE:O	2.02	0.59
1:A:432:TYR:O	1:A:435:GLN:HG2	2.02	0.59
1:D:161:LEU:HD12	1:D:161:LEU:N	2.17	0.59
1:I:432:TYR:O	1:I:435:GLN:HG2	2.03	0.59
1:C:119:GLU:HA	1:C:122:LEU:HD23	1.84	0.59
1:H:174:VAL:O	1:H:174:VAL:HG12	2.03	0.59
1:I:161:LEU:HD12	1:I:161:LEU:N	2.17	0.59
1:E:88:LEU:HD22	1:F:58:MET:HE2	1.84	0.59
1:G:358:GLU:HG3	1:G:360:ARG:HH22	1.67	0.59
1:A:260:LEU:HD12	1:A:260:LEU:C	2.17	0.58
1:D:432:TYR:O	1:D:435:GLN:HG2	2.03	0.58



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:432:TYR:O	1:E:435:GLN:HG2	2.02	0.58
1:F:174:VAL:O	1:F:174:VAL:HG12	2.03	0.58
1:G:161:LEU:HD12	1:G:161:LEU:N	2.17	0.58
1:G:432:TYR:O	1:G:435:GLN:HG2	2.02	0.58
1:H:161:LEU:N	1:H:161:LEU:HD12	2.17	0.58
1:H:432:TYR:O	1:H:435:GLN:HG2	2.03	0.58
1:B:153:VAL:CG2	1:B:160:LEU:HD23	2.33	0.58
1:F:127:HIS:HD2	1:F:129:THR:HB	1.68	0.58
1:F:256:GLU:C	1:F:258:PRO:HD3	2.22	0.58
1:F:502:VAL:O	1:F:502:VAL:HG12	2.02	0.58
1:I:153:VAL:CG2	1:I:160:LEU:HD23	2.33	0.58
1:E:450:ALA:O	1:E:453:SER:HB2	2.04	0.58
1:G:153:VAL:CG2	1:G:160:LEU:HD23	2.33	0.58
1:H:127:HIS:HD2	1:H:129:THR:HB	1.69	0.58
1:A:450:ALA:O	1:A:453:SER:HB2	2.04	0.58
1:F:432:TYR:O	1:F:435:GLN:HG2	2.03	0.58
1:G:127:HIS:HD2	1:G:129:THR:HB	1.69	0.58
1:H:153:VAL:CG2	1:H:160:LEU:HD23	2.34	0.58
1:I:119:GLU:HA	1:I:122:LEU:HD23	1.84	0.58
1:I:450:ALA:O	1:I:453:SER:HB2	2.04	0.58
1:B:142:ALA:HA	1:B:425:ILE:HG23	1.86	0.58
1:B:450:ALA:O	1:B:453:SER:HB2	2.04	0.58
1:C:450:ALA:O	1:C:453:SER:HB2	2.04	0.58
1:D:450:ALA:O	1:D:453:SER:HB2	2.04	0.58
1:F:415:ILE:HG23	1:F:506:ALA:HB2	1.84	0.58
1:D:324:LYS:O	1:D:327:ASP:OD2	2.21	0.58
1:I:142:ALA:HA	1:I:425:ILE:HG23	1.86	0.58
1:A:127:HIS:HD2	1:A:129:THR:HB	1.69	0.58
1:C:142:ALA:HA	1:C:425:ILE:HG23	1.86	0.58
1:D:415:ILE:HD13	1:D:415:ILE:H	1.69	0.58
1:D:415:ILE:HG23	1:D:506:ALA:HB2	1.84	0.58
1:G:174:VAL:HG12	1:G:174:VAL:O	2.03	0.58
1:G:222:LEU:H	1:G:222:LEU:HD23	1.69	0.58
1:H:207:ILE:HA	1:H:379:ILE:O	2.02	0.58
1:H:433:ALA:HB3	1:H:434:PRO:HD3	1.86	0.58
1:A:222:LEU:HD23	1:A:222:LEU:H	1.69	0.58
1:C:174:VAL:O	1:C:174:VAL:HG12	2.03	0.58
1:C:222:LEU:HD23	1:C:222:LEU:H	1.69	0.58
1:C:324:LYS:O	1:C:327:ASP:OD2	2.21	0.58
1:F:324:LYS:O	1:F:327:ASP:OD2	2.21	0.58
1:I:415:ILE:HD13	1:I:415:ILE:H	1.69	0.58



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:415:ILE:HD13	1:A:415:ILE:H	1.69	0.58
1:B:415:ILE:H	1:B:415:ILE:HD13	1.69	0.58
1:F:528:ASP:HB3	1:G:57:LYS:CD	2.34	0.58
1:H:450:ALA:O	1:H:453:SER:HB2	2.04	0.58
1:D:226:ILE:HG13	1:D:331:LEU:HA	1.86	0.58
1:E:222:LEU:HD23	1:E:222:LEU:H	1.69	0.58
1:F:415:ILE:HD13	1:F:415:ILE:H	1.69	0.58
1:A:142:ALA:HA	1:A:425:ILE:HG23	1.86	0.57
1:A:260:LEU:HD12	1:A:261:ASP:CA	2.29	0.57
1:B:222:LEU:HD23	1:B:222:LEU:H	1.69	0.57
1:C:232:VAL:CG1	1:C:318:LEU:HD11	2.34	0.57
1:E:226:ILE:HG13	1:E:331:LEU:HA	1.86	0.57
1:F:527:ASP:HB2	1:G:55:MET:CB	2.33	0.57
1:G:142:ALA:HA	1:G:425:ILE:HG23	1.86	0.57
1:G:232:VAL:CG1	1:G:318:LEU:HD11	2.34	0.57
1:I:433:ALA:HB3	1:I:434:PRO:HD3	1.86	0.57
1:A:324:LYS:O	1:A:327:ASP:OD2	2.21	0.57
1:B:433:ALA:HB3	1:B:434:PRO:HD3	1.86	0.57
1:C:415:ILE:HD13	1:C:415:ILE:H	1.69	0.57
1:C:433:ALA:HB3	1:C:434:PRO:HD3	1.86	0.57
1:D:153:VAL:CG2	1:D:160:LEU:HD23	2.33	0.57
1:E:433:ALA:HB3	1:E:434:PRO:HD3	1.86	0.57
1:F:433:ALA:HB3	1:F:434:PRO:HD3	1.86	0.57
1:H:226:ILE:HG13	1:H:331:LEU:HA	1.86	0.57
1:H:265:ARG:O	1:H:266:ILE:HG12	2.04	0.57
1:I:265:ARG:O	1:I:266:ILE:HG12	2.04	0.57
1:A:153:VAL:CG2	1:A:160:LEU:HD23	2.33	0.57
1:B:174:VAL:O	1:B:174:VAL:HG12	2.03	0.57
1:C:265:ARG:O	1:C:266:ILE:HG12	2.04	0.57
1:E:127:HIS:HD2	1:E:129:THR:HB	1.68	0.57
1:F:260:LEU:HD12	1:F:261:ASP:CA	2.29	0.57
1:I:222:LEU:HD23	1:I:222:LEU:H	1.69	0.57
1:A:245:LYS:HG2	1:A:353:TYR:CD1	2.40	0.57
1:C:98:GLU:HG3	1:C:99:GLU:H	1.69	0.57
1:C:127:HIS:HD2	1:C:129:THR:HB	1.68	0.57
1:D:142:ALA:HA	1:D:425:ILE:HG23	1.86	0.57
1:D:174:VAL:O	1:D:174:VAL:HG12	2.03	0.57
1:E:153:VAL:CG2	1:E:160:LEU:HD23	2.33	0.57
1:F:232:VAL:CG1	1:F:318:LEU:HD11	2.35	0.57
1:I:174:VAL:O	1:I:174:VAL:HG12	2.03	0.57
1:I:226:ILE:HG13	1:I:331:LEU:HA	1.86	0.57



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:232:VAL:CG1	1:I:318:LEU:HD11	2.34	0.57
1:B:245:LYS:HG2	1:B:353:TYR:CD1	2.40	0.57
1:E:174:VAL:O	1:E:174:VAL:HG12	2.03	0.57
1:E:245:LYS:HG2	1:E:353:TYR:CD1	2.40	0.57
1:C:245:LYS:HG2	1:C:353:TYR:CD1	2.40	0.57
1:D:260:LEU:HD12	1:D:260:LEU:C	2.17	0.57
1:F:226:ILE:HG13	1:F:331:LEU:HA	1.86	0.57
1:G:245:LYS:HG2	1:G:353:TYR:CD1	2.40	0.57
1:G:450:ALA:O	1:G:453:SER:HB2	2.04	0.57
1:H:222:LEU:HD23	1:H:222:LEU:H	1.69	0.57
1:I:127:HIS:HD2	1:I:129:THR:HB	1.68	0.57
1:A:232:VAL:CG1	1:A:318:LEU:HD11	2.35	0.57
1:A:433:ALA:HB3	1:A:434:PRO:HD3	1.86	0.57
1:C:153:VAL:CG2	1:C:160:LEU:HD23	2.33	0.57
1:D:147:GLN:HE21	1:D:413:ARG:HH22	1.53	0.57
1:F:222:LEU:HD23	1:F:222:LEU:H	1.69	0.57
1:G:351:LEU:H	1:G:351:LEU:CD2	2.17	0.57
1:H:98:GLU:HG3	1:H:99:GLU:H	1.69	0.57
1:A:383:ILE:HG22	1:A:391:VAL:HG23	1.87	0.57
1:D:265:ARG:O	1:D:266:ILE:HG12	2.04	0.57
1:E:265:ARG:O	1:E:266:ILE:HG12	2.04	0.57
1:F:162:ARG:HB2	1:F:162:ARG:HH11	1.70	0.57
1:G:265:ARG:O	1:G:266:ILE:HG12	2.04	0.57
1:H:299:ILE:HD13	1:H:299:ILE:N	2.20	0.57
1:H:383:ILE:HG22	1:H:391:VAL:HG23	1.87	0.57
1:I:245:LYS:HG2	1:I:353:TYR:CD1	2.40	0.57
1:A:174:VAL:O	1:A:174:VAL:HG12	2.03	0.57
1:B:98:GLU:HG3	1:B:99:GLU:H	1.69	0.57
1:B:232:VAL:CG1	1:B:318:LEU:HD11	2.35	0.57
1:D:98:GLU:HG3	1:D:99:GLU:H	1.69	0.57
1:D:433:ALA:HB3	1:D:434:PRO:HD3	1.86	0.57
1:D:520:ALA:O	1:D:524:LEU:HD13	2.05	0.57
1:F:245:LYS:HG2	1:F:353:TYR:CD1	2.40	0.57
1:G:147:GLN:HE21	1:G:413:ARG:HH22	1.53	0.57
1:H:245:LYS:HG2	1:H:353:TYR:CD1	2.40	0.57
1:B:383:ILE:HG22	1:B:391:VAL:HG23	1.87	0.57
1:C:147:GLN:HE21	1:C:413:ARG:HH22	1.53	0.57
1:D:222:LEU:HD23	1:D:222:LEU:H	1.69	0.57
1:D:256:GLU:C	1:D:258:PRO:HD3	2.22	0.57
1:E:88:LEU:CD2	1:F:58:MET:HE1	2.35	0.57
1:E:415:ILE:H	1:E:415:ILE:HD13	1.69	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:147:GLN:HE21	1:F:413:ARG:HH22	1.53	0.57
1:F:166:MET:HE1	1:F:179:GLU:HG2	1.87	0.57
1:F:265:ARG:O	1:F:266:ILE:HG12	2.04	0.57
1:F:299:ILE:HD13	1:F:299:ILE:N	2.20	0.57
1:H:142:ALA:HA	1:H:425:ILE:HG23	1.86	0.57
1:H:415:ILE:H	1:H:415:ILE:HD13	1.69	0.57
1:A:162:ARG:HB2	1:A:162:ARG:HH11	1.70	0.56
1:A:351:LEU:H	1:A:351:LEU:CD2	2.17	0.56
1:E:462:ALA:HB2	1:E:489:LEU:HD12	1.87	0.56
1:H:147:GLN:HE21	1:H:413:ARG:HH22	1.53	0.56
1:H:260:LEU:HD12	1:H:261:ASP:CA	2.29	0.56
1:A:147:GLN:HE21	1:A:413:ARG:HH22	1.53	0.56
1:D:245:LYS:HG2	1:D:353:TYR:CD1	2.40	0.56
1:D:508:VAL:HG13	1:D:509:LYS:N	2.20	0.56
1:E:244:ALA:HA	1:E:296:ASN:ND2	2.21	0.56
1:H:244:ALA:HA	1:H:296:ASN:ND2	2.21	0.56
1:I:462:ALA:HB2	1:I:489:LEU:HD12	1.87	0.56
1:A:226:ILE:HG13	1:A:331:LEU:HA	1.86	0.56
1:A:265:ARG:O	1:A:266:ILE:HG12	2.04	0.56
1:A:520:ALA:O	1:A:524:LEU:HD13	2.05	0.56
1:B:147:GLN:HE21	1:B:413:ARG:HH22	1.53	0.56
1:B:226:ILE:HG13	1:B:331:LEU:HA	1.86	0.56
1:C:99:GLU:HG3	1:C:407:ASP:OD2	2.06	0.56
1:C:520:ALA:O	1:C:524:LEU:HD13	2.05	0.56
1:D:232:VAL:CG1	1:D:318:LEU:HD11	2.34	0.56
1:D:462:ALA:HB2	1:D:489:LEU:HD12	1.87	0.56
1:E:88:LEU:HD23	1:F:58:MET:HE1	1.86	0.56
1:E:98:GLU:HG3	1:E:99:GLU:H	1.69	0.56
1:E:142:ALA:HA	1:E:425:ILE:HG23	1.86	0.56
1:F:98:GLU:HG3	1:F:99:GLU:H	1.69	0.56
1:F:244:ALA:HA	1:F:296:ASN:ND2	2.21	0.56
1:F:508:VAL:HG13	1:F:509:LYS:N	2.20	0.56
1:F:520:ALA:O	1:F:524:LEU:HD13	2.05	0.56
1:G:162:ARG:HB2	1:G:162:ARG:HH11	1.70	0.56
1:G:256:GLU:C	1:G:258:PRO:HD3	2.22	0.56
1:H:162:ARG:HB2	1:H:162:ARG:HH11	1.70	0.56
1:H:462:ALA:HB2	1:H:489:LEU:HD12	1.87	0.56
1:I:98:GLU:HG3	1:I:99:GLU:H	1.69	0.56
1:I:147:GLN:HE21	1:I:413:ARG:HH22	1.53	0.56
1:A:508:VAL:HG13	1:A:509:LYS:N	2.20	0.56
1:D:180:TYR:O	1:D:184:ILE:HG12	2.06	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:88:LEU:O	1:I:92:ILE:HG13	2.06	0.56
1:A:244:ALA:HA	1:A:296:ASN:ND2	2.21	0.56
1:B:88:LEU:O	1:B:92:ILE:HG13	2.06	0.56
1:C:180:TYR:O	1:C:184:ILE:HG12	2.06	0.56
1:C:226:ILE:HG13	1:C:331:LEU:HA	1.86	0.56
1:D:299:ILE:HD13	1:D:299:ILE:N	2.20	0.56
1:G:415:ILE:HD13	1:G:415:ILE:H	1.69	0.56
1:G:433:ALA:HB3	1:G:434:PRO:HD3	1.86	0.56
1:G:520:ALA:O	1:G:524:LEU:HD13	2.05	0.56
1:I:508:VAL:HG13	1:I:509:LYS:N	2.20	0.56
1:I:520:ALA:O	1:I:524:LEU:HD13	2.05	0.56
1:A:88:LEU:O	1:A:92:ILE:HG13	2.06	0.56
1:B:180:TYR:O	1:B:184:ILE:HG12	2.06	0.56
1:B:520:ALA:O	1:B:524:LEU:HD13	2.05	0.56
1:D:127:HIS:HD2	1:D:129:THR:HB	1.69	0.56
1:F:450:ALA:O	1:F:453:SER:HB2	2.04	0.56
1:H:520:ALA:O	1:H:524:LEU:HD13	2.05	0.56
1:I:244:ALA:HA	1:I:296:ASN:ND2	2.20	0.56
1:I:443:ALA:O	1:I:446:ALA:HB3	2.06	0.56
1:A:99:GLU:HG3	1:A:407:ASP:OD2	2.06	0.56
1:B:265:ARG:O	1:B:266:ILE:HG12	2.04	0.56
1:E:99:GLU:HG3	1:E:407:ASP:OD2	2.06	0.56
1:E:232:VAL:CG1	1:E:318:LEU:HD11	2.35	0.56
1:E:260:LEU:HD12	1:E:261:ASP:CA	2.29	0.56
1:G:226:ILE:HG13	1:G:331:LEU:HA	1.86	0.56
1:H:126:VAL:HG23	1:H:126:VAL:O	2.06	0.56
1:B:99:GLU:HG3	1:B:407:ASP:OD2	2.06	0.56
1:B:127:HIS:HD2	1:B:129:THR:HB	1.69	0.56
1:B:244:ALA:HA	1:B:296:ASN:ND2	2.20	0.56
1:D:99:GLU:HG3	1:D:407:ASP:OD2	2.06	0.56
1:E:88:LEU:O	1:E:92:ILE:HG13	2.05	0.56
1:G:443:ALA:O	1:G:446:ALA:HB3	2.06	0.56
1:H:180:TYR:O	1:H:184:ILE:HG12	2.06	0.56
1:A:98:GLU:HG3	1:A:99:GLU:H	1.69	0.56
1:A:443:ALA:O	1:A:446:ALA:HB3	2.06	0.56
1:B:462:ALA:HB2	1:B:489:LEU:HD12	1.87	0.56
1:C:443:ALA:O	1:C:446:ALA:HB3	2.06	0.56
1:D:88:LEU:O	1:D:92:ILE:HG13	2.06	0.56
1:E:88:LEU:HD22	1:F:58:MET:CE	2.36	0.56
1:E:383:ILE:HG22	1:E:391:VAL:HG23	1.87	0.56
1:F:88:LEU:O	1:F:92:ILE:HG13	2.06	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:180:TYR:O	1:F:184:ILE:HG12	2.06	0.56
1:G:88:LEU:O	1:G:92:ILE:HG13	2.06	0.56
1:G:98:GLU:HG3	1:G:99:GLU:H	1.69	0.56
1:H:232:VAL:CG1	1:H:318:LEU:HD11	2.34	0.56
1:H:430:ARG:O	1:H:434:PRO:HD3	2.06	0.56
1:A:126:VAL:HG23	1:A:126:VAL:O	2.06	0.56
1:C:192:VAL:HG11	1:C:206:ASN:HB2	1.88	0.56
1:C:299:ILE:HD13	1:C:299:ILE:N	2.20	0.56
1:D:244:ALA:HA	1:D:296:ASN:ND2	2.21	0.56
1:D:443:ALA:O	1:D:446:ALA:HB3	2.06	0.56
1:E:39:VAL:HG13	1:E:89:LEU:HD22	1.88	0.56
1:F:99:GLU:HG3	1:F:407:ASP:OD2	2.06	0.56
1:F:126:VAL:HG23	1:F:126:VAL:O	2.06	0.56
1:F:142:ALA:HA	1:F:425:ILE:HG23	1.86	0.56
1:F:153:VAL:CG2	1:F:160:LEU:HD23	2.33	0.56
1:F:462:ALA:HB2	1:F:489:LEU:HD12	1.87	0.56
1:H:99:GLU:HG3	1:H:407:ASP:OD2	2.06	0.56
1:H:443:ALA:O	1:H:446:ALA:HB3	2.06	0.56
1:B:39:VAL:HG13	1:B:89:LEU:HD22	1.88	0.55
1:C:470:LEU:CD2	1:C:474:ARG:HD2	2.37	0.55
1:D:383:ILE:HG22	1:D:391:VAL:HG23	1.87	0.55
1:D:470:LEU:CD2	1:D:474:ARG:HD2	2.37	0.55
1:G:244:ALA:HA	1:G:296:ASN:ND2	2.20	0.55
1:H:470:LEU:CD2	1:H:474:ARG:HD2	2.37	0.55
1:I:162:ARG:HB2	1:I:162:ARG:HH11	1.70	0.55
1:I:180:TYR:O	1:I:184:ILE:HG12	2.06	0.55
1:A:363:GLY:HA2	1:A:384:ARG:NH2	2.21	0.55
1:B:299:ILE:HD13	1:B:299:ILE:N	2.20	0.55
1:B:470:LEU:CD2	1:B:474:ARG:HD2	2.37	0.55
1:C:88:LEU:O	1:C:92:ILE:HG13	2.06	0.55
1:C:462:ALA:HB2	1:C:489:LEU:HD12	1.87	0.55
1:C:508:VAL:HG13	1:C:509:LYS:N	2.20	0.55
1:D:430:ARG:O	1:D:434:PRO:HD3	2.06	0.55
1:E:470:LEU:CD2	1:E:474:ARG:HD2	2.37	0.55
1:E:508:VAL:HG13	1:E:509:LYS:N	2.20	0.55
1:G:383:ILE:HG22	1:G:391:VAL:HG23	1.87	0.55
1:I:126:VAL:HG23	1:I:126:VAL:O	2.06	0.55
1:I:363:GLY:HA2	1:I:384:ARG:NH2	2.21	0.55
1:A:430:ARG:O	1:A:434:PRO:HD3	2.06	0.55
1:B:88:LEU:CD2	1:C:58:MET:HE1	2.35	0.55
1:B:192:VAL:HG11	1:B:206:ASN:HB2	1.88	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:508:VAL:HG13	1:B:509:LYS:N	2.21	0.55
1:C:244:ALA:HA	1:C:296:ASN:ND2	2.21	0.55
1:D:363:GLY:HA2	1:D:384:ARG:NH2	2.21	0.55
1:G:212:LYS:HA	1:G:212:LYS:CE	2.33	0.55
1:H:63:LEU:O	1:H:63:LEU:HD23	2.06	0.55
1:I:383:ILE:HG22	1:I:391:VAL:HG23	1.87	0.55
1:I:430:ARG:O	1:I:434:PRO:HD3	2.06	0.55
1:A:180:TYR:O	1:A:184:ILE:HG12	2.06	0.55
1:C:363:GLY:HA2	1:C:384:ARG:NH2	2.21	0.55
1:C:430:ARG:O	1:C:434:PRO:HD3	2.06	0.55
1:D:192:VAL:HG11	1:D:206:ASN:HB2	1.88	0.55
1:E:63:LEU:HD23	1:E:63:LEU:O	2.06	0.55
1:E:126:VAL:HG23	1:E:126:VAL:O	2.06	0.55
1:F:63:LEU:O	1:F:63:LEU:HD23	2.06	0.55
1:F:192:VAL:HG11	1:F:206:ASN:HB2	1.88	0.55
1:F:230:LYS:HZ1	1:F:321:ARG:NH1	2.04	0.55
1:F:383:ILE:HG22	1:F:391:VAL:HG23	1.87	0.55
1:G:299:ILE:HD13	1:G:299:ILE:N	2.20	0.55
1:H:255:VAL:HG13	1:H:305:ASP:OD1	2.07	0.55
1:I:39:VAL:HG13	1:I:89:LEU:HD22	1.88	0.55
1:I:351:LEU:H	1:I:351:LEU:CD2	2.17	0.55
1:A:63:LEU:O	1:A:63:LEU:HD23	2.06	0.55
1:A:462:ALA:HB2	1:A:489:LEU:HD12	1.87	0.55
1:D:39:VAL:HG13	1:D:89:LEU:HD22	1.88	0.55
1:D:126:VAL:HG23	1:D:126:VAL:O	2.06	0.55
1:D:162:ARG:HB2	1:D:162:ARG:HH11	1.70	0.55
1:E:430:ARG:O	1:E:434:PRO:HD3	2.06	0.55
1:F:363:GLY:HA2	1:F:384:ARG:NH2	2.21	0.55
1:F:443:ALA:O	1:F:446:ALA:HB3	2.06	0.55
1:F:470:LEU:CD2	1:F:474:ARG:HD2	2.37	0.55
1:G:192:VAL:HG11	1:G:206:ASN:HB2	1.88	0.55
1:G:255:VAL:HG13	1:G:305:ASP:OD1	2.07	0.55
1:G:508:VAL:HG13	1:G:509:LYS:N	2.20	0.55
1:H:363:GLY:HA2	1:H:384:ARG:NH2	2.21	0.55
1:I:63:LEU:O	1:I:63:LEU:HD23	2.06	0.55
1:I:470:LEU:CD2	1:I:474:ARG:HD2	2.37	0.55
1:A:39:VAL:HG13	1:A:89:LEU:HD22	1.88	0.55
1:A:470:LEU:CD2	1:A:474:ARG:HD2	2.37	0.55
1:B:162:ARG:HB2	1:B:162:ARG:HH11	1.70	0.55
1:B:363:GLY:HA2	1:B:384:ARG:NH2	2.21	0.55
1:C:256:GLU:C	1:C:258:PRO:HD3	2.22	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:D:255:VAL:HG13	1:D:305:ASP:OD1	2.07	0.55
1:E:180:TYR:O	1:E:184:ILE:HG12	2.06	0.55
1:A:178:ARG:H	1:A:178:ARG:HE	1.55	0.55
1:B:443:ALA:O	1:B:446:ALA:HB3	2.06	0.55
1:C:162:ARG:HB2	1:C:162:ARG:HH11	1.70	0.55
1:D:232:VAL:HG22	1:D:359:GLU:OE2	2.07	0.55
1:E:147:GLN:HE21	1:E:413:ARG:HH22	1.53	0.55
1:E:363:GLY:HA2	1:E:384:ARG:NH2	2.21	0.55
1:E:520:ALA:O	1:E:524:LEU:HD13	2.05	0.55
1:F:430:ARG:O	1:F:434:PRO:HD3	2.06	0.55
1:H:88:LEU:O	1:H:92:ILE:HG13	2.06	0.55
1:I:99:GLU:HG3	1:I:407:ASP:OD2	2.06	0.55
1:I:230:LYS:HZ2	1:I:321:ARG:NH1	2.05	0.55
1:I:383:ILE:HD12	1:I:383:ILE:N	2.22	0.55
1:E:212:LYS:HA	1:E:212:LYS:CE	2.33	0.55
1:E:256:GLU:C	1:E:258:PRO:HD3	2.22	0.55
1:E:351:LEU:H	1:E:351:LEU:CD2	2.17	0.55
1:G:99:GLU:HG3	1:G:407:ASP:OD2	2.06	0.55
1:G:180:TYR:O	1:G:184:ILE:HG12	2.06	0.55
1:G:462:ALA:HB2	1:G:489:LEU:HD12	1.87	0.55
1:G:470:LEU:CD2	1:G:474:ARG:HD2	2.37	0.55
1:H:351:LEU:H	1:H:351:LEU:CD2	2.17	0.55
1:H:508:VAL:HG13	1:H:509:LYS:N	2.20	0.55
1:B:126:VAL:O	1:B:126:VAL:HG23	2.06	0.55
1:C:383:ILE:HD12	1:C:383:ILE:N	2.22	0.55
1:C:383:ILE:HG22	1:C:391:VAL:HG23	1.87	0.55
1:E:443:ALA:O	1:E:446:ALA:HB3	2.06	0.55
1:G:430:ARG:O	1:G:434:PRO:HD3	2.06	0.55
1:H:423:ILE:HD12	1:H:424:GLU:HG2	1.89	0.55
1:A:76:LEU:CD2	1:A:90:VAL:HG12	2.36	0.55
1:A:232:VAL:HG22	1:A:359:GLU:OE2	2.07	0.55
1:D:383:ILE:N	1:D:383:ILE:HD12	2.22	0.55
1:E:383:ILE:HD12	1:E:383:ILE:N	2.22	0.55
1:F:255:VAL:HG13	1:F:305:ASP:OD1	2.07	0.55
1:F:351:LEU:H	1:F:351:LEU:CD2	2.17	0.55
1:G:63:LEU:HD23	1:G:63:LEU:O	2.06	0.55
1:A:299:ILE:HD13	1:A:299:ILE:N	2.20	0.54
1:B:430:ARG:O	1:B:434:PRO:HD3	2.06	0.54
1:C:126:VAL:HG23	1:C:126:VAL:O	2.06	0.54
$1:\overline{C:255:VAL:HG13}$	1:C:305:ASP:OD1	2.07	0.54
1:G:126:VAL:HG23	1:G:126:VAL:O	2.06	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:232:VAL:HG22	1:G:359:GLU:OE2	2.07	0.54
1:G:423:ILE:HD12	1:G:424:GLU:HG2	1.89	0.54
1:H:383:ILE:HD12	1:H:383:ILE:N	2.22	0.54
1:B:63:LEU:HD23	1:B:63:LEU:O	2.06	0.54
1:B:232:VAL:HG22	1:B:359:GLU:OE2	2.07	0.54
1:C:39:VAL:HG13	1:C:89:LEU:HD22	1.88	0.54
1:C:178:ARG:H	1:C:178:ARG:HE	1.55	0.54
1:E:111:SER:O	1:E:115:VAL:HG23	2.08	0.54
1:E:347:SER:C	1:E:349:GLN:H	2.11	0.54
1:E:487:ILE:O	1:E:489:LEU:HD22	2.08	0.54
1:I:192:VAL:HG11	1:I:206:ASN:HB2	1.88	0.54
1:B:256:GLU:C	1:B:258:PRO:HD3	2.22	0.54
1:C:63:LEU:O	1:C:63:LEU:HD23	2.06	0.54
1:C:232:VAL:HG22	1:C:359:GLU:OE2	2.07	0.54
1:D:63:LEU:HD23	1:D:63:LEU:O	2.06	0.54
1:F:232:VAL:HG22	1:F:359:GLU:OE2	2.07	0.54
1:G:363:GLY:HA2	1:G:384:ARG:NH2	2.21	0.54
1:I:487:ILE:O	1:I:489:LEU:HD22	2.08	0.54
1:A:347:SER:C	1:A:349:GLN:H	2.11	0.54
1:B:178:ARG:HE	1:B:178:ARG:H	1.55	0.54
1:B:255:VAL:HG13	1:B:305:ASP:OD1	2.07	0.54
1:I:178:ARG:H	1:I:178:ARG:HE	1.55	0.54
1:A:192:VAL:HG11	1:A:206:ASN:HB2	1.88	0.54
1:B:111:SER:O	1:B:115:VAL:HG23	2.08	0.54
1:B:487:ILE:O	1:B:489:LEU:HD22	2.08	0.54
1:F:178:ARG:H	1:F:178:ARG:HE	1.55	0.54
1:F:347:SER:C	1:F:349:GLN:H	2.11	0.54
1:H:192:VAL:HG11	1:H:206:ASN:HB2	1.88	0.54
1:H:230:LYS:HZ1	1:H:321:ARG:NH1	2.05	0.54
1:H:232:VAL:HG22	1:H:359:GLU:OE2	2.07	0.54
1:H:256:GLU:C	1:H:258:PRO:HD3	2.22	0.54
1:I:299:ILE:HD13	1:I:299:ILE:N	2.20	0.54
1:B:118:ALA:O	1:B:122:LEU:HD22	2.08	0.54
1:B:166:MET:HE1	1:B:179:GLU:HG2	1.89	0.54
1:C:487:ILE:O	1:C:489:LEU:HD22	2.08	0.54
1:D:178:ARG:HE	1:D:178:ARG:H	1.55	0.54
1:F:39:VAL:HG13	1:F:89:LEU:HD22	1.88	0.54
1:G:39:VAL:HG13	1:G:89:LEU:HD22	1.88	0.54
1:G:347:SER:C	1:G:349:GLN:H	2.11	0.54
1:H:39:VAL:HG13	1:H:89:LEU:HD22	1.88	0.54
1:A:255:VAL:HG13	1:A:305:ASP:OD1	2.07	0.54



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:299:ILE:HD13	1:E:299:ILE:N	2.20	0.54
1:I:255:VAL:HG13	1:I:305:ASP:OD1	2.07	0.54
1:A:111:SER:O	1:A:115:VAL:HG23	2.08	0.54
1:A:383:ILE:HD12	1:A:383:ILE:N	2.22	0.54
1:B:181:ILE:O	1:B:185:VAL:HG23	2.08	0.54
1:B:383:ILE:N	1:B:383:ILE:HD12	2.22	0.54
1:D:351:LEU:H	1:D:351:LEU:CD2	2.17	0.54
1:D:529:VAL:HG12	1:E:58:MET:SD	2.48	0.54
1:F:383:ILE:HD12	1:F:383:ILE:N	2.22	0.54
1:F:487:ILE:O	1:F:489:LEU:HD22	2.08	0.54
1:G:118:ALA:O	1:G:122:LEU:HD22	2.08	0.54
1:I:232:VAL:HG22	1:I:359:GLU:OE2	2.07	0.54
1:I:256:GLU:C	1:I:258:PRO:HD3	2.22	0.54
1:B:347:SER:C	1:B:349:GLN:H	2.11	0.54
1:C:265:ARG:HD2	1:C:266:ILE:N	2.23	0.54
1:C:284:LYS:HD3	1:C:311:TYR:CE2	2.43	0.54
1:C:347:SER:C	1:C:349:GLN:H	2.11	0.54
1:C:470:LEU:HD22	1:C:474:ARG:HD2	1.90	0.54
1:E:255:VAL:HG13	1:E:305:ASP:OD1	2.07	0.54
1:G:470:LEU:HD22	1:G:474:ARG:HD2	1.90	0.54
1:H:284:LYS:HD3	1:H:311:TYR:CE2	2.43	0.54
1:H:482:ASN:O	1:H:483:LYS:C	2.47	0.54
1:D:118:ALA:O	1:D:122:LEU:HD22	2.08	0.54
1:D:284:LYS:HD3	1:D:311:TYR:CE2	2.43	0.54
1:E:284:LYS:HD3	1:E:311:TYR:CE2	2.43	0.54
1:F:423:ILE:HD12	1:F:424:GLU:HG2	1.89	0.54
1:H:76:LEU:CD2	1:H:90:VAL:HG12	2.36	0.54
1:B:76:LEU:CD2	1:B:90:VAL:HG12	2.36	0.53
1:B:351:LEU:H	1:B:351:LEU:CD2	2.17	0.53
1:C:233:VAL:HG22	1:C:309:GLN:OE1	2.08	0.53
1:D:423:ILE:HD12	1:D:424:GLU:HG2	1.90	0.53
1:D:504:GLU:OE1	2:D:800:ADP:H2'	2.09	0.53
1:D:530:VAL:O	1:E:59:LEU:HD23	2.07	0.53
1:E:192:VAL:HG11	1:E:206:ASN:HB2	1.88	0.53
1:E:423:ILE:HD12	1:E:424:GLU:HG2	1.90	0.53
1:G:111:SER:O	1:G:115:VAL:HG23	2.08	0.53
1:G:482:ASN:O	1:G:483:LYS:C	2.47	0.53
1:A:265:ARG:HD2	1:A:266:ILE:N	2.23	0.53
1:C:423:ILE:HD12	1:C:424:GLU:HG2	1.90	0.53
1:E:118:ALA:O	1:E:122:LEU:HD22	2.08	0.53
1:E:232:VAL:HG22	1:E:359:GLU:OE2	2.07	0.53



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:233:VAL:HG22	1:E:309:GLN:OE1	2.09	0.53
1:E:470:LEU:HD22	1:E:474:ARG:HD2	1.90	0.53
1:F:111:SER:O	1:F:115:VAL:HG23	2.08	0.53
1:F:470:LEU:HD22	1:F:474:ARG:HD2	1.90	0.53
1:G:383:ILE:N	1:G:383:ILE:HD12	2.22	0.53
1:H:487:ILE:O	1:H:489:LEU:HD22	2.08	0.53
1:I:347:SER:C	1:I:349:GLN:H	2.11	0.53
1:B:284:LYS:HD3	1:B:311:TYR:CE2	2.43	0.53
1:D:111:SER:O	1:D:115:VAL:HG23	2.08	0.53
1:F:529:VAL:HG12	1:G:58:MET:SD	2.47	0.53
1:G:178:ARG:HE	1:G:178:ARG:H	1.55	0.53
1:G:361:LYS:CB	1:G:366:LYS:HG2	2.36	0.53
1:G:524:LEU:N	1:G:524:LEU:HD12	2.24	0.53
1:I:504:GLU:OE1	2:I:800:ADP:H2'	2.09	0.53
1:A:487:ILE:O	1:A:489:LEU:HD22	2.08	0.53
1:D:487:ILE:O	1:D:489:LEU:HD22	2.08	0.53
1:F:284:LYS:HD3	1:F:311:TYR:CE2	2.43	0.53
1:G:265:ARG:HD2	1:G:266:ILE:N	2.23	0.53
1:H:111:SER:O	1:H:115:VAL:HG23	2.08	0.53
1:A:423:ILE:HD12	1:A:424:GLU:HG2	1.90	0.53
1:B:185:VAL:O	1:B:189:VAL:HG23	2.09	0.53
1:C:111:SER:O	1:C:115:VAL:HG23	2.08	0.53
1:D:470:LEU:HD22	1:D:474:ARG:HD2	1.90	0.53
1:F:118:ALA:O	1:F:122:LEU:HD22	2.08	0.53
1:F:524:LEU:HD12	1:F:524:LEU:N	2.24	0.53
1:G:487:ILE:O	1:G:489:LEU:HD22	2.08	0.53
1:H:347:SER:C	1:H:349:GLN:H	2.11	0.53
1:I:181:ILE:O	1:I:185:VAL:HG23	2.08	0.53
1:I:265:ARG:HD2	1:I:266:ILE:N	2.23	0.53
1:I:423:ILE:HD12	1:I:424:GLU:HG2	1.90	0.53
1:I:470:LEU:HD22	1:I:474:ARG:HD2	1.90	0.53
1:B:265:ARG:HD2	1:B:266:ILE:N	2.23	0.53
1:B:423:ILE:HD12	1:B:424:GLU:HG2	1.90	0.53
1:C:118:ALA:O	1:C:122:LEU:HD22	2.08	0.53
1:C:351:LEU:H	1:C:351:LEU:CD2	2.17	0.53
1:C:524:LEU:HD12	1:C:524:LEU:N	2.24	0.53
1:D:66:ILE:HD13	1:D:66:ILE:N	2.13	0.53
1:E:162:ARG:HB2	1:E:162:ARG:HH11	1.70	0.53
1:E:178:ARG:HE	1:E:178:ARG:H	1.55	0.53
1:E:265:ARG:HD2	1:E:266:ILE:N	2.23	0.53
1:E:524:LEU:HD12	1:E:524:LEU:N	2.24	0.53



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:58:MET:HG3	1:F:68:ILE:HG22	1.91	0.53
1:F:185:VAL:O	1:F:189:VAL:HG23	2.09	0.53
1:I:111:SER:O	1:I:115:VAL:HG23	2.08	0.53
1:I:118:ALA:O	1:I:122:LEU:HD22	2.08	0.53
1:B:482:ASN:O	1:B:483:LYS:C	2.47	0.53
1:D:58:MET:HG3	1:D:68:ILE:HG22	1.91	0.53
1:D:265:ARG:HD2	1:D:266:ILE:N	2.23	0.53
1:E:181:ILE:O	1:E:185:VAL:HG23	2.08	0.53
1:F:181:ILE:O	1:F:185:VAL:HG23	2.08	0.53
1:G:181:ILE:O	1:G:185:VAL:HG23	2.08	0.53
1:G:185:VAL:O	1:G:189:VAL:HG23	2.09	0.53
1:G:504:GLU:OE1	2:G:800:ADP:H2'	2.09	0.53
1:H:181:ILE:O	1:H:185:VAL:HG23	2.08	0.53
1:I:231:GLU:HG3	1:I:366:LYS:NZ	2.24	0.53
1:A:284:LYS:HD3	1:A:311:TYR:CE2	2.43	0.53
1:A:504:GLU:OE1	2:A:800:ADP:H2'	2.09	0.53
1:C:185:VAL:O	1:C:189:VAL:HG23	2.09	0.53
1:C:230:LYS:HZ1	1:C:321:ARG:NH1	2.05	0.53
1:D:181:ILE:O	1:D:185:VAL:HG23	2.08	0.53
1:F:212:LYS:HA	1:F:212:LYS:CE	2.33	0.53
1:F:265:ARG:HD2	1:F:266:ILE:N	2.23	0.53
1:F:530:VAL:HG21	1:G:79:MET:CE	2.39	0.53
1:G:530:VAL:O	1:H:59:LEU:HD23	2.08	0.53
1:H:178:ARG:HE	1:H:178:ARG:H	1.55	0.53
1:H:233:VAL:HG22	1:H:309:GLN:OE1	2.09	0.53
1:H:265:ARG:HD2	1:H:266:ILE:N	2.23	0.53
1:H:423:ILE:CD1	1:H:424:GLU:HG2	2.39	0.53
1:I:185:VAL:O	1:I:189:VAL:HG23	2.09	0.53
1:B:233:VAL:HG22	1:B:309:GLN:OE1	2.08	0.53
1:C:58:MET:HG3	1:C:68:ILE:HG22	1.91	0.53
1:C:361:LYS:CB	1:C:366:LYS:HG2	2.36	0.53
1:E:185:VAL:O	1:E:189:VAL:HG23	2.09	0.53
1:E:361:LYS:CB	1:E:366:LYS:HG2	2.36	0.53
1:E:482:ASN:O	1:E:483:LYS:C	2.47	0.53
1:E:504:GLU:OE1	2:E:800:ADP:H2'	2.09	0.53
1:G:284:LYS:HD3	1:G:311:TYR:CE2	2.43	0.53
1:A:118:ALA:O	1:A:122:LEU:HD22	2.08	0.53
1:A:423:ILE:CD1	1:A:424:GLU:HG2	2.39	0.53
1:B:470:LEU:HD22	1:B:474:ARG:HD2	1.90	0.53
1:D:233:VAL:HG22	1:D:309:GLN:OE1	2.09	0.53
1:D:347:SER:C	1:D:349:GLN:H	2.11	0.53



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:482:ASN:O	1:D:483:LYS:C	2.47	0.53
1:F:230:LYS:HZ1	1:F:321:ARG:HH12	1.57	0.53
1:F:504:GLU:OE1	2:F:800:ADP:H2'	2.09	0.53
1:G:423:ILE:CD1	1:G:424:GLU:HG2	2.39	0.53
1:H:58:MET:HG3	1:H:68:ILE:HG22	1.91	0.53
1:H:244:ALA:C	1:H:296:ASN:HD22	2.12	0.53
1:I:212:LYS:HA	1:I:212:LYS:CE	2.33	0.53
1:A:482:ASN:O	1:A:483:LYS:C	2.47	0.52
1:C:181:ILE:O	1:C:185:VAL:HG23	2.08	0.52
1:G:244:ALA:C	1:G:296:ASN:HD22	2.12	0.52
1:H:118:ALA:O	1:H:122:LEU:HD22	2.08	0.52
1:B:230:LYS:HZ2	1:B:321:ARG:NH1	2.07	0.52
1:B:423:ILE:CD1	1:B:424:GLU:HG2	2.39	0.52
1:C:482:ASN:O	1:C:483:LYS:C	2.47	0.52
1:E:58:MET:HG3	1:E:68:ILE:HG22	1.91	0.52
1:E:231:GLU:HG3	1:E:366:LYS:NZ	2.24	0.52
1:I:233:VAL:HG22	1:I:309:GLN:OE1	2.09	0.52
1:A:233:VAL:HG22	1:A:309:GLN:OE1	2.09	0.52
1:A:423:ILE:HD12	1:A:423:ILE:C	2.30	0.52
1:B:423:ILE:HD12	1:B:423:ILE:C	2.30	0.52
1:E:272:MET:O	1:E:275:PHE:HB3	2.10	0.52
1:F:363:GLY:HA2	1:F:384:ARG:HH22	1.75	0.52
1:G:233:VAL:HG22	1:G:309:GLN:OE1	2.08	0.52
1:H:185:VAL:O	1:H:189:VAL:HG23	2.09	0.52
1:H:363:GLY:HA2	1:H:384:ARG:HH22	1.74	0.52
1:A:185:VAL:O	1:A:189:VAL:HG23	2.09	0.52
1:B:524:LEU:HD12	1:B:524:LEU:N	2.24	0.52
1:C:231:GLU:HG3	1:C:366:LYS:NZ	2.24	0.52
1:D:244:ALA:C	1:D:296:ASN:HD22	2.12	0.52
1:D:423:ILE:HD12	1:D:423:ILE:C	2.30	0.52
1:D:524:LEU:N	1:D:524:LEU:HD12	2.24	0.52
1:G:58:MET:HG3	1:G:68:ILE:HG22	1.91	0.52
1:H:166:MET:HE1	1:H:179:GLU:HG2	1.92	0.52
1:H:231:GLU:HG3	1:H:366:LYS:NZ	2.24	0.52
1:H:272:MET:O	1:H:275:PHE:HB3	2.10	0.52
1:I:423:ILE:CD1	1:I:424:GLU:HG2	2.39	0.52
1:A:181:ILE:O	1:A:185:VAL:HG23	2.08	0.52
1:A:231:GLU:HG3	1:A:366:LYS:NZ	2.24	0.52
1:A:272:MET:O	1:A:275:PHE:HB3	2.10	0.52
1:B:272:MET:O	1:B:275:PHE:HB3	2.10	0.52
1:D:306:GLU:HA	1:D:309:GLN:NE2	2.25	0.52



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:234:HIS:CD2	1:E:236:GLY:H	2.28	0.52
1:F:233:VAL:HG22	1:F:309:GLN:OE1	2.08	0.52
1:F:234:HIS:CD2	1:F:236:GLY:H	2.28	0.52
1:F:272:MET:O	1:F:275:PHE:HB3	2.10	0.52
1:G:272:MET:O	1:G:275:PHE:HB3	2.10	0.52
1:G:306:GLU:HA	1:G:309:GLN:NE2	2.25	0.52
1:H:504:GLU:OE1	2:H:800:ADP:H2'	2.09	0.52
1:H:524:LEU:HD12	1:H:524:LEU:N	2.24	0.52
1:I:234:HIS:CD2	1:I:236:GLY:H	2.28	0.52
1:A:470:LEU:HD22	1:A:474:ARG:HD2	1.90	0.52
1:C:423:ILE:CD1	1:C:424:GLU:HG2	2.39	0.52
1:D:185:VAL:O	1:D:189:VAL:HG23	2.09	0.52
1:D:234:HIS:CD2	1:D:236:GLY:H	2.28	0.52
1:E:162:ARG:HH11	1:E:162:ARG:CB	2.23	0.52
1:F:423:ILE:CD1	1:F:424:GLU:HG2	2.39	0.52
1:H:361:LYS:CB	1:H:366:LYS:HG2	2.36	0.52
1:I:482:ASN:O	1:I:483:LYS:C	2.47	0.52
1:I:524:LEU:N	1:I:524:LEU:HD12	2.24	0.52
1:A:58:MET:HG3	1:A:68:ILE:HG22	1.91	0.52
1:A:524:LEU:N	1:A:524:LEU:HD12	2.24	0.52
1:C:363:GLY:HA2	1:C:384:ARG:HH22	1.74	0.52
1:G:127:HIS:ND1	1:G:128:PRO:HD2	2.25	0.52
1:G:166:MET:HE1	1:G:179:GLU:HG2	1.91	0.52
1:G:234:HIS:CD2	1:G:236:GLY:H	2.28	0.52
1:G:363:GLY:HA2	1:G:384:ARG:HH22	1.74	0.52
1:A:256:GLU:C	1:A:258:PRO:HD3	2.22	0.52
1:B:361:LYS:CB	1:B:366:LYS:HG2	2.36	0.52
1:B:504:GLU:OE1	2:B:800:ADP:H2'	2.09	0.52
1:C:234:HIS:CD2	1:C:236:GLY:H	2.28	0.52
1:D:361:LYS:CB	1:D:366:LYS:HG2	2.36	0.52
1:D:423:ILE:CD1	1:D:424:GLU:HG2	2.39	0.52
1:E:360:ARG:NH1	1:E:371:GLU:OE2	2.43	0.52
1:F:231:GLU:HG3	1:F:366:LYS:NZ	2.24	0.52
1:F:244:ALA:C	1:F:296:ASN:HD22	2.12	0.52
1:F:360:ARG:NH1	1:F:371:GLU:OE2	2.43	0.52
1:I:76:LEU:CD2	1:I:90:VAL:HG12	2.36	0.52
1:A:68:ILE:O	1:A:68:ILE:HG13	2.10	0.52
1:B:58:MET:HG3	1:B:68:ILE:HG22	1.91	0.52
1:C:230:LYS:HZ1	1:C:321:ARG:HH12	1.58	0.52
1:C:423:ILE:HD12	1:C:423:ILE:C	2.30	0.52
1:D:363:GLY:HA2	1:D:384:ARG:HH22	1.74	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:127:HIS:ND1	1:F:128:PRO:HD2	2.25	0.52
1:H:127:HIS:ND1	1:H:128:PRO:HD2	2.25	0.52
1:H:306:GLU:HA	1:H:309:GLN:NE2	2.25	0.52
1:B:68:ILE:HG13	1:B:68:ILE:O	2.10	0.52
1:C:162:ARG:HH11	1:C:162:ARG:CB	2.23	0.52
1:C:504:GLU:OE1	2:C:800:ADP:H2'	2.09	0.52
1:G:68:ILE:HG13	1:G:68:ILE:O	2.10	0.52
1:G:162:ARG:HH11	1:G:162:ARG:CB	2.23	0.52
1:A:127:HIS:ND1	1:A:128:PRO:HD2	2.25	0.51
1:B:234:HIS:CD2	1:B:236:GLY:H	2.28	0.51
1:C:68:ILE:O	1:C:68:ILE:HG13	2.10	0.51
1:C:272:MET:O	1:C:275:PHE:HB3	2.10	0.51
1:D:272:MET:O	1:D:275:PHE:HB3	2.10	0.51
1:E:306:GLU:HA	1:E:309:GLN:NE2	2.25	0.51
1:E:423:ILE:HD11	1:E:477:HIS:NE2	2.26	0.51
1:A:363:GLY:HA2	1:A:384:ARG:HH22	1.75	0.51
1:E:127:HIS:ND1	1:E:128:PRO:HD2	2.25	0.51
1:G:66:ILE:HD13	1:G:66:ILE:N	2.14	0.51
1:G:360:ARG:NH1	1:G:371:GLU:OE2	2.43	0.51
1:H:234:HIS:CD2	1:H:236:GLY:H	2.28	0.51
1:H:423:ILE:HD12	1:H:423:ILE:C	2.30	0.51
1:H:470:LEU:HD22	1:H:474:ARG:HD2	1.90	0.51
1:I:58:MET:HG3	1:I:68:ILE:HG22	1.91	0.51
1:I:306:GLU:HA	1:I:309:GLN:NE2	2.25	0.51
1:E:363:GLY:HA2	1:E:384:ARG:HH22	1.75	0.51
1:H:212:LYS:HA	1:H:212:LYS:CE	2.33	0.51
1:H:423:ILE:HD11	1:H:477:HIS:NE2	2.26	0.51
1:I:127:HIS:ND1	1:I:128:PRO:HD2	2.25	0.51
1:I:363:GLY:HA2	1:I:384:ARG:HH22	1.75	0.51
1:B:363:GLY:HA2	1:B:384:ARG:HH22	1.75	0.51
1:B:423:ILE:HD11	1:B:477:HIS:NE2	2.26	0.51
1:D:68:ILE:HG13	1:D:68:ILE:O	2.10	0.51
1:H:162:ARG:HH11	1:H:162:ARG:CB	2.23	0.51
1:H:230:LYS:HZ1	1:H:321:ARG:HH12	1.58	0.51
1:A:360:ARG:NH1	1:A:371:GLU:OE2	2.43	0.51
1:B:306:GLU:HA	1:B:309:GLN:NE2	2.25	0.51
1:D:162:ARG:HH11	1:D:162:ARG:CB	2.23	0.51
1:D:423:ILE:HD11	1:D:477:HIS:NE2	2.26	0.51
1:E:68:ILE:HG13	1:E:68:ILE:O	2.10	0.51
1:I:272:MET:O	1:I:275:PHE:HB3	2.10	0.51
1:A:162:ARG:HH11	1:A:162:ARG:CB	2.23	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:423:ILE:HD11	1:A:477:HIS:NE2	2.26	0.51
1:B:244:ALA:C	1:B:296:ASN:HD22	2.12	0.51
1:E:230:LYS:HZ2	1:E:321:ARG:NH1	2.08	0.51
1:F:68:ILE:O	1:F:68:ILE:HG13	2.10	0.51
1:F:129:THR:HG23	1:G:53:ARG:NH1	2.25	0.51
1:H:68:ILE:O	1:H:68:ILE:HG13	2.10	0.51
1:H:360:ARG:NH1	1:H:371:GLU:OE2	2.43	0.51
1:I:360:ARG:NH1	1:I:371:GLU:OE2	2.43	0.51
1:I:415:ILE:O	1:I:503:ILE:HG23	2.11	0.51
1:I:423:ILE:HD12	1:I:424:GLU:H	1.73	0.51
1:A:415:ILE:O	1:A:503:ILE:HG23	2.11	0.51
1:B:360:ARG:NH1	1:B:371:GLU:OE2	2.43	0.51
1:C:306:GLU:HA	1:C:309:GLN:NE2	2.25	0.51
1:D:360:ARG:NH1	1:D:371:GLU:OE2	2.43	0.51
1:E:423:ILE:CD1	1:E:424:GLU:HG2	2.39	0.51
1:F:162:ARG:HH11	1:F:162:ARG:CB	2.23	0.51
1:G:423:ILE:HD12	1:G:423:ILE:C	2.30	0.51
1:I:423:ILE:HD11	1:I:477:HIS:NE2	2.26	0.51
1:B:245:LYS:HG2	1:B:353:TYR:HD1	1.76	0.51
1:C:360:ARG:NH1	1:C:371:GLU:OE2	2.43	0.51
1:E:255:VAL:HA	1:E:283:ILE:CD1	2.41	0.51
1:F:76:LEU:CD2	1:F:90:VAL:HG12	2.36	0.51
1:F:361:LYS:CB	1:F:366:LYS:HG2	2.36	0.51
1:F:423:ILE:HD11	1:F:477:HIS:NE2	2.26	0.51
1:I:162:ARG:HH11	1:I:162:ARG:CB	2.23	0.51
1:A:127:HIS:HD2	1:A:129:THR:CG2	2.24	0.51
1:B:71:ASP:O	1:B:75:ILE:HG12	2.11	0.51
1:B:127:HIS:ND1	1:B:128:PRO:HD2	2.25	0.51
1:B:290:ILE:HG21	1:B:298:ILE:CD1	2.40	0.51
1:C:108:VAL:O	1:C:111:SER:HB3	2.11	0.51
1:C:127:HIS:ND1	1:C:128:PRO:HD2	2.25	0.51
1:D:415:ILE:O	1:D:503:ILE:HG23	2.11	0.51
1:E:244:ALA:C	1:E:296:ASN:HD22	2.12	0.51
1:E:423:ILE:HD12	1:E:423:ILE:C	2.30	0.51
1:G:423:ILE:HD11	1:G:477:HIS:NE2	2.26	0.51
1:A:108:VAL:O	1:A:111:SER:HB3	2.11	0.51
1:B:127:HIS:HD2	1:B:129:THR:CG2	2.24	0.51
1:C:127:HIS:HD2	1:C:129:THR:CG2	2.24	0.51
1:C:163:LYS:HD3	1:C:501:GLY:HA2	1.93	0.51
1:C:415:ILE:O	1:C:503:ILE:HG23	2.11	0.51
1:F:482:ASN:O	1:F:483:LYS:C	2.47	0.51



	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:255:VAL:HA	1:H:283:ILE:CD1	2.41	0.51
1:I:245:LYS:HG2	1:I:353:TYR:HD1	1.76	0.51
1:A:234:HIS:CD2	1:A:236:GLY:H	2.28	0.50
1:B:161:LEU:HD12	1:B:161:LEU:H	1.77	0.50
1:B:163:LYS:HD3	1:B:501:GLY:HA2	1.93	0.50
1:C:166:MET:HE1	1:C:179:GLU:HG2	1.93	0.50
1:C:244:ALA:C	1:C:296:ASN:HD22	2.12	0.50
1:C:245:LYS:HG2	1:C:353:TYR:HD1	1.76	0.50
1:C:505:PRO:O	1:C:508:VAL:HG12	2.12	0.50
1:D:71:ASP:O	1:D:75:ILE:HG12	2.11	0.50
1:D:127:HIS:ND1	1:D:128:PRO:HD2	2.25	0.50
1:D:230:LYS:HZ1	1:D:321:ARG:NH1	2.09	0.50
1:D:231:GLU:HG3	1:D:366:LYS:NZ	2.24	0.50
1:F:415:ILE:O	1:F:503:ILE:HG23	2.11	0.50
1:G:231:GLU:HG3	1:G:366:LYS:NZ	2.24	0.50
1:G:415:ILE:O	1:G:503:ILE:HG23	2.11	0.50
1:I:108:VAL:O	1:I:111:SER:HB3	2.11	0.50
1:I:280:GLU:O	1:I:284:LYS:HG3	2.12	0.50
1:C:255:VAL:HA	1:C:283:ILE:CD1	2.41	0.50
1:D:34:ALA:O	1:D:37:ALA:HB3	2.12	0.50
1:E:108:VAL:O	1:E:111:SER:HB3	2.11	0.50
1:F:108:VAL:O	1:F:111:SER:HB3	2.11	0.50
1:F:208:GLN:HE22	1:F:227:VAL:H	1.60	0.50
1:F:306:GLU:HA	1:F:309:GLN:NE2	2.25	0.50
1:G:71:ASP:O	1:G:75:ILE:HG12	2.11	0.50
1:G:76:LEU:CD2	1:G:90:VAL:HG12	2.36	0.50
1:H:280:GLU:O	1:H:284:LYS:HG3	2.12	0.50
1:H:415:ILE:O	1:H:503:ILE:HG23	2.11	0.50
1:I:505:PRO:O	1:I:508:VAL:HG12	2.11	0.50
1:A:71:ASP:O	1:A:75:ILE:HG12	2.11	0.50
1:A:280:GLU:O	1:A:284:LYS:HG3	2.12	0.50
1:A:306:GLU:HA	1:A:309:GLN:NE2	2.25	0.50
1:A:479:ASN:CB	1:A:482:ASN:OD1	2.59	0.50
1:B:231:GLU:HG3	1:B:366:LYS:NZ	2.24	0.50
1:D:76:LEU:CD2	1:D:90:VAL:HG12	2.36	0.50
1:G:208:GLN:HE22	1:G:227:VAL:H	1.60	0.50
1:G:230:LYS:HZ2	1:G:321:ARG:NH1	2.10	0.50
1:G:245:LYS:HG2	1:G:353:TYR:HD1	1.76	0.50
1:H:479:ASN:CB	1:H:482:ASN:OD1	2.59	0.50
1:C:423:ILE:HD11	1:C:477:HIS:NE2	2.26	0.50
1:D:127:HIS:HD2	1:D:129:THR:CG2	2.24	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:245:LYS:HG2	1:D:353:TYR:HD1	1.76	0.50
1:E:290:ILE:HG21	1:E:298:ILE:CD1	2.40	0.50
1:E:505:PRO:O	1:E:508:VAL:HG12	2.12	0.50
1:F:127:HIS:HD2	1:F:129:THR:CG2	2.24	0.50
1:H:108:VAL:O	1:H:111:SER:HB3	2.11	0.50
1:I:85:ALA:O	1:I:88:LEU:HB3	2.12	0.50
1:I:244:ALA:C	1:I:296:ASN:HD22	2.12	0.50
1:A:230:LYS:HZ2	1:A:321:ARG:NH1	2.08	0.50
1:A:422:GLU:OE1	1:A:422:GLU:N	2.45	0.50
1:C:34:ALA:O	1:C:37:ALA:HB3	2.12	0.50
1:C:85:ALA:O	1:C:88:LEU:HB3	2.12	0.50
1:F:280:GLU:O	1:F:284:LYS:HG3	2.12	0.50
1:F:393:GLU:HG3	1:F:396:ARG:HH21	1.77	0.50
1:H:245:LYS:HG2	1:H:353:TYR:HD1	1.76	0.50
1:I:68:ILE:O	1:I:68:ILE:HG13	2.10	0.50
1:I:284:LYS:HD3	1:I:311:TYR:CE2	2.43	0.50
1:I:479:ASN:CB	1:I:482:ASN:OD1	2.59	0.50
1:A:85:ALA:O	1:A:88:LEU:HB3	2.12	0.50
1:B:422:GLU:OE1	1:B:422:GLU:N	2.45	0.50
1:E:88:LEU:HD11	1:F:389:ARG:NH1	2.18	0.50
1:E:127:HIS:HD2	1:E:129:THR:CG2	2.24	0.50
1:G:34:ALA:O	1:G:37:ALA:HB3	2.12	0.50
1:G:423:ILE:HG21	1:G:473:LEU:CD1	2.42	0.50
1:H:393:GLU:HG3	1:H:396:ARG:HH21	1.77	0.50
1:H:470:LEU:O	1:H:470:LEU:HD23	2.12	0.50
1:I:255:VAL:HA	1:I:283:ILE:CD1	2.41	0.50
1:I:422:GLU:OE1	1:I:422:GLU:N	2.45	0.50
1:I:423:ILE:HG21	1:I:473:LEU:CD1	2.42	0.50
1:A:91:GLN:NE2	1:B:387:LEU:HD21	2.26	0.50
1:B:162:ARG:HH11	1:B:162:ARG:CB	2.23	0.50
1:D:470:LEU:O	1:D:470:LEU:HD23	2.12	0.50
1:F:71:ASP:O	1:F:75:ILE:HG12	2.11	0.50
1:F:470:LEU:O	1:F:470:LEU:HD23	2.12	0.50
1:G:108:VAL:O	1:G:111:SER:HB3	2.11	0.50
1:G:479:ASN:CB	1:G:482:ASN:OD1	2.59	0.50
1:H:71:ASP:O	1:H:75:ILE:HG12	2.11	0.50
1:I:209:ILE:HD12	1:I:209:ILE:N	2.27	0.50
1:A:437:GLY:O	1:A:441:GLN:HB2	2.12	0.50
1:A:470:LEU:O	1:A:470:LEU:HD23	2.12	0.50
1:B:212:LYS:HA	1:B:212:LYS:CE	2.33	0.50
1:B:220:THR:HB	1:B:382:LEU:O	2.12	0.50



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:505:PRO:O	1:B:508:VAL:HG12	2.12	0.50
1:E:393:GLU:HG3	1:E:396:ARG:HH21	1.77	0.50
1:G:209:ILE:HD12	1:G:209:ILE:N	2.27	0.50
1:G:470:LEU:O	1:G:470:LEU:HD23	2.12	0.50
1:H:163:LYS:HD3	1:H:501:GLY:HA2	1.93	0.50
1:H:208:GLN:HE22	1:H:227:VAL:H	1.60	0.50
1:H:423:ILE:HG21	1:H:473:LEU:CD1	2.42	0.50
1:I:376:PRO:HG2	1:I:377:LYS:H	1.77	0.50
1:A:290:ILE:HG21	1:A:298:ILE:CD1	2.40	0.50
1:B:108:VAL:O	1:B:111:SER:HB3	2.11	0.50
1:B:470:LEU:O	1:B:470:LEU:HD23	2.12	0.50
1:D:423:ILE:HG21	1:D:473:LEU:CD1	2.42	0.50
1:F:163:LYS:HD3	1:F:501:GLY:HA2	1.93	0.50
1:F:220:THR:HB	1:F:382:LEU:O	2.12	0.50
1:F:245:LYS:HG2	1:F:353:TYR:HD1	1.76	0.50
1:F:505:PRO:O	1:F:508:VAL:HG12	2.11	0.50
1:G:393:GLU:HG3	1:G:396:ARG:HH21	1.77	0.50
1:H:376:PRO:HG2	1:H:377:LYS:H	1.77	0.50
1:I:470:LEU:O	1:I:470:LEU:HD23	2.12	0.50
1:B:415:ILE:O	1:B:503:ILE:HG23	2.11	0.49
1:B:426:ALA:O	1:B:429:LEU:N	2.46	0.49
1:C:208:GLN:HE22	1:C:227:VAL:H	1.59	0.49
1:C:422:GLU:N	1:C:422:GLU:OE1	2.45	0.49
1:C:437:GLY:O	1:C:441:GLN:HB2	2.12	0.49
1:D:85:ALA:O	1:D:88:LEU:HB3	2.12	0.49
1:D:230:LYS:HZ2	1:D:321:ARG:NH1	2.09	0.49
1:E:36:ILE:HG23	1:E:115:VAL:HG12	1.94	0.49
1:E:85:ALA:O	1:E:88:LEU:HB3	2.12	0.49
1:E:208:GLN:HE22	1:E:227:VAL:H	1.60	0.49
1:E:220:THR:HB	1:E:382:LEU:O	2.12	0.49
1:E:245:LYS:HG2	1:E:353:TYR:HD1	1.76	0.49
1:E:422:GLU:OE1	1:E:422:GLU:N	2.45	0.49
1:F:85:ALA:O	1:F:88:LEU:HB3	2.12	0.49
1:H:127:HIS:HD2	1:H:129:THR:CG2	2.24	0.49
1:H:209:ILE:N	1:H:209:ILE:HD12	2.27	0.49
1:I:71:ASP:O	1:I:75:ILE:HG12	2.11	0.49
1:A:34:ALA:O	1:A:37:ALA:HB3	2.12	0.49
1:A:163:LYS:HD3	1:A:501:GLY:HA2	1.93	0.49
1:A:208:GLN:HE22	1:A:227:VAL:H	1.60	0.49
1:A:255:VAL:HA	1:A:283:ILE:CD1	2.41	0.49
1:B:208:GLN:HE22	1:B:227:VAL:H	1.60	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:280:GLU:O	1:B:284:LYS:HG3	2.12	0.49
1:B:423:ILE:HG21	1:B:473:LEU:CD1	2.42	0.49
1:C:280:GLU:O	1:C:284:LYS:HG3	2.12	0.49
1:D:163:LYS:HD3	1:D:501:GLY:HA2	1.93	0.49
1:D:209:ILE:HD12	1:D:209:ILE:N	2.27	0.49
1:D:422:GLU:OE1	1:D:422:GLU:N	2.45	0.49
1:F:423:ILE:HG21	1:F:473:LEU:CD1	2.42	0.49
1:F:426:ALA:O	1:F:429:LEU:N	2.45	0.49
1:G:127:HIS:HD2	1:G:129:THR:CG2	2.24	0.49
1:G:505:PRO:O	1:G:508:VAL:HG12	2.11	0.49
1:H:437:GLY:O	1:H:441:GLN:HB2	2.12	0.49
1:I:127:HIS:HD2	1:I:129:THR:CG2	2.24	0.49
1:I:393:GLU:HG3	1:I:396:ARG:HH21	1.77	0.49
1:A:209:ILE:HD12	1:A:209:ILE:N	2.27	0.49
1:A:393:GLU:HG3	1:A:396:ARG:HH21	1.77	0.49
1:B:85:ALA:O	1:B:88:LEU:HB3	2.12	0.49
1:B:437:GLY:O	1:B:441:GLN:HB2	2.12	0.49
1:C:71:ASP:O	1:C:75:ILE:HG12	2.11	0.49
1:C:376:PRO:HG2	1:C:377:LYS:H	1.77	0.49
1:C:393:GLU:HG3	1:C:396:ARG:HH21	1.77	0.49
1:D:280:GLU:O	1:D:284:LYS:HG3	2.12	0.49
1:D:479:ASN:CB	1:D:482:ASN:OD1	2.59	0.49
1:E:34:ALA:O	1:E:37:ALA:HB3	2.12	0.49
1:E:71:ASP:O	1:E:75:ILE:HG12	2.11	0.49
1:E:437:GLY:O	1:E:441:GLN:HB2	2.12	0.49
1:G:230:LYS:HZ1	1:G:321:ARG:HH12	1.60	0.49
1:G:422:GLU:OE1	1:G:422:GLU:N	2.45	0.49
1:A:246:ILE:HA	1:A:297:VAL:HG13	1.94	0.49
1:A:505:PRO:O	1:A:508:VAL:HG12	2.11	0.49
1:C:246:ILE:HA	1:C:297:VAL:HG13	1.94	0.49
1:C:470:LEU:O	1:C:470:LEU:HD23	2.12	0.49
1:D:108:VAL:O	1:D:111:SER:HB3	2.11	0.49
1:F:423:ILE:HD12	1:F:423:ILE:C	2.30	0.49
1:I:163:LYS:HD3	1:I:501:GLY:HA2	1.93	0.49
1:A:161:LEU:HD12	1:A:161:LEU:H	1.77	0.49
1:B:209:ILE:N	1:B:209:ILE:HD12	2.27	0.49
1:B:210:VAL:HG23	1:B:382:LEU:HD12	1.95	0.49
1:E:230:LYS:HZ1	1:E:321:ARG:NH1	2.10	0.49
1:E:280:GLU:O	1:E:284:LYS:HG3	2.12	0.49
1:E:415:ILE:O	1:E:503:1LE:HG23	2.11	0.49
1:E:423:ILE:HG21	1:E:473:LEU:CD1	2.42	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:34:ALA:O	1:F:37:ALA:HB3	2.12	0.49
1:F:422:GLU:OE1	1:F:422:GLU:N	2.45	0.49
1:F:530:VAL:O	1:G:59:LEU:HA	2.12	0.49
1:G:280:GLU:O	1:G:284:LYS:HG3	2.12	0.49
1:H:36:ILE:HG23	1:H:115:VAL:HG12	1.95	0.49
1:I:34:ALA:O	1:I:37:ALA:HB3	2.12	0.49
1:C:220:THR:HB	1:C:382:LEU:O	2.12	0.49
1:C:423:ILE:HG21	1:C:473:LEU:CD1	2.42	0.49
1:C:503:ILE:HG22	1:C:504:GLU:N	2.28	0.49
1:D:505:PRO:O	1:D:508:VAL:HG12	2.11	0.49
1:E:161:LEU:HD12	1:E:161:LEU:H	1.77	0.49
1:E:209:ILE:N	1:E:209:ILE:HD12	2.27	0.49
1:G:36:ILE:HG23	1:G:115:VAL:HG12	1.94	0.49
1:G:163:LYS:HD3	1:G:501:GLY:HA2	1.93	0.49
1:G:376:PRO:HG2	1:G:377:LYS:H	1.77	0.49
1:H:34:ALA:O	1:H:37:ALA:HB3	2.12	0.49
1:H:85:ALA:O	1:H:88:LEU:HB3	2.12	0.49
1:I:220:THR:HB	1:I:382:LEU:O	2.12	0.49
1:I:503:ILE:N	1:I:503:ILE:HD12	2.28	0.49
1:A:212:LYS:HA	1:A:212:LYS:CE	2.33	0.49
1:A:220:THR:HB	1:A:382:LEU:O	2.12	0.49
1:B:34:ALA:O	1:B:37:ALA:HB3	2.12	0.49
1:B:36:ILE:HG23	1:B:115:VAL:HG12	1.95	0.49
1:B:255:VAL:HA	1:B:283:ILE:CD1	2.41	0.49
1:B:503:ILE:HG22	1:B:504:GLU:N	2.28	0.49
1:C:36:ILE:HG23	1:C:115:VAL:HG12	1.94	0.49
1:C:503:ILE:HD12	1:C:503:ILE:N	2.28	0.49
1:D:393:GLU:HG3	1:D:396:ARG:HH21	1.77	0.49
1:D:437:GLY:O	1:D:441:GLN:HB2	2.12	0.49
1:E:470:LEU:O	1:E:470:LEU:HD23	2.12	0.49
1:E:503:ILE:HG22	1:E:504:GLU:N	2.28	0.49
1:F:36:ILE:HG23	1:F:115:VAL:HG12	1.94	0.49
1:F:246:ILE:HA	1:F:297:VAL:HG13	1.94	0.49
1:G:85:ALA:O	1:G:88:LEU:HB3	2.12	0.49
1:I:36:ILE:HG23	1:I:115:VAL:HG12	1.95	0.49
1:A:426:ALA:O	1:A:429:LEU:N	2.45	0.49
1:B:393:GLU:HG3	1:B:396:ARG:HH21	1.77	0.49
1:C:209:ILE:N	1:C:209:ILE:HD12	2.27	0.49
1:D:208:GLN:HE22	1:D:227:VAL:H	1.59	0.49
1:D:220:THR:HB	1:D:382:LEU:O	2.12	0.49
1:E:163:LYS:HD3	1:E:501:GLY:HA2	1.93	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:209:ILE:HD12	1:F:209:ILE:N	2.27	0.49
1:F:376:PRO:HG2	1:F:377:LYS:H	1.77	0.49
1:G:220:THR:HB	1:G:382:LEU:O	2.12	0.49
1:G:246:ILE:HA	1:G:297:VAL:HG13	1.95	0.49
1:G:437:GLY:O	1:G:441:GLN:HB2	2.12	0.49
1:H:505:PRO:O	1:H:508:VAL:HG12	2.11	0.49
1:C:426:ALA:O	1:C:429:LEU:N	2.45	0.49
1:D:161:LEU:HD12	1:D:161:LEU:H	1.77	0.49
1:D:230:LYS:HZ1	1:D:321:ARG:HH12	1.60	0.49
1:E:76:LEU:CD2	1:E:90:VAL:HG12	2.36	0.49
1:E:376:PRO:HG2	1:E:377:LYS:H	1.77	0.49
1:E:479:ASN:CB	1:E:482:ASN:OD1	2.59	0.49
1:F:290:ILE:HG21	1:F:298:ILE:CD1	2.40	0.49
1:G:161:LEU:HD12	1:G:161:LEU:H	1.77	0.49
1:H:422:GLU:N	1:H:422:GLU:OE1	2.45	0.49
1:H:423:ILE:HD12	1:H:424:GLU:H	1.73	0.49
1:H:503:ILE:HG22	1:H:504:GLU:N	2.28	0.49
1:I:161:LEU:HD12	1:I:161:LEU:H	1.76	0.49
1:I:290:ILE:HG21	1:I:298:ILE:CD1	2.40	0.49
1:A:245:LYS:HG2	1:A:353:TYR:HD1	1.76	0.49
1:C:127:HIS:HD2	1:C:129:THR:CB	2.26	0.49
1:D:503:ILE:N	1:D:503:ILE:HD12	2.28	0.49
1:D:503:ILE:HG22	1:D:504:GLU:N	2.28	0.49
1:H:127:HIS:HD2	1:H:129:THR:CB	2.26	0.49
1:A:127:HIS:HD2	1:A:129:THR:CB	2.26	0.48
1:A:423:ILE:HG21	1:A:473:LEU:CD1	2.42	0.48
1:A:503:ILE:HG22	1:A:504:GLU:N	2.28	0.48
1:B:110:PHE:O	1:B:114:LEU:HD13	2.13	0.48
1:C:58:MET:HG3	1:C:68:ILE:CG2	2.43	0.48
1:C:479:ASN:CB	1:C:482:ASN:OD1	2.59	0.48
1:D:66:ILE:CD1	1:D:66:ILE:N	2.76	0.48
1:E:426:ALA:O	1:E:429:LEU:N	2.45	0.48
1:F:255:VAL:HA	1:F:283:ILE:CD1	2.41	0.48
1:F:263:GLU:C	1:F:264:ILE:HG22	2.34	0.48
1:F:423:ILE:HD12	1:F:424:GLU:H	1.73	0.48
1:G:230:LYS:HZ1	1:G:321:ARG:NH1	2.09	0.48
1:H:246:ILE:HA	1:H:297:VAL:HG13	1.94	0.48
1:I:210:VAL:HG23	1:I:382:LEU:HD12	1.95	0.48
1:I:423:ILE:HD12	1:I:423:ILE:C	2.30	0.48
1:I:503:ILE:HG22	1:I:504:GLU:N	2.28	0.48
1:A:36:ILE:HG23	1:A:115:VAL:HG12	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:110:PHE:O	1:D:114:LEU:HD13	2.13	0.48
1:D:255:VAL:HA	1:D:283:ILE:CD1	2.41	0.48
1:D:482:ASN:O	1:D:485:TYR:N	2.40	0.48
1:E:263:GLU:C	1:E:264:ILE:HG22	2.34	0.48
1:F:58:MET:HG3	1:F:68:ILE:CG2	2.44	0.48
1:F:210:VAL:HG23	1:F:382:LEU:HD12	1.95	0.48
1:G:110:PHE:O	1:G:114:LEU:HD13	2.13	0.48
1:H:110:PHE:O	1:H:114:LEU:HD13	2.13	0.48
1:H:217:ILE:HD11	1:H:390:LEU:CD2	2.44	0.48
1:H:220:THR:HB	1:H:382:LEU:O	2.12	0.48
1:H:522:LEU:HD11	1:I:68:ILE:CD1	2.43	0.48
1:I:208:GLN:HE22	1:I:227:VAL:H	1.60	0.48
1:B:127:HIS:HD2	1:B:129:THR:CB	2.26	0.48
1:B:217:ILE:HD11	1:B:390:LEU:CD2	2.44	0.48
1:B:358:GLU:CG	1:B:360:ARG:HH22	2.27	0.48
1:B:376:PRO:HG2	1:B:377:LYS:H	1.77	0.48
1:E:127:HIS:HD2	1:E:129:THR:CB	2.26	0.48
1:F:161:LEU:HD12	1:F:161:LEU:H	1.77	0.48
1:H:58:MET:HG3	1:H:68:ILE:CG2	2.44	0.48
1:H:232:VAL:HG12	1:H:318:LEU:HD11	1.95	0.48
1:H:263:GLU:C	1:H:264:ILE:HG22	2.34	0.48
1:H:426:ALA:O	1:H:429:LEU:N	2.45	0.48
1:I:246:ILE:HA	1:I:297:VAL:HG13	1.94	0.48
1:I:437:GLY:O	1:I:441:GLN:HB2	2.12	0.48
1:I:482:ASN:O	1:I:485:TYR:N	2.40	0.48
1:A:110:PHE:O	1:A:114:LEU:HD13	2.13	0.48
1:A:423:ILE:HD12	1:A:424:GLU:H	1.73	0.48
1:E:255:VAL:HG13	1:E:305:ASP:CG	2.34	0.48
1:E:330:LYS:O	1:E:334:ALA:HB2	2.14	0.48
1:F:437:GLY:O	1:F:441:GLN:HB2	2.12	0.48
1:G:66:ILE:CD1	1:G:66:ILE:N	2.76	0.48
1:G:232:VAL:HG12	1:G:318:LEU:HD11	1.95	0.48
1:I:232:VAL:HG12	1:I:318:LEU:HD11	1.95	0.48
1:I:426:ALA:O	1:I:429:LEU:N	2.45	0.48
1:A:244:ALA:C	1:A:296:ASN:HD22	2.12	0.48
1:B:255:VAL:HG13	1:B:305:ASP:CG	2.34	0.48
1:B:263:GLU:C	1:B:264:ILE:HG22	2.34	0.48
1:C:469:LEU:HB3	1:C:487:ILE:CD1	2.43	0.48
1:D:36:ILE:HG23	1:D:115:VAL:HG12	1.94	0.48
1:D:127:HIS:HD2	1:D:129:THR:CB	2.26	0.48
1:D:210:VAL:HG23	1:D:382:LEU:HD12	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:232:VAL:HG11	1:D:318:LEU:HD11	1.95	0.48
1:D:376:PRO:HG2	1:D:377:LYS:H	1.77	0.48
1:E:246:ILE:HA	1:E:297:VAL:HG13	1.94	0.48
1:G:426:ALA:O	1:G:429:LEU:N	2.45	0.48
1:G:503:ILE:HG22	1:G:504:GLU:N	2.28	0.48
1:H:255:VAL:HG13	1:H:305:ASP:CG	2.34	0.48
1:I:358:GLU:CG	1:I:360:ARG:HH22	2.27	0.48
1:A:361:LYS:CB	1:A:366:LYS:HG2	2.36	0.48
1:B:58:MET:HG3	1:B:68:ILE:CG2	2.44	0.48
1:B:66:ILE:CD1	1:B:66:ILE:N	2.76	0.48
1:C:161:LEU:HD12	1:C:161:LEU:H	1.77	0.48
1:C:232:VAL:HG12	1:C:318:LEU:HD11	1.95	0.48
1:C:263:GLU:C	1:C:264:ILE:HG22	2.34	0.48
1:D:58:MET:HG3	1:D:68:ILE:CG2	2.44	0.48
1:D:166:MET:HE1	1:D:179:GLU:HG2	1.96	0.48
1:D:246:ILE:HA	1:D:297:VAL:HG13	1.94	0.48
1:D:263:GLU:C	1:D:264:ILE:HG22	2.34	0.48
1:F:110:PHE:O	1:F:114:LEU:HD13	2.13	0.48
1:F:503:ILE:N	1:F:503:ILE:HD12	2.28	0.48
1:G:58:MET:HG3	1:G:68:ILE:CG2	2.44	0.48
1:G:255:VAL:HG13	1:G:305:ASP:CG	2.34	0.48
1:A:227:VAL:HG22	1:A:369:PHE:HD1	1.79	0.48
1:C:210:VAL:HG23	1:C:382:LEU:HD12	1.95	0.48
1:D:255:VAL:HG13	1:D:305:ASP:CG	2.34	0.48
1:E:58:MET:HG3	1:E:68:ILE:CG2	2.44	0.48
1:E:358:GLU:CG	1:E:360:ARG:HH22	2.27	0.48
1:E:473:LEU:C	1:E:473:LEU:HD13	2.34	0.48
1:F:479:ASN:CB	1:F:482:ASN:OD1	2.59	0.48
1:G:127:HIS:HD2	1:G:129:THR:CB	2.26	0.48
1:G:227:VAL:HG22	1:G:369:PHE:HD1	1.79	0.48
1:G:232:VAL:HG11	1:G:318:LEU:HD11	1.95	0.48
1:G:358:GLU:CG	1:G:360:ARG:HH22	2.27	0.48
1:G:503:ILE:N	1:G:503:ILE:HD12	2.28	0.48
1:H:503:ILE:HD12	1:H:503:ILE:N	2.28	0.48
1:H:529:VAL:HG12	1:I:58:MET:HB3	1.95	0.48
1:I:110:PHE:O	1:I:114:LEU:HD13	2.13	0.48
1:I:127:HIS:HD2	1:I:129:THR:CB	2.26	0.48
1:A:58:MET:HG3	1:A:68:ILE:CG2	2.44	0.48
1:A:473:LEU:HD13	1:A:473:LEU:C	2.34	0.48
1:B:479:ASN:CB	1:B:482:ASN:OD1	2.59	0.48
1:C:358:GLU:CG	1:C:360:ARG:HH22	2.27	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:263:GLU:C	1:D:264:ILE:CG2	2.82	0.48
1:H:260:LEU:CD1	1:H:260:LEU:C	2.81	0.48
1:I:263:GLU:C	1:I:264:ILE:HG22	2.34	0.48
1:A:255:VAL:HG13	1:A:305:ASP:CG	2.34	0.48
1:A:299:ILE:HG22	1:A:320:VAL:HG23	1.96	0.48
1:A:503:ILE:N	1:A:503:ILE:HD12	2.28	0.48
1:B:330:LYS:O	1:B:334:ALA:HB2	2.14	0.48
1:B:503:ILE:HD12	1:B:503:ILE:N	2.28	0.48
1:C:232:VAL:HG11	1:C:318:LEU:HD11	1.95	0.48
1:C:423:ILE:HD12	1:C:424:GLU:H	1.73	0.48
1:D:212:LYS:HA	1:D:212:LYS:CE	2.33	0.48
1:F:232:VAL:HG12	1:F:318:LEU:HD11	1.95	0.48
1:F:246:ILE:O	1:F:351:LEU:HB2	2.14	0.48
1:F:299:ILE:HG22	1:F:320:VAL:HG23	1.96	0.48
1:F:358:GLU:CG	1:F:360:ARG:HH22	2.27	0.48
1:F:503:ILE:HG22	1:F:504:GLU:N	2.28	0.48
1:H:246:ILE:O	1:H:351:LEU:HB2	2.14	0.48
1:A:263:GLU:C	1:A:264:ILE:HG22	2.34	0.48
1:A:376:PRO:HG2	1:A:377:LYS:H	1.77	0.48
1:B:469:LEU:HB3	1:B:487:ILE:CD1	2.43	0.48
1:C:110:PHE:O	1:C:114:LEU:HD13	2.13	0.48
1:F:217:ILE:HD11	1:F:390:LEU:CD2	2.44	0.48
1:G:330:LYS:O	1:G:334:ALA:HB2	2.14	0.48
1:A:210:VAL:HG23	1:A:382:LEU:HD12	1.95	0.47
1:B:473:LEU:C	1:B:473:LEU:HD13	2.34	0.47
1:C:290:ILE:HG21	1:C:298:ILE:CD1	2.40	0.47
1:D:227:VAL:HG22	1:D:369:PHE:HD1	1.79	0.47
1:D:469:LEU:HB3	1:D:487:ILE:CD1	2.43	0.47
1:F:255:VAL:HG13	1:F:305:ASP:CG	2.34	0.47
1:G:263:GLU:C	1:G:264:ILE:CG2	2.82	0.47
1:H:263:GLU:C	1:H:264:ILE:CG2	2.82	0.47
1:H:330:LYS:O	1:H:334:ALA:HB2	2.14	0.47
1:I:58:MET:HG3	1:I:68:ILE:CG2	2.44	0.47
1:I:178:ARG:H	1:I:178:ARG:NE	2.12	0.47
1:A:178:ARG:H	1:A:178:ARG:NE	2.12	0.47
1:A:232:VAL:HG11	1:A:318:LEU:HD11	1.95	0.47
1:B:230:LYS:HZ1	1:B:321:ARG:HH12	1.62	0.47
1:C:217:ILE:HD11	1:C:390:LEU:CD2	2.44	0.47
1:C:260:LEU:CD1	1:C:260:LEU:C	2.81	0.47
1:E:110:PHE:O	1:E:114:LEU:HD13	2.13	0.47
1:E:503:ILE:HD12	1:E:503:ILE:N	2.28	0.47



	i a s pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:210:VAL:HG23	1:G:382:LEU:HD12	1.95	0.47
1:G:217:ILE:HD11	1:G:390:LEU:CD2	2.44	0.47
1:G:263:GLU:C	1:G:264:ILE:HG22	2.34	0.47
1:H:214:GLY:HA3	1:H:384:ARG:HH21	1.79	0.47
1:H:227:VAL:HG22	1:H:369:PHE:HD1	1.79	0.47
1:I:436:VAL:HG23	1:I:437:GLY:N	2.30	0.47
1:A:246:ILE:O	1:A:351:LEU:HB2	2.14	0.47
1:B:232:VAL:HG12	1:B:318:LEU:HD11	1.95	0.47
1:B:246:ILE:O	1:B:351:LEU:HB2	2.14	0.47
1:C:76:LEU:CD2	1:C:90:VAL:HG12	2.36	0.47
1:C:227:VAL:HG22	1:C:369:PHE:HD1	1.79	0.47
1:D:214:GLY:HA3	1:D:384:ARG:HH21	1.79	0.47
1:D:249:ILE:HD12	1:D:346:ILE:HD11	1.96	0.47
1:D:299:ILE:HG22	1:D:320:VAL:HG23	1.96	0.47
1:E:232:VAL:HG11	1:E:318:LEU:HD11	1.96	0.47
1:F:127:HIS:HD2	1:F:129:THR:CB	2.26	0.47
1:F:214:GLY:HA3	1:F:384:ARG:HH21	1.79	0.47
1:F:482:ASN:O	1:F:485:TYR:N	2.40	0.47
1:G:178:ARG:H	1:G:178:ARG:NE	2.12	0.47
1:I:249:ILE:HD12	1:I:346:ILE:HD11	1.96	0.47
1:A:121:LEU:HB3	1:A:126:VAL:CG2	2.44	0.47
1:A:214:GLY:HA3	1:A:384:ARG:HH21	1.79	0.47
1:A:528:ASP:OD2	1:A:529:VAL:N	2.48	0.47
1:B:227:VAL:HG22	1:B:369:PHE:HD1	1.79	0.47
1:B:246:ILE:HA	1:B:297:VAL:HG13	1.94	0.47
1:B:249:ILE:HD12	1:B:346:ILE:HD11	1.96	0.47
1:C:211:LYS:HE3	1:C:395:GLU:OE2	2.14	0.47
1:D:121:LEU:HB3	1:D:126:VAL:CG2	2.44	0.47
1:D:246:ILE:O	1:D:351:LEU:HB2	2.14	0.47
1:D:258:PRO:CG	1:D:279:GLU:OE2	2.56	0.47
1:E:210:VAL:HG23	1:E:382:LEU:HD12	1.95	0.47
1:E:423:ILE:HD12	1:E:424:GLU:H	1.73	0.47
1:F:211:LYS:HE3	1:F:395:GLU:OE2	2.14	0.47
1:H:211:LYS:HE3	1:H:395:GLU:OE2	2.14	0.47
1:H:299:ILE:HG22	1:H:320:VAL:HG23	1.96	0.47
1:H:436:VAL:HG23	1:H:437:GLY:N	2.30	0.47
1:I:246:ILE:O	1:I:351:LEU:HB2	2.14	0.47
1:A:330:LYS:O	1:A:334:ALA:HB2	2.14	0.47
1:B:528:ASP:OD2	1:B:529:VAL:N	2.48	0.47
1:C:141:VAL:CG2	1:C:432:TYR:CE1	2.97	0.47
1:D:358:GLU:CG	1:D:360:ARG:HH22	2.27	0.47



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:230:LYS:HZ1	1:E:321:ARG:HH12	1.61	0.47
1:F:232:VAL:HG11	1:F:318:LEU:HD11	1.95	0.47
1:F:473:LEU:HD13	1:F:473:LEU:C	2.34	0.47
1:G:299:ILE:HG22	1:G:320:VAL:HG23	1.96	0.47
1:G:473:LEU:C	1:G:473:LEU:HD13	2.34	0.47
1:H:178:ARG:H	1:H:178:ARG:NE	2.12	0.47
1:H:473:LEU:HD13	1:H:473:LEU:C	2.34	0.47
1:I:361:LYS:CB	1:I:366:LYS:HG2	2.36	0.47
1:I:528:ASP:OD2	1:I:529:VAL:N	2.48	0.47
1:B:436:VAL:HG23	1:B:437:GLY:N	2.30	0.47
1:C:330:LYS:O	1:C:334:ALA:HB2	2.14	0.47
1:G:121:LEU:HB3	1:G:126:VAL:CG2	2.44	0.47
1:G:211:LYS:HE3	1:G:395:GLU:OE2	2.14	0.47
1:H:46:LEU:O	1:H:47:LYS:C	2.53	0.47
1:A:46:LEU:O	1:A:47:LYS:C	2.53	0.47
1:A:230:LYS:HZ1	1:A:321:ARG:NH1	2.10	0.47
1:A:232:VAL:HG12	1:A:318:LEU:HD11	1.95	0.47
1:A:249:ILE:HD12	1:A:346:ILE:HD11	1.96	0.47
1:A:263:GLU:C	1:A:264:ILE:CG2	2.82	0.47
1:A:271:GLN:OE1	1:A:271:GLN:HA	2.15	0.47
1:A:358:GLU:CG	1:A:360:ARG:HH22	2.27	0.47
1:A:359:GLU:O	1:A:359:GLU:HG2	2.15	0.47
1:A:469:LEU:HB3	1:A:487:ILE:CD1	2.43	0.47
1:B:75:ILE:O	1:B:79:MET:HB3	2.15	0.47
1:B:121:LEU:HB3	1:B:126:VAL:CG2	2.44	0.47
1:B:230:LYS:HZ1	1:B:321:ARG:NH1	2.12	0.47
1:C:46:LEU:O	1:C:47:LYS:C	2.53	0.47
1:C:56:ASP:OD1	1:C:70:ASN:HB3	2.15	0.47
1:C:75:ILE:O	1:C:79:MET:HB3	2.15	0.47
1:C:234:HIS:ND1	1:C:235:PRO:HD2	2.30	0.47
1:C:255:VAL:HG13	1:C:305:ASP:CG	2.34	0.47
1:C:430:ARG:HG2	1:C:430:ARG:NH1	2.29	0.47
1:C:436:VAL:HG23	1:C:437:GLY:N	2.30	0.47
1:D:46:LEU:O	1:D:47:LYS:C	2.53	0.47
1:D:75:ILE:O	1:D:79:MET:HB3	2.15	0.47
1:D:211:LYS:HE3	1:D:395:GLU:OE2	2.14	0.47
1:D:282:LEU:O	1:D:285:GLU:HB3	2.15	0.47
1:D:430:ARG:HG2	1:D:430:ARG:NH1	2.29	0.47
1:D:436:VAL:HG23	1:D:437:GLY:N	2.30	0.47
1:E:211:LYS:HE3	1:E:395:GLU:OE2	2.14	0.47
1:E:246:ILE:O	1:E:351:LEU:HB2	2.14	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:436:VAL:HG23	1:E:437:GLY:N	2.30	0.47
1:F:330:LYS:O	1:F:334:ALA:HB2	2.14	0.47
1:F:436:VAL:HG23	1:F:437:GLY:N	2.30	0.47
1:G:234:HIS:ND1	1:G:235:PRO:HD2	2.30	0.47
1:G:258:PRO:CG	1:G:279:GLU:OE2	2.56	0.47
1:G:290:ILE:HG21	1:G:298:ILE:CD1	2.40	0.47
1:I:121:LEU:HB3	1:I:126:VAL:CG2	2.44	0.47
1:I:211:LYS:HE3	1:I:395:GLU:OE2	2.15	0.47
1:I:214:GLY:HA3	1:I:384:ARG:HH21	1.80	0.47
1:I:255:VAL:HG13	1:I:305:ASP:CG	2.34	0.47
1:I:330:LYS:O	1:I:334:ALA:HB2	2.14	0.47
1:I:473:LEU:HD13	1:I:473:LEU:C	2.35	0.47
1:A:234:HIS:ND1	1:A:235:PRO:HD2	2.30	0.47
1:B:232:VAL:HG11	1:B:318:LEU:HD11	1.95	0.47
1:C:214:GLY:HA3	1:C:384:ARG:HH21	1.79	0.47
1:C:473:LEU:HD13	1:C:473:LEU:C	2.34	0.47
1:C:482:ASN:O	1:C:485:TYR:N	2.40	0.47
1:D:217:ILE:HD11	1:D:390:LEU:CD2	2.43	0.47
1:D:234:HIS:ND1	1:D:235:PRO:HD2	2.30	0.47
1:D:473:LEU:C	1:D:473:LEU:HD13	2.34	0.47
1:D:528:ASP:OD2	1:D:529:VAL:N	2.48	0.47
1:F:75:ILE:O	1:F:79:MET:HB3	2.15	0.47
1:F:227:VAL:HG22	1:F:369:PHE:HD1	1.79	0.47
1:F:234:HIS:ND1	1:F:235:PRO:HD2	2.30	0.47
1:F:469:LEU:HB3	1:F:487:ILE:CD1	2.43	0.47
1:F:528:ASP:OD2	1:F:529:VAL:N	2.48	0.47
1:G:359:GLU:HG2	1:G:359:GLU:O	2.15	0.47
1:H:161:LEU:HD12	1:H:161:LEU:H	1.77	0.47
1:H:210:VAL:HG23	1:H:382:LEU:HD12	1.95	0.47
1:H:271:GLN:OE1	1:H:271:GLN:HA	2.15	0.47
1:H:290:ILE:HG21	1:H:298:ILE:CD1	2.40	0.47
1:A:166:MET:HE1	1:A:179:GLU:HG2	1.96	0.47
1:B:46:LEU:O	1:B:47:LYS:C	2.53	0.47
1:B:214:GLY:HA3	1:B:384:ARG:HH21	1.79	0.47
1:B:271:GLN:OE1	1:B:271:GLN:HA	2.15	0.47
1:B:299:ILE:HG22	1:B:320:VAL:HG23	1.96	0.47
1:E:75:ILE:O	1:E:79:MET:HB3	2.15	0.47
1:E:227:VAL:HG22	1:E:369:PHE:HD1	1.79	0.47
1:E:299:ILE:HG22	1:E:320:VAL:HG23	1.96	0.47
1:F:263:GLU:C	1:F:264:ILE:CG2	2.82	0.47
1:F:529:VAL:CG1	1:G:58:MET:SD	3.03	0.47



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:530:VAL:O	1:G:59:LEU:HD22	2.13	0.47
1:G:255:VAL:HA	1:G:283:ILE:CD1	2.41	0.47
1:G:271:GLN:OE1	1:G:271:GLN:HA	2.15	0.47
1:G:528:ASP:OD2	1:G:529:VAL:N	2.48	0.47
1:H:121:LEU:HB3	1:H:126:VAL:HG21	1.97	0.47
1:H:406:ALA:O	1:H:410:LYS:HG3	2.15	0.47
1:A:150:ALA:HA	1:A:415:ILE:HG22	1.97	0.47
1:A:230:LYS:HZ1	1:A:321:ARG:HH12	1.61	0.47
1:A:259:GLU:C	1:A:259:GLU:CD	2.74	0.47
1:C:84:PRO:HG2	1:C:85:ALA:H	1.80	0.47
1:C:178:ARG:H	1:C:178:ARG:NE	2.12	0.47
1:C:249:ILE:HD12	1:C:346:ILE:HD11	1.96	0.47
1:D:290:ILE:HG21	1:D:298:ILE:CD1	2.40	0.47
1:D:359:GLU:HG2	1:D:359:GLU:O	2.15	0.47
1:E:121:LEU:HB3	1:E:126:VAL:HG21	1.97	0.47
1:F:121:LEU:HB3	1:F:126:VAL:CG2	2.44	0.47
1:G:246:ILE:O	1:G:351:LEU:HB2	2.14	0.47
1:G:249:ILE:HD12	1:G:346:ILE:HD11	1.96	0.47
1:G:282:LEU:O	1:G:285:GLU:HB3	2.15	0.47
1:H:83:HIS:CD2	1:H:84:PRO:HD2	2.50	0.47
1:H:232:VAL:HG11	1:H:318:LEU:HD11	1.95	0.47
1:H:528:ASP:OD2	1:H:529:VAL:N	2.48	0.47
1:I:66:ILE:CD1	1:I:66:ILE:N	2.76	0.47
1:I:259:GLU:C	1:I:259:GLU:CD	2.74	0.47
1:I:271:GLN:HA	1:I:271:GLN:OE1	2.15	0.47
1:A:436:VAL:HG23	1:A:437:GLY:N	2.30	0.46
1:B:121:LEU:HB3	1:B:126:VAL:HG21	1.97	0.46
1:B:505:PRO:C	1:B:507:LEU:N	2.69	0.46
1:C:259:GLU:C	1:C:259:GLU:CD	2.74	0.46
1:D:178:ARG:H	1:D:178:ARG:NE	2.12	0.46
1:D:330:LYS:O	1:D:334:ALA:HB2	2.14	0.46
1:E:232:VAL:HG12	1:E:318:LEU:HD11	1.95	0.46
1:E:406:ALA:O	1:E:410:LYS:HG3	2.16	0.46
1:E:526:ILE:HD11	1:F:68:ILE:HG21	1.96	0.46
1:F:56:ASP:OD1	1:F:70:ASN:HB3	2.15	0.46
1:F:249:ILE:HD12	1:F:346:ILE:HD11	1.96	0.46
1:H:56:ASP:OD1	1:H:70:ASN:HB3	2.15	0.46
1:H:66:ILE:CD1	1:H:66:ILE:N	2.76	0.46
1:I:194:GLU:C	1:I:195:LEU:HD12	2.36	0.46
1:I:227:VAL:HG22	1:I:369:PHE:HD1	1.79	0.46
1:I:299:ILE:HG22	1:I:320:VAL:HG23	1.96	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:260:LEU:CD1	1:A:260:LEU:C	2.81	0.46
1:A:406:ALA:O	1:A:410:LYS:HG3	2.16	0.46
1:B:56:ASP:OD1	1:B:70:ASN:HB3	2.15	0.46
1:C:45:ALA:C	1:C:46:LEU:HD12	2.36	0.46
1:C:121:LEU:HB3	1:C:126:VAL:CG2	2.44	0.46
1:C:271:GLN:OE1	1:C:271:GLN:HA	2.15	0.46
1:D:194:GLU:C	1:D:195:LEU:HD12	2.36	0.46
1:E:194:GLU:C	1:E:195:LEU:HD12	2.36	0.46
1:F:259:GLU:C	1:F:259:GLU:CD	2.74	0.46
1:H:75:ILE:O	1:H:79:MET:HB3	2.15	0.46
1:I:75:ILE:O	1:I:79:MET:HB3	2.15	0.46
1:I:212:LYS:O	1:I:213:ALA:O	2.33	0.46
1:I:359:GLU:O	1:I:359:GLU:HG2	2.15	0.46
1:A:84:PRO:HG2	1:A:85:ALA:H	1.80	0.46
1:A:121:LEU:HB3	1:A:126:VAL:HG21	1.97	0.46
1:A:194:GLU:C	1:A:195:LEU:HD12	2.36	0.46
1:A:282:LEU:O	1:A:285:GLU:HB3	2.15	0.46
1:B:84:PRO:HG2	1:B:85:ALA:H	1.80	0.46
1:B:188:ALA:HA	1:B:379:ILE:HD11	1.97	0.46
1:B:211:LYS:HE3	1:B:395:GLU:OE2	2.14	0.46
1:B:263:GLU:C	1:B:264:ILE:CG2	2.82	0.46
1:B:406:ALA:O	1:B:410:LYS:HG3	2.15	0.46
1:C:212:LYS:HA	1:C:212:LYS:CE	2.33	0.46
1:C:230:LYS:HZ2	1:C:321:ARG:NH1	2.13	0.46
1:C:505:PRO:C	1:C:507:LEU:N	2.69	0.46
1:C:528:ASP:OD2	1:C:529:VAL:N	2.48	0.46
1:D:208:GLN:C	1:D:209:ILE:HD12	2.36	0.46
1:D:232:VAL:HG12	1:D:318:LEU:HD11	1.95	0.46
1:E:121:LEU:HB3	1:E:126:VAL:CG2	2.44	0.46
1:E:141:VAL:CG2	1:E:432:TYR:CE1	2.97	0.46
1:E:217:ILE:HD11	1:E:390:LEU:CD2	2.43	0.46
1:E:271:GLN:OE1	1:E:271:GLN:HA	2.15	0.46
1:E:505:PRO:C	1:E:507:LEU:N	2.69	0.46
1:F:406:ALA:O	1:F:410:LYS:HG3	2.16	0.46
1:G:406:ALA:O	1:G:410:LYS:HG3	2.16	0.46
1:H:141:VAL:CG2	1:H:432:TYR:CE1	2.97	0.46
1:H:249:ILE:HD12	1:H:346:ILE:HD11	1.96	0.46
1:I:56:ASP:OD1	1:I:70:ASN:HB3	2.15	0.46
1:I:282:LEU:O	1:I:285:GLU:HB3	2.15	0.46
1:A:208:GLN:C	1:A:209:ILE:HD12	2.36	0.46
1:A:212:LYS:O	1:A:213:ALA:O	2.34	0.46



	to ac pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:224:TYR:HA	1:A:379:ILE:HG22	1.98	0.46
1:B:194:GLU:C	1:B:195:LEU:HD12	2.36	0.46
1:C:121:LEU:HB3	1:C:126:VAL:HG21	1.97	0.46
1:C:150:ALA:HA	1:C:415:ILE:HG22	1.97	0.46
1:C:246:ILE:O	1:C:351:LEU:HB2	2.14	0.46
1:C:282:LEU:O	1:C:285:GLU:HB3	2.15	0.46
1:D:84:PRO:HG2	1:D:85:ALA:H	1.80	0.46
1:E:56:ASP:OD1	1:E:70:ASN:HB3	2.15	0.46
1:E:234:HIS:ND1	1:E:235:PRO:HD2	2.30	0.46
1:E:263:GLU:C	1:E:264:ILE:CG2	2.82	0.46
1:E:282:LEU:O	1:E:285:GLU:HB3	2.15	0.46
1:E:525:ARG:HG3	1:F:56:ASP:OD2	2.13	0.46
1:F:46:LEU:O	1:F:47:LYS:C	2.53	0.46
1:F:528:ASP:HB3	1:G:57:LYS:HD3	1.97	0.46
1:G:45:ALA:C	1:G:46:LEU:HD12	2.36	0.46
1:G:150:ALA:HA	1:G:415:ILE:HG22	1.97	0.46
1:G:194:GLU:C	1:G:195:LEU:HD12	2.36	0.46
1:G:212:LYS:O	1:G:213:ALA:O	2.33	0.46
1:H:282:LEU:O	1:H:285:GLU:HB3	2.15	0.46
1:H:290:ILE:HG12	1:H:346:ILE:CD1	2.46	0.46
1:H:359:GLU:O	1:H:359:GLU:HG2	2.15	0.46
1:I:45:ALA:C	1:I:46:LEU:HD12	2.36	0.46
1:I:84:PRO:HG2	1:I:85:ALA:H	1.80	0.46
1:I:121:LEU:HB3	1:I:126:VAL:HG21	1.97	0.46
1:I:232:VAL:HG11	1:I:318:LEU:HD11	1.95	0.46
1:I:263:GLU:C	1:I:264:ILE:CG2	2.82	0.46
1:A:528:ASP:HB3	1:B:57:LYS:HE3	1.97	0.46
1:B:259:GLU:C	1:B:259:GLU:CD	2.74	0.46
1:D:56:ASP:OD1	1:D:70:ASN:HB3	2.15	0.46
1:D:212:LYS:O	1:D:213:ALA:O	2.34	0.46
1:D:271:GLN:OE1	1:D:271:GLN:HA	2.15	0.46
1:D:423:ILE:HD12	1:D:424:GLU:H	1.73	0.46
1:E:208:GLN:C	1:E:209:ILE:HD12	2.36	0.46
1:F:83:HIS:CD2	1:F:84:PRO:HD2	2.50	0.46
1:F:121:LEU:HB3	1:F:126:VAL:HG21	1.97	0.46
1:F:212:LYS:O	1:F:213:ALA:O	2.34	0.46
1:G:153:VAL:O	1:G:153:VAL:HG13	2.16	0.46
1:G:436:VAL:HG23	1:G:437:GLY:N	2.30	0.46
1:H:234:HIS:ND1	1:H:235:PRO:HD2	2.30	0.46
1:I:469:LEU:HB3	1:I:487:ILE:CD1	2.43	0.46
1:A:56:ASP:OD1	1:A:70:ASN:HB3	2.15	0.46



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:210:VAL:O	1:A:382:LEU:HD12	2.16	0.46
1:A:211:LYS:HE3	1:A:395:GLU:OE2	2.15	0.46
1:B:83:HIS:CD2	1:B:84:PRO:HD2	2.50	0.46
1:B:153:VAL:HG13	1:B:153:VAL:O	2.16	0.46
1:B:234:HIS:ND1	1:B:235:PRO:HD2	2.30	0.46
1:D:188:ALA:HA	1:D:379:ILE:HD11	1.98	0.46
1:D:211:LYS:HD2	1:D:391:VAL:HG22	1.98	0.46
1:F:359:GLU:O	1:F:359:GLU:HG2	2.15	0.46
1:G:423:ILE:HD12	1:G:424:GLU:H	1.73	0.46
1:H:84:PRO:HG2	1:H:85:ALA:H	1.80	0.46
1:I:46:LEU:O	1:I:47:LYS:C	2.53	0.46
1:I:83:HIS:CD2	1:I:84:PRO:HD2	2.50	0.46
1:I:234:HIS:ND1	1:I:235:PRO:HD2	2.30	0.46
1:A:75:ILE:O	1:A:79:MET:HB3	2.15	0.46
1:A:290:ILE:HG12	1:A:346:ILE:CD1	2.46	0.46
1:B:178:ARG:H	1:B:178:ARG:NE	2.12	0.46
1:B:212:LYS:O	1:B:213:ALA:O	2.34	0.46
1:B:359:GLU:HG2	1:B:359:GLU:O	2.15	0.46
1:C:208:GLN:C	1:C:209:ILE:HD12	2.36	0.46
1:C:224:TYR:HA	1:C:379:ILE:HG22	1.98	0.46
1:E:46:LEU:O	1:E:47:LYS:C	2.53	0.46
1:E:214:GLY:HA3	1:E:384:ARG:HH21	1.79	0.46
1:F:178:ARG:H	1:F:178:ARG:NE	2.12	0.46
1:F:224:TYR:HA	1:F:379:ILE:HG22	1.98	0.46
1:F:271:GLN:HA	1:F:271:GLN:OE1	2.15	0.46
1:F:528:ASP:O	1:G:58:MET:N	2.41	0.46
1:G:56:ASP:OD1	1:G:70:ASN:HB3	2.15	0.46
1:G:208:GLN:C	1:G:209:ILE:HD12	2.36	0.46
1:G:210:VAL:O	1:G:382:LEU:HD12	2.16	0.46
1:G:214:GLY:HA3	1:G:384:ARG:HH21	1.79	0.46
1:H:194:GLU:C	1:H:195:LEU:HD12	2.36	0.46
1:H:210:VAL:O	1:H:382:LEU:HD12	2.16	0.46
1:I:141:VAL:CG2	1:I:432:TYR:CE1	2.97	0.46
1:I:208:GLN:C	1:I:209:ILE:HD12	2.36	0.46
1:I:290:ILE:HG12	1:I:346:ILE:CD1	2.46	0.46
1:A:45:ALA:C	1:A:46:LEU:HD12	2.36	0.46
1:A:430:ARG:HG2	1:A:430:ARG:NH1	2.29	0.46
1:A:505:PRO:C	1:A:507:LEU:N	2.69	0.46
1:C:194:GLU:C	1:C:195:LEU:HD12	2.36	0.46
1:C:299:ILE:HG22	1:C:320:VAL:HG23	1.96	0.46
1:D:150:ALA:HA	1:D:415:ILE:HG22	1.97	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:359:GLU:HG2	1:E:359:GLU:O	2.15	0.46
1:E:430:ARG:HG2	1:E:430:ARG:NH1	2.29	0.46
1:F:153:VAL:O	1:F:153:VAL:HG13	2.16	0.46
1:F:282:LEU:O	1:F:285:GLU:HB3	2.15	0.46
1:G:505:PRO:C	1:G:507:LEU:N	2.69	0.46
1:G:522:LEU:O	1:G:526:ILE:HG12	2.16	0.46
1:H:150:ALA:HA	1:H:415:ILE:HG22	1.98	0.46
1:H:208:GLN:C	1:H:209:ILE:HD12	2.36	0.46
1:H:259:GLU:C	1:H:259:GLU:CD	2.74	0.46
1:B:224:TYR:HA	1:B:379:ILE:HG22	1.98	0.46
1:B:290:ILE:HG12	1:B:346:ILE:CD1	2.46	0.46
1:C:263:GLU:C	1:C:264:ILE:CG2	2.82	0.46
1:C:522:LEU:O	1:C:526:ILE:HG12	2.16	0.46
1:D:121:LEU:HB3	1:D:126:VAL:HG21	1.97	0.46
1:E:259:GLU:C	1:E:259:GLU:CD	2.74	0.46
1:E:492:GLY:O	1:E:493:GLN:HB2	2.16	0.46
1:E:528:ASP:OD2	1:E:529:VAL:N	2.48	0.46
1:F:150:ALA:HA	1:F:415:ILE:HG22	1.98	0.46
1:G:46:LEU:O	1:G:47:LYS:C	2.53	0.46
1:G:84:PRO:HG2	1:G:85:ALA:H	1.80	0.46
1:G:430:ARG:HG2	1:G:430:ARG:NH1	2.29	0.46
1:H:211:LYS:HD2	1:H:391:VAL:HG22	1.98	0.46
1:I:230:LYS:HZ1	1:I:321:ARG:HH12	1.64	0.46
1:C:127:HIS:CG	1:C:128:PRO:HD2	2.51	0.46
1:C:290:ILE:HG12	1:C:346:ILE:CD1	2.46	0.46
1:C:359:GLU:O	1:C:359:GLU:HG2	2.15	0.46
1:E:127:HIS:CG	1:E:128:PRO:HD2	2.51	0.46
1:E:178:ARG:H	1:E:178:ARG:NE	2.13	0.46
1:E:522:LEU:O	1:E:526:ILE:HG12	2.16	0.46
1:F:84:PRO:HG2	1:F:85:ALA:H	1.80	0.46
1:F:141:VAL:CG2	1:F:432:TYR:CE1	2.97	0.46
1:G:127:HIS:CG	1:G:128:PRO:HD2	2.51	0.46
1:G:259:GLU:C	1:G:259:GLU:CD	2.74	0.46
1:H:153:VAL:HG13	1:H:153:VAL:O	2.16	0.46
1:H:230:LYS:HZ2	1:H:321:ARG:NH1	2.13	0.46
1:H:522:LEU:O	1:H:526:ILE:HG12	2.16	0.46
1:I:217:ILE:HD11	1:I:390:LEU:CD2	2.44	0.46
1:I:406:ALA:O	1:I:410:LYS:HG3	2.15	0.46
1:A:522:LEU:O	1:A:526:ILE:HG12	2.16	0.45
1:B:166:MET:CE	1:B:178:ARG:HG2	2.47	0.45
1:B:211:LYS:HD2	1:B:391:VAL:HG22	1.98	0.45


	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:260:LEU:CD1	1:B:261:ASP:CG	2.85	0.45
1:B:282:LEU:O	1:B:285:GLU:HB3	2.15	0.45
1:D:31:ALA:O	1:D:34:ALA:N	2.49	0.45
1:D:40:LYS:HD3	1:D:116:LYS:HG2	1.99	0.45
1:D:83:HIS:CD2	1:D:84:PRO:HD2	2.50	0.45
1:D:153:VAL:O	1:D:153:VAL:HG13	2.16	0.45
1:E:469:LEU:HB3	1:E:487:ILE:CD1	2.43	0.45
1:F:210:VAL:O	1:F:382:LEU:HD12	2.16	0.45
1:G:83:HIS:CD2	1:G:84:PRO:HD2	2.50	0.45
1:G:121:LEU:HB3	1:G:126:VAL:HG21	1.97	0.45
1:H:45:ALA:C	1:H:46:LEU:HD12	2.36	0.45
1:H:121:LEU:HB3	1:H:126:VAL:CG2	2.44	0.45
1:I:166:MET:CE	1:I:178:ARG:HG2	2.47	0.45
1:I:258:PRO:CG	1:I:279:GLU:OE2	2.56	0.45
1:A:141:VAL:CG2	1:A:432:TYR:CE1	2.97	0.45
1:A:188:ALA:HA	1:A:379:ILE:HD11	1.98	0.45
1:B:208:GLN:C	1:B:209:ILE:HD12	2.36	0.45
1:C:40:LYS:HD3	1:C:116:LYS:HG2	1.99	0.45
1:D:224:TYR:HA	1:D:379:ILE:HG22	1.98	0.45
1:D:406:ALA:O	1:D:410:LYS:HG3	2.16	0.45
1:E:31:ALA:O	1:E:34:ALA:N	2.49	0.45
1:E:45:ALA:C	1:E:46:LEU:HD12	2.36	0.45
1:E:432:TYR:CZ	1:E:436:VAL:HG12	2.52	0.45
1:E:527:ASP:N	1:F:56:ASP:O	2.46	0.45
1:F:194:GLU:C	1:F:195:LEU:HD12	2.36	0.45
1:F:290:ILE:HG12	1:F:346:ILE:CD1	2.46	0.45
1:G:75:ILE:O	1:G:79:MET:HB3	2.15	0.45
1:G:290:ILE:HG12	1:G:346:ILE:CD1	2.46	0.45
1:H:224:TYR:HA	1:H:379:ILE:HG22	1.98	0.45
1:H:358:GLU:CG	1:H:360:ARG:HH22	2.27	0.45
1:H:505:PRO:C	1:H:507:LEU:N	2.69	0.45
1:I:127:HIS:CG	1:I:128:PRO:HD2	2.51	0.45
1:I:150:ALA:HA	1:I:415:ILE:HG22	1.98	0.45
1:I:153:VAL:O	1:I:153:VAL:HG13	2.16	0.45
1:I:224:TYR:HA	1:I:379:ILE:HG22	1.98	0.45
1:I:432:TYR:CZ	1:I:436:VAL:HG12	2.52	0.45
1:I:522:LEU:O	1:I:526:ILE:HG12	2.16	0.45
1:A:83:HIS:CD2	1:A:84:PRO:HD2	2.50	0.45
1:A:492:GLY:O	1:A:493:GLN:HB2	2.16	0.45
1:A:527:ASP:HB2	1:B:55:MET:CG	2.45	0.45
1:B:45:ALA:C	1:B:46:LEU:HD12	2.36	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:432:TYR:CZ	1:B:436:VAL:HG12	2.52	0.45
1:B:522:LEU:O	1:B:526:ILE:HG12	2.16	0.45
1:C:211:LYS:HD2	1:C:391:VAL:HG22	1.98	0.45
1:D:210:VAL:O	1:D:382:LEU:HD12	2.16	0.45
1:D:426:ALA:O	1:D:429:LEU:N	2.45	0.45
1:D:522:LEU:O	1:D:526:ILE:HG12	2.16	0.45
1:E:66:ILE:CD1	1:E:66:ILE:N	2.76	0.45
1:E:84:PRO:HG2	1:E:85:ALA:H	1.80	0.45
1:E:166:MET:CE	1:E:178:ARG:HG2	2.47	0.45
1:E:188:ALA:HA	1:E:379:ILE:HD11	1.98	0.45
1:F:31:ALA:O	1:F:34:ALA:N	2.49	0.45
1:F:40:LYS:HD3	1:F:116:LYS:HG2	1.99	0.45
1:F:188:ALA:HA	1:F:379:ILE:HD11	1.98	0.45
1:F:250:ASP:O	1:F:251:ALA:HB2	2.17	0.45
1:G:492:GLY:O	1:G:493:GLN:HB2	2.16	0.45
1:H:260:LEU:CD1	1:H:261:ASP:CG	2.85	0.45
1:H:492:GLY:O	1:H:493:GLN:HB2	2.16	0.45
1:I:31:ALA:O	1:I:34:ALA:N	2.49	0.45
1:B:31:ALA:O	1:B:34:ALA:N	2.49	0.45
1:C:210:VAL:O	1:C:382:LEU:HD12	2.16	0.45
1:C:212:LYS:O	1:C:213:ALA:O	2.34	0.45
1:D:166:MET:CE	1:D:178:ARG:HG2	2.47	0.45
1:E:150:ALA:HA	1:E:415:ILE:HG22	1.98	0.45
1:E:250:ASP:O	1:E:251:ALA:HB2	2.17	0.45
1:F:166:MET:CE	1:F:178:ARG:HG2	2.47	0.45
1:F:211:LYS:HD2	1:F:391:VAL:HG22	1.98	0.45
1:G:166:MET:CE	1:G:178:ARG:HG2	2.47	0.45
1:H:166:MET:CE	1:H:178:ARG:HG2	2.47	0.45
1:I:250:ASP:O	1:I:251:ALA:HB2	2.17	0.45
1:B:40:LYS:HD3	1:B:116:LYS:HG2	1.99	0.45
1:B:127:HIS:CG	1:B:128:PRO:HD2	2.51	0.45
1:B:210:VAL:O	1:B:382:LEU:HD12	2.16	0.45
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.29	0.45
1:B:492:GLY:O	1:B:493:GLN:HB2	2.16	0.45
1:C:83:HIS:CD2	1:C:84:PRO:HD2	2.50	0.45
1:C:406:ALA:O	1:C:410:LYS:HG3	2.15	0.45
1:D:127:HIS:CG	1:D:128:PRO:HD2	2.51	0.45
1:D:505:PRO:C	1:D:507:LEU:N	2.69	0.45
1:E:83:HIS:CD2	1:E:84:PRO:HD2	2.50	0.45
1:E:260:LEU:CD1	1:E:261:ASP:CG	2.85	0.45
1:E:321:ARG:HB3	1:E:322:ARG:H	1.56	0.45



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:436:VAL:HG21	1:E:441:GLN:HA	1.99	0.45
1:F:430:ARG:HG2	1:F:430:ARG:NH1	2.29	0.45
1:G:224:TYR:HA	1:G:379:ILE:HG22	1.98	0.45
1:H:436:VAL:HG21	1:H:441:GLN:HA	1.99	0.45
1:I:244:ALA:HA	1:I:296:ASN:HD22	1.82	0.45
1:I:260:LEU:CD1	1:I:260:LEU:C	2.81	0.45
1:I:505:PRO:C	1:I:507:LEU:N	2.69	0.45
1:A:153:VAL:O	1:A:153:VAL:HG13	2.16	0.45
1:A:161:LEU:H	1:A:161:LEU:CD1	2.30	0.45
1:B:150:ALA:HA	1:B:415:ILE:HG22	1.98	0.45
1:B:250:ASP:O	1:B:251:ALA:HB2	2.17	0.45
1:B:423:ILE:HD12	1:B:424:GLU:H	1.73	0.45
1:C:153:VAL:HG13	1:C:153:VAL:O	2.16	0.45
1:D:45:ALA:C	1:D:46:LEU:HD12	2.36	0.45
1:E:40:LYS:HD3	1:E:116:LYS:HG2	1.99	0.45
1:E:166:MET:HE1	1:E:179:GLU:HG2	1.99	0.45
1:E:212:LYS:O	1:E:213:ALA:O	2.34	0.45
1:E:224:TYR:HA	1:E:379:ILE:HG22	1.98	0.45
1:E:249:ILE:HD12	1:E:346:ILE:HD11	1.97	0.45
1:E:290:ILE:HG12	1:E:346:ILE:CD1	2.46	0.45
1:F:45:ALA:C	1:F:46:LEU:HD12	2.36	0.45
1:F:208:GLN:C	1:F:209:ILE:HD12	2.36	0.45
1:F:230:LYS:HZ2	1:F:321:ARG:NH1	2.15	0.45
1:G:31:ALA:O	1:G:34:ALA:N	2.49	0.45
1:G:211:LYS:HD2	1:G:391:VAL:HG22	1.98	0.45
1:H:40:LYS:HD3	1:H:116:LYS:HG2	1.99	0.45
1:I:260:LEU:CD1	1:I:261:ASP:CG	2.85	0.45
1:B:476:THR:HG21	1:B:494:PRO:HB3	1.99	0.45
1:C:142:ALA:O	1:C:425:ILE:HD12	2.17	0.45
1:C:244:ALA:HA	1:C:296:ASN:HD22	1.82	0.45
1:C:432:TYR:CZ	1:C:436:VAL:HG12	2.52	0.45
1:D:250:ASP:O	1:D:251:ALA:HB2	2.17	0.45
1:D:290:ILE:HG12	1:D:346:ILE:CD1	2.46	0.45
1:D:436:VAL:HG21	1:D:441:GLN:HA	1.99	0.45
1:D:492:GLY:O	1:D:493:GLN:HB2	2.16	0.45
1:E:142:ALA:O	1:E:425:ILE:HD12	2.17	0.45
1:F:127:HIS:CG	1:F:128:PRO:HD2	2.51	0.45
1:F:172:LYS:HG3	1:F:397:ALA:HB2	1.99	0.45
1:F:209:ILE:CB	1:F:399:ARG:HH22	2.28	0.45
1:F:529:VAL:HG12	1:G:58:MET:CG	2.46	0.45
1:G:188:ALA:HA	1:G:379:ILE:HD11	1.98	0.45



	lo us puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:127:HIS:CG	1:H:128:PRO:HD2	2.51	0.45
1:C:188:ALA:HA	1:C:379:ILE:HD11	1.98	0.45
1:E:153:VAL:HG23	1:E:160:LEU:CD2	2.45	0.45
1:E:211:LYS:HD2	1:E:391:VAL:HG22	1.98	0.45
1:G:172:LYS:HG3	1:G:397:ALA:HB2	1.99	0.45
1:G:432:TYR:CZ	1:G:436:VAL:HG12	2.52	0.45
1:G:436:VAL:HG21	1:G:441:GLN:HA	1.99	0.45
1:H:172:LYS:HG3	1:H:397:ALA:HB2	1.99	0.45
1:H:321:ARG:HB3	1:H:322:ARG:H	1.56	0.45
1:I:210:VAL:O	1:I:382:LEU:HD12	2.16	0.45
1:A:68:ILE:HD12	1:I:522:LEU:HD11	1.98	0.45
1:A:146:ILE:HB	1:A:510:MET:HE2	1.99	0.45
1:A:172:LYS:HG3	1:A:397:ALA:HB2	1.99	0.45
1:C:31:ALA:O	1:C:34:ALA:N	2.49	0.45
1:C:146:ILE:HB	1:C:510:MET:HE3	1.99	0.45
1:C:166:MET:CE	1:C:178:ARG:HG2	2.46	0.45
1:C:172:LYS:HG3	1:C:397:ALA:HB2	1.99	0.45
1:E:210:VAL:O	1:E:382:LEU:HD12	2.16	0.45
1:H:31:ALA:O	1:H:34:ALA:N	2.49	0.45
1:A:40:LYS:HD3	1:A:116:LYS:HG2	1.99	0.45
1:D:142:ALA:O	1:D:425:ILE:HD12	2.17	0.45
1:D:260:LEU:CD1	1:D:261:ASP:CG	2.85	0.45
1:E:153:VAL:HG13	1:E:153:VAL:O	2.16	0.45
1:F:142:ALA:O	1:F:425:ILE:HD12	2.17	0.45
1:G:161:LEU:H	1:G:161:LEU:CD1	2.30	0.45
1:H:432:TYR:CZ	1:H:436:VAL:HG12	2.52	0.45
1:I:40:LYS:HD3	1:I:116:LYS:HG2	1.99	0.45
1:I:188:ALA:HA	1:I:379:ILE:HD11	1.98	0.45
1:A:31:ALA:O	1:A:34:ALA:N	2.49	0.44
1:A:98:GLU:HA	1:A:98:GLU:OE1	2.17	0.44
1:A:142:ALA:O	1:A:425:ILE:HD12	2.17	0.44
1:E:165:ALA:O	1:E:169:LEU:HG	2.18	0.44
1:F:432:TYR:CZ	1:F:436:VAL:HG12	2.52	0.44
1:G:98:GLU:OE1	1:G:98:GLU:HA	2.17	0.44
1:H:165:ALA:O	1:H:169:LEU:HG	2.17	0.44
1:I:89:LEU:CD2	1:I:108:VAL:HG23	2.44	0.44
1:I:161:LEU:H	1:I:161:LEU:CD1	2.30	0.44
1:A:153:VAL:HG23	1:A:160:LEU:CD2	2.45	0.44
1:A:166:MET:CE	1:A:178:ARG:HG2	2.47	0.44
1:B:165:ALA:O	1:B:169:LEU:HG	2.18	0.44
1:E:244:ALA:HA	1:E:296:ASN:HD22	1.82	0.44



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:161:LEU:H	1:F:161:LEU:CD1	2.30	0.44
1:F:165:ALA:O	1:F:169:LEU:HG	2.18	0.44
1:F:265:ARG:HD2	1:F:265:ARG:C	2.38	0.44
1:F:492:GLY:O	1:F:493:GLN:HB2	2.16	0.44
1:G:321:ARG:HB3	1:G:322:ARG:H	1.56	0.44
1:I:211:LYS:HD2	1:I:391:VAL:HG22	1.98	0.44
1:C:436:VAL:HG21	1:C:441:GLN:HA	1.99	0.44
1:C:492:GLY:O	1:C:493:GLN:HB2	2.16	0.44
1:D:82:GLN:O	1:D:83:HIS:C	2.56	0.44
1:F:522:LEU:O	1:F:526:ILE:HG12	2.16	0.44
1:H:212:LYS:O	1:H:213:ALA:O	2.34	0.44
1:I:492:GLY:O	1:I:493:GLN:HB2	2.16	0.44
1:A:82:GLN:O	1:A:83:HIS:C	2.56	0.44
1:A:127:HIS:CG	1:A:128:PRO:HD2	2.51	0.44
1:A:260:LEU:CD1	1:A:261:ASP:CG	2.85	0.44
1:B:260:LEU:CD1	1:B:260:LEU:C	2.81	0.44
1:C:414:ALA:HA	1:C:506:ALA:H	1.83	0.44
1:D:259:GLU:C	1:D:259:GLU:CD	2.74	0.44
1:E:265:ARG:HD2	1:E:265:ARG:C	2.38	0.44
1:G:59:LEU:HD13	1:G:78:LYS:HB2	2.00	0.44
1:G:82:GLN:O	1:G:83:HIS:C	2.56	0.44
1:G:260:LEU:CD1	1:G:261:ASP:CG	2.85	0.44
1:G:469:LEU:HB3	1:G:487:ILE:CD1	2.43	0.44
1:H:529:VAL:HG12	1:I:58:MET:SD	2.57	0.44
1:I:82:GLN:O	1:I:83:HIS:C	2.56	0.44
1:I:142:ALA:O	1:I:425:ILE:HD12	2.17	0.44
1:I:265:ARG:HD2	1:I:265:ARG:C	2.38	0.44
1:I:414:ALA:HA	1:I:506:ALA:H	1.83	0.44
1:A:39:VAL:HG11	1:A:115:VAL:HG21	2.00	0.44
1:A:66:ILE:CD1	1:A:66:ILE:N	2.76	0.44
1:A:165:ALA:O	1:A:169:LEU:HG	2.17	0.44
1:B:142:ALA:O	1:B:425:ILE:HD12	2.17	0.44
1:C:39:VAL:HG11	1:C:115:VAL:HG21	2.00	0.44
1:C:476:THR:HG21	1:C:494:PRO:HB3	1.99	0.44
1:C:515:ALA:O	1:C:518:GLU:HB3	2.18	0.44
1:C:529:VAL:HG12	1:D:58:MET:SD	2.57	0.44
1:D:530:VAL:O	1:E:59:LEU:CD2	2.65	0.44
1:E:82:GLN:O	1:E:83:HIS:C	2.56	0.44
1:E:161:LEU:H	1:E:161:LEU:CD1	2.30	0.44
1:E:260:LEU:CD1	1:E:260:LEU:C	2.81	0.44
1:F:145:THR:O	1:F:145:THR:HG22	2.18	0.44



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:141:VAL:CG2	1:G:432:TYR:CE1	2.97	0.44
1:G:165:ALA:O	1:G:169:LEU:HG	2.17	0.44
1:I:172:LYS:HG3	1:I:397:ALA:HB2	1.99	0.44
1:A:250:ASP:O	1:A:251:ALA:HB2	2.17	0.44
1:A:432:TYR:CZ	1:A:436:VAL:HG12	2.52	0.44
1:B:391:VAL:HG13	1:B:392:ASP:N	2.33	0.44
1:B:414:ALA:HA	1:B:506:ALA:H	1.83	0.44
1:B:440:GLU:O	1:B:444:VAL:HG23	2.18	0.44
1:C:82:GLN:O	1:C:83:HIS:C	2.56	0.44
1:C:110:PHE:CZ	1:C:114:LEU:HD11	2.53	0.44
1:D:98:GLU:HA	1:D:98:GLU:OE1	2.17	0.44
1:D:260:LEU:CD1	1:D:260:LEU:C	2.81	0.44
1:D:515:ALA:O	1:D:518:GLU:HB3	2.18	0.44
1:E:391:VAL:HG13	1:E:392:ASP:N	2.33	0.44
1:F:98:GLU:OE1	1:F:98:GLU:HA	2.17	0.44
1:F:110:PHE:HD1	1:F:516:ALA:CB	2.31	0.44
1:F:391:VAL:HG13	1:F:392:ASP:N	2.33	0.44
1:F:505:PRO:C	1:F:507:LEU:N	2.69	0.44
1:G:440:GLU:O	1:G:444:VAL:HG23	2.18	0.44
1:H:59:LEU:HD13	1:H:78:LYS:HB2	2.00	0.44
1:H:110:PHE:CZ	1:H:114:LEU:HD11	2.53	0.44
1:H:249:ILE:HD13	1:H:340:VAL:HB	2.00	0.44
1:H:265:ARG:HD2	1:H:265:ARG:C	2.38	0.44
1:H:515:ALA:O	1:H:518:GLU:HB3	2.18	0.44
1:I:98:GLU:OE1	1:I:98:GLU:HA	2.17	0.44
1:I:146:ILE:HB	1:I:510:MET:HE3	1.98	0.44
1:I:430:ARG:HG2	1:I:430:ARG:NH1	2.29	0.44
1:A:110:PHE:CZ	1:A:114:LEU:HD11	2.53	0.44
1:A:217:ILE:HD11	1:A:390:LEU:CD2	2.43	0.44
1:A:436:VAL:HG21	1:A:441:GLN:HA	1.99	0.44
1:A:476:THR:HG21	1:A:494:PRO:HB3	1.99	0.44
1:B:89:LEU:CD2	1:B:108:VAL:HG23	2.44	0.44
1:B:265:ARG:HD2	1:B:265:ARG:C	2.38	0.44
1:C:249:ILE:HD13	1:C:340:VAL:HB	2.00	0.44
1:C:265:ARG:HD2	1:C:265:ARG:C	2.38	0.44
1:D:391:VAL:HG13	1:D:392:ASP:N	2.33	0.44
1:D:440:GLU:O	1:D:444:VAL:HG23	2.18	0.44
1:E:59:LEU:HD13	1:E:78:LYS:HB2	2.00	0.44
1:E:110:PHE:CZ	1:E:114:LEU:HD11	2.53	0.44
1:E:110:PHE:HD1	1:E:516:ALA:CB	2.31	0.44
1:E:172:LYS:HG3	1:E:397:ALA:HB2	1.99	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:153:VAL:HG23	1:F:160:LEU:CD2	2.45	0.44
1:G:110:PHE:CZ	1:G:114:LEU:HD11	2.53	0.44
1:G:145:THR:O	1:G:145:THR:HG22	2.18	0.44
1:G:250:ASP:O	1:G:251:ALA:HB2	2.17	0.44
1:G:414:ALA:HA	1:G:506:ALA:H	1.83	0.44
1:H:89:LEU:CD2	1:H:108:VAL:HG23	2.44	0.44
1:H:469:LEU:HB3	1:H:487:ILE:CD1	2.43	0.44
1:I:110:PHE:CZ	1:I:114:LEU:HD11	2.53	0.44
1:I:165:ALA:O	1:I:169:LEU:HG	2.18	0.44
1:A:265:ARG:HD2	1:A:265:ARG:C	2.38	0.44
1:B:110:PHE:HD1	1:B:516:ALA:CB	2.31	0.44
1:C:110:PHE:HD1	1:C:516:ALA:CB	2.31	0.44
1:C:165:ALA:O	1:C:169:LEU:HG	2.17	0.44
1:D:145:THR:O	1:D:145:THR:HG22	2.18	0.44
1:D:146:ILE:HB	1:D:510:MET:HE3	2.00	0.44
1:D:165:ALA:O	1:D:169:LEU:HG	2.17	0.44
1:D:172:LYS:HG3	1:D:397:ALA:HB2	1.99	0.44
1:D:209:ILE:CB	1:D:399:ARG:HH22	2.28	0.44
1:D:265:ARG:HD2	1:D:265:ARG:C	2.38	0.44
1:E:145:THR:HG22	1:E:145:THR:O	2.18	0.44
1:E:515:ALA:O	1:E:518:GLU:HB3	2.18	0.44
1:H:142:ALA:O	1:H:425:ILE:HD12	2.17	0.44
1:H:476:THR:HG21	1:H:494:PRO:HB3	1.99	0.44
1:I:440:GLU:O	1:I:444:VAL:HG23	2.18	0.44
1:I:476:THR:HG21	1:I:494:PRO:HB3	1.99	0.44
1:I:515:ALA:O	1:I:518:GLU:HB3	2.18	0.44
1:A:211:LYS:HD2	1:A:391:VAL:HG22	1.98	0.44
1:B:59:LEU:HD13	1:B:78:LYS:HB2	2.00	0.44
1:B:146:ILE:HB	1:B:510:MET:HE3	1.99	0.44
1:B:244:ALA:HA	1:B:296:ASN:HD22	1.82	0.44
1:B:249:ILE:HD13	1:B:340:VAL:HB	2.00	0.44
1:C:250:ASP:O	1:C:251:ALA:HB2	2.17	0.44
1:D:414:ALA:HA	1:D:506:ALA:H	1.83	0.44
1:E:505:PRO:C	1:E:507:LEU:H	2.22	0.44
1:G:89:LEU:CD2	1:G:108:VAL:HG23	2.44	0.44
1:H:81:LEU:HD12	1:H:81:LEU:N	2.28	0.44
1:H:146:ILE:HB	1:H:510:MET:HE3	1.99	0.44
1:H:161:LEU:H	1:H:161:LEU:CD1	2.30	0.44
1:H:250:ASP:O	1:H:251:ALA:HB2	2.17	0.44
1:A:59:LEU:HD13	1:A:78:LYS:HB2	2.00	0.43
1:A:66:ILE:HD13	1:A:66:ILE:N	2.13	0.43



	hi a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:440:GLU:O	1:A:444:VAL:HG23	2.18	0.43
1:C:145:THR:HG22	1:C:145:THR:O	2.18	0.43
1:E:414:ALA:HA	1:E:506:ALA:H	1.83	0.43
1:F:233:VAL:HG22	1:F:309:GLN:CD	2.39	0.43
1:F:258:PRO:CG	1:F:279:GLU:OE2	2.56	0.43
1:F:436:VAL:HG21	1:F:441:GLN:HA	1.99	0.43
1:G:142:ALA:O	1:G:425:ILE:HD12	2.17	0.43
1:G:233:VAL:HG22	1:G:309:GLN:CD	2.39	0.43
1:G:244:ALA:HA	1:G:296:ASN:HD22	1.82	0.43
1:H:82:GLN:O	1:H:83:HIS:C	2.56	0.43
1:H:145:THR:HG22	1:H:145:THR:O	2.18	0.43
1:I:58:MET:CB	1:I:68:ILE:HG22	2.48	0.43
1:I:110:PHE:HD1	1:I:516:ALA:CB	2.31	0.43
1:I:145:THR:O	1:I:145:THR:HG22	2.18	0.43
1:I:436:VAL:HG21	1:I:441:GLN:HA	1.99	0.43
1:A:233:VAL:HG22	1:A:309:GLN:CD	2.39	0.43
1:A:244:ALA:HA	1:A:296:ASN:HD22	1.82	0.43
1:B:110:PHE:CZ	1:B:114:LEU:HD11	2.53	0.43
1:B:233:VAL:HG22	1:B:309:GLN:CD	2.39	0.43
1:C:72:GLY:O	1:C:73:ALA:C	2.57	0.43
1:C:88:LEU:HD11	1:D:389:ARG:HH12	1.83	0.43
1:C:98:GLU:OE1	1:C:98:GLU:HA	2.17	0.43
1:C:161:LEU:H	1:C:161:LEU:CD1	2.30	0.43
1:C:260:LEU:CD1	1:C:261:ASP:CG	2.85	0.43
1:C:391:VAL:HG13	1:C:392:ASP:N	2.33	0.43
1:D:476:THR:HG21	1:D:494:PRO:HB3	1.99	0.43
1:D:484:TRP:HA	1:D:484:TRP:CE3	2.53	0.43
1:F:260:LEU:CD1	1:F:261:ASP:CG	2.85	0.43
1:F:515:ALA:O	1:F:518:GLU:HB3	2.18	0.43
1:G:110:PHE:HD1	1:G:516:ALA:CB	2.31	0.43
1:G:391:VAL:HG13	1:G:392:ASP:N	2.33	0.43
1:G:525:ARG:HG2	1:G:525:ARG:NH1	2.31	0.43
1:H:188:ALA:HA	1:H:379:ILE:HD11	1.98	0.43
1:H:298:ILE:O	1:H:319:ALA:HA	2.19	0.43
1:I:72:GLY:O	1:I:73:ALA:C	2.57	0.43
1:B:98:GLU:OE1	1:B:98:GLU:HA	2.17	0.43
1:C:58:MET:CB	1:C:68:ILE:HG22	2.48	0.43
1:C:233:VAL:HG22	1:C:309:GLN:CD	2.39	0.43
1:D:161:LEU:H	1:D:161:LEU:CD1	2.30	0.43
1:D:432:TYR:CZ	1:D:436:VAL:HG12	2.52	0.43
1:D:505:PRO:C	1:D:507:LEU:H	2.22	0.43



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:233:VAL:HG22	1:E:309:GLN:CD	2.39	0.43
1:F:59:LEU:HD13	1:F:78:LYS:HB2	2.00	0.43
1:F:249:ILE:HD13	1:F:340:VAL:HB	2.00	0.43
1:F:440:GLU:O	1:F:444:VAL:HG23	2.18	0.43
1:F:505:PRO:C	1:F:507:LEU:H	2.22	0.43
1:G:58:MET:CB	1:G:68:ILE:HG22	2.48	0.43
1:G:249:ILE:HD13	1:G:340:VAL:HB	2.00	0.43
1:G:482:ASN:O	1:G:485:TYR:N	2.40	0.43
1:H:98:GLU:OE1	1:H:98:GLU:HA	2.17	0.43
1:H:482:ASN:O	1:H:485:TYR:N	2.40	0.43
1:A:414:ALA:HA	1:A:506:ALA:H	1.83	0.43
1:A:515:ALA:O	1:A:518:GLU:HB3	2.18	0.43
1:B:58:MET:CB	1:B:68:ILE:HG22	2.48	0.43
1:B:258:PRO:CG	1:B:279:GLU:OE2	2.56	0.43
1:D:58:MET:CB	1:D:68:ILE:HG22	2.48	0.43
1:D:110:PHE:HD1	1:D:516:ALA:CB	2.31	0.43
1:F:476:THR:HG21	1:F:494:PRO:HB3	1.99	0.43
1:H:39:VAL:HG11	1:H:115:VAL:HG21	2.00	0.43
1:I:249:ILE:HD13	1:I:340:VAL:HB	2.00	0.43
1:I:391:VAL:HG13	1:I:392:ASP:N	2.33	0.43
1:I:505:PRO:C	1:I:507:LEU:H	2.22	0.43
1:A:110:PHE:HD1	1:A:516:ALA:CB	2.31	0.43
1:B:81:LEU:HD22	1:B:86:ALA:HB1	2.01	0.43
1:B:161:LEU:H	1:B:161:LEU:CD1	2.30	0.43
1:B:415:ILE:HG23	1:B:506:ALA:CB	2.48	0.43
1:B:436:VAL:HG21	1:B:441:GLN:HA	1.99	0.43
1:B:515:ALA:O	1:B:518:GLU:HB3	2.18	0.43
1:E:39:VAL:HG11	1:E:115:VAL:HG21	2.00	0.43
1:E:98:GLU:OE1	1:E:98:GLU:HA	2.17	0.43
1:G:265:ARG:HD2	1:G:265:ARG:C	2.38	0.43
1:G:476:THR:HG21	1:G:494:PRO:HB3	1.99	0.43
1:G:484:TRP:HA	1:G:484:TRP:CE3	2.54	0.43
1:H:110:PHE:HD1	1:H:516:ALA:CB	2.31	0.43
1:H:414:ALA:HA	1:H:506:ALA:H	1.83	0.43
1:I:415:ILE:HG23	1:I:506:ALA:CB	2.48	0.43
1:A:59:LEU:HD23	1:I:530:VAL:O	2.19	0.43
1:A:145:THR:O	1:A:145:THR:HG22	2.18	0.43
1:B:94:LYS:O	1:B:96:GLN:N	2.48	0.43
1:B:482:ASN:O	1:B:485:TYR:N	2.40	0.43
1:B:484:TRP:CE3	1:B:484:TRP:HA	2.53	0.43
1:B:505:PRO:C	1:B:507:LEU:H	2.22	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:59:LEU:HD13	1:D:78:LYS:HB2	2.00	0.43
1:E:81:LEU:HD22	1:E:86:ALA:HB1	2.01	0.43
1:E:128:PRO:HG3	1:F:55:MET:CE	2.48	0.43
1:E:484:TRP:CE3	1:E:484:TRP:HA	2.54	0.43
1:F:58:MET:CB	1:F:68:ILE:HG22	2.48	0.43
1:F:244:ALA:HA	1:F:296:ASN:HD22	1.82	0.43
1:G:40:LYS:HD3	1:G:116:LYS:HG2	1.99	0.43
1:G:46:LEU:O	1:G:49:THR:N	2.43	0.43
1:G:146:ILE:HB	1:G:510:MET:HE3	2.01	0.43
1:G:515:ALA:O	1:G:518:GLU:HB3	2.18	0.43
1:H:233:VAL:HG22	1:H:309:GLN:CD	2.39	0.43
1:H:244:ALA:HA	1:H:296:ASN:HD22	1.82	0.43
1:H:440:GLU:O	1:H:444:VAL:HG23	2.18	0.43
1:H:505:PRO:C	1:H:507:LEU:H	2.22	0.43
1:A:88:LEU:CD1	1:B:389:ARG:HH12	2.32	0.43
1:A:132:ILE:HD12	1:A:521:THR:HB	2.01	0.43
1:C:81:LEU:HD22	1:C:86:ALA:HB1	2.01	0.43
1:C:484:TRP:HA	1:C:484:TRP:CE3	2.54	0.43
1:D:298:ILE:O	1:D:319:ALA:HA	2.19	0.43
1:E:146:ILE:HB	1:E:510:MET:HE3	2.01	0.43
1:E:298:ILE:O	1:E:319:ALA:HA	2.19	0.43
1:F:110:PHE:CZ	1:F:114:LEU:HD11	2.53	0.43
1:F:415:ILE:HG23	1:F:506:ALA:CB	2.48	0.43
1:G:72:GLY:O	1:G:73:ALA:C	2.57	0.43
1:G:81:LEU:HD22	1:G:86:ALA:HB1	2.01	0.43
1:H:58:MET:CB	1:H:68:ILE:HG22	2.48	0.43
1:H:118:ALA:O	1:H:122:LEU:CD2	2.67	0.43
1:H:391:VAL:HG13	1:H:392:ASP:N	2.33	0.43
1:A:298:ILE:O	1:A:319:ALA:HA	2.19	0.43
1:B:141:VAL:CG2	1:B:432:TYR:CE1	2.97	0.43
1:B:145:THR:O	1:B:145:THR:HG22	2.18	0.43
1:B:172:LYS:HG3	1:B:397:ALA:HB2	1.99	0.43
1:C:94:LYS:O	1:C:96:GLN:N	2.48	0.43
1:D:110:PHE:CZ	1:D:114:LEU:HD11	2.53	0.43
1:D:233:VAL:HG22	1:D:309:GLN:CD	2.39	0.43
1:F:161:LEU:N	1:F:161:LEU:CD1	2.82	0.43
1:F:264:ILE:HD12	1:F:265:ARG:HH22	1.84	0.43
1:F:298:ILE:O	1:F:319:ALA:HA	2.18	0.43
1:F:414:ALA:HA	1:F:506:ALA:H	1.83	0.43
1:G:118:ALA:O	1:G:122:LEU:CD2	2.67	0.43
1:G:155:ILE:O	1:G:155:ILE:HG12	2.19	0.43



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:161:LEU:N	1:H:161:LEU:CD1	2.82	0.43
1:H:264:ILE:HD12	1:H:265:ARG:HH22	1.84	0.43
1:H:430:ARG:HG2	1:H:430:ARG:NH1	2.29	0.43
1:H:484:TRP:HA	1:H:484:TRP:CE3	2.54	0.43
1:I:39:VAL:HG11	1:I:115:VAL:HG21	2.00	0.43
1:A:284:LYS:HB3	1:A:311:TYR:CE2	2.54	0.43
1:A:415:ILE:HG23	1:A:506:ALA:CB	2.48	0.43
1:B:72:GLY:O	1:B:73:ALA:C	2.57	0.43
1:B:134:GLY:HA3	1:B:443:ALA:CB	2.49	0.43
1:B:298:ILE:O	1:B:319:ALA:HA	2.19	0.43
1:C:209:ILE:CB	1:C:399:ARG:HH22	2.28	0.43
1:C:298:ILE:O	1:C:319:ALA:HA	2.19	0.43
1:E:58:MET:CB	1:E:68:ILE:HG22	2.48	0.43
1:E:72:GLY:O	1:E:73:ALA:C	2.57	0.43
1:E:249:ILE:HD13	1:E:340:VAL:HB	2.00	0.43
1:F:484:TRP:HA	1:F:484:TRP:CE3	2.53	0.43
1:G:161:LEU:N	1:G:161:LEU:CD1	2.82	0.43
1:H:155:ILE:O	1:H:155:ILE:HG12	2.19	0.43
1:I:134:GLY:HA3	1:I:443:ALA:CB	2.49	0.43
1:I:230:LYS:HZ1	1:I:321:ARG:NH1	2.14	0.43
1:I:233:VAL:HG22	1:I:309:GLN:CD	2.39	0.43
1:I:298:ILE:O	1:I:319:ALA:HA	2.19	0.43
1:A:58:MET:CB	1:A:68:ILE:HG22	2.48	0.43
1:A:134:GLY:HA3	1:A:443:ALA:CB	2.49	0.43
1:A:505:PRO:C	1:A:507:LEU:H	2.22	0.43
1:C:440:GLU:O	1:C:444:VAL:HG23	2.18	0.43
1:D:81:LEU:HD22	1:D:86:ALA:HB1	2.01	0.43
1:E:118:ALA:O	1:E:122:LEU:CD2	2.67	0.43
1:E:440:GLU:O	1:E:444:VAL:HG23	2.18	0.43
1:E:476:THR:HG21	1:E:494:PRO:HB3	1.99	0.43
1:F:155:ILE:O	1:F:155:ILE:HG12	2.19	0.43
1:H:459:ILE:O	1:H:462:ALA:HB3	2.19	0.43
1:I:264:ILE:HD12	1:I:265:ARG:HH22	1.84	0.43
1:A:482:ASN:O	1:A:485:TYR:N	2.40	0.42
1:A:484:TRP:HA	1:A:484:TRP:CE3	2.54	0.42
1:C:134:GLY:HA3	1:C:443:ALA:CB	2.49	0.42
1:C:415:ILE:HG23	1:C:506:ALA:CB	2.48	0.42
1:D:46:LEU:N	1:D:46:LEU:CD1	2.82	0.42
1:D:46:LEU:O	1:D:49:THR:N	2.43	0.42
1:D:249:ILE:HD13	1:D:340:VAL:HB	2.00	0.42
1:D:321:ARG:HB3	1:D:322:ARG:H	1.56	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:459:ILE:O	1:D:462:ALA:HB3	2.19	0.42
1:E:134:GLY:HA3	1:E:443:ALA:CB	2.49	0.42
1:E:505:PRO:O	1:E:507:LEU:N	2.52	0.42
1:F:89:LEU:CD2	1:F:108:VAL:HG23	2.44	0.42
1:G:39:VAL:HG11	1:G:115:VAL:HG21	2.00	0.42
1:G:134:GLY:HA3	1:G:443:ALA:CB	2.49	0.42
1:G:505:PRO:C	1:G:507:LEU:H	2.22	0.42
1:H:258:PRO:CG	1:H:279:GLU:OE2	2.56	0.42
1:H:284:LYS:HB3	1:H:311:TYR:CE2	2.54	0.42
1:H:525:ARG:HG2	1:H:525:ARG:NH1	2.31	0.42
1:A:391:VAL:HG13	1:A:392:ASP:N	2.33	0.42
1:A:505:PRO:O	1:A:507:LEU:N	2.52	0.42
1:B:39:VAL:HG11	1:B:115:VAL:HG21	2.00	0.42
1:B:118:ALA:O	1:B:122:LEU:CD2	2.67	0.42
1:B:459:ILE:O	1:B:462:ALA:HB3	2.19	0.42
1:C:284:LYS:HB3	1:C:311:TYR:CE2	2.54	0.42
1:C:298:ILE:O	1:C:298:ILE:HG23	2.19	0.42
1:D:134:GLY:HA3	1:D:443:ALA:CB	2.49	0.42
1:D:153:VAL:HG23	1:D:160:LEU:CD2	2.45	0.42
1:D:244:ALA:HA	1:D:296:ASN:HD22	1.82	0.42
1:E:508:VAL:CG1	1:E:509:LYS:N	2.83	0.42
1:F:46:LEU:N	1:F:46:LEU:CD1	2.82	0.42
1:F:508:VAL:CG1	1:F:509:LYS:N	2.83	0.42
1:I:484:TRP:HA	1:I:484:TRP:CE3	2.54	0.42
1:A:72:GLY:O	1:A:73:ALA:C	2.57	0.42
1:A:155:ILE:O	1:A:155:ILE:HG12	2.19	0.42
1:A:298:ILE:O	1:A:298:ILE:HG23	2.20	0.42
1:B:82:GLN:O	1:B:83:HIS:C	2.56	0.42
1:C:505:PRO:C	1:C:507:LEU:H	2.22	0.42
1:D:39:VAL:HG11	1:D:115:VAL:HG21	2.00	0.42
1:D:245:LYS:H	1:D:296:ASN:ND2	2.07	0.42
1:F:82:GLN:O	1:F:83:HIS:C	2.56	0.42
1:F:321:ARG:HB3	1:F:322:ARG:H	1.56	0.42
1:H:298:ILE:O	1:H:298:ILE:HG23	2.20	0.42
1:I:268:ASP:HB3	1:I:269:PRO:HD2	2.02	0.42
1:I:298:ILE:O	1:I:298:ILE:HG23	2.20	0.42
1:A:89:LEU:CD2	1:A:108:VAL:HG23	2.44	0.42
1:A:264:ILE:HD12	1:A:265:ARG:HH22	1.84	0.42
1:A:459:ILE:O	1:A:462:ALA:HB3	2.19	0.42
1:B:155:ILE:O	1:B:155:ILE:HG12	2.19	0.42
1:C:59:LEU:HD13	1:C:78:LYS:HB2	2.00	0.42



	A 4 O	Interatomic	Clash		
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
1:C:118:ALA:O	1:C:122:LEU:CD2	2.67	0.42		
1:C:398:LEU:HD12	1:C:398:LEU:HA	1.88	0.42		
1:C:459:ILE:O	1:C:462:ALA:HB3	2.19	0.42		
1:E:132:ILE:HD12	1:E:521:THR:HB	2.01	0.42		
1:E:155:ILE:HG12	1:E:155:ILE:O	2.19	0.42		
1:E:161:LEU:N	1:E:161:LEU:CD1	2.82	0.42		
1:E:284:LYS:HB3	1:E:311:TYR:CE2	2.54	0.42		
1:F:118:ALA:O	1:F:122:LEU:CD2	2.67	0.42		
1:G:459:ILE:O	1:G:462:ALA:HB3	2.19	0.42		
1:G:505:PRO:O	1:G:507:LEU:N	2.52	0.42		
1:H:505:PRO:O	1:H:507:LEU:N	2.52	0.42		
1:H:508:VAL:CG1	1:H:509:LYS:N	2.83	0.42		
1:I:132:ILE:HD12	1:I:521:THR:HB	2.01	0.42		
1:A:81:LEU:HD22	1:A:86:ALA:HB1	2.01	0.42		
1:A:249:ILE:HD13	1:A:340:VAL:HB	2.00	0.42		
1:A:433:ALA:O	1:A:434:PRO:C	2.58	0.42		
1:C:46:LEU:O	1:C:49:THR:N	2.43	0.42		
1:C:268:ASP:HB3	1:C:269:PRO:HD2	2.02	0.42		
1:D:505:PRO:O	1:D:507:LEU:N	2.52	0.42		
1:D:508:VAL:CG1	1:D:509:LYS:N	2.83	0.42		
1:D:529:VAL:CG1	1:E:58:MET:HB3	2.29	0.42		
1:E:482:ASN:O	1:E:485:TYR:N	2.40	0.42		
1:F:351:LEU:HD23	1:F:351:LEU:N	2.26	0.42		
1:G:298:ILE:O	1:G:319:ALA:HA	2.19	0.42		
1:H:106:THR:O	1:H:107:ALA:C	2.58	0.42		
1:H:209:ILE:CB	1:H:399:ARG:HH22	2.28	0.42		
1:I:81:LEU:HD22	1:I:86:ALA:HB1	2.01	0.42		
1:I:155:ILE:O	1:I:155:ILE:HG12	2.19	0.42		
1:I:161:LEU:N	1:I:161:LEU:CD1	2.82	0.42		
1:I:284:LYS:HB3	1:I:311:TYR:CE2	2.54	0.42		
1:B:284:LYS:HB3	1:B:311:TYR:CE2	2.54	0.42		
1:C:46:LEU:N	1:C:46:LEU:CD1	2.82	0.42		
1:C:106:THR:O	1:C:107:ALA:C	2.58	0.42		
1:C:153:VAL:HG23	1:C:160:LEU:CD2	2.45	0.42		
1:C:258:PRO:CG	1:C:279:GLU:OE2	2.56	0.42		
1:D:72:GLY:O	1:D:73:ALA:C	2.57	0.42		
1:D:106:THR:O	1:D:107:ALA:C	2.58	0.42		
1:D:118:ALA:O	1:D:122:LEU:CD2	2.67	0.42		
1:D:141:VAL:CG2	1:D:432:TYR:CE1	2.97	0.42		
1:E:264:ILE:HD12	1:E:265:ARG:HH22	1.84	0.42		
1:F:132:ILE:HD12	1:F:521:THR:HB	2.01	0.42		



		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (\AA)		
1:F:260:LEU:CD1	1:F:260:LEU:C	2.81	0.42	
1:G:153:VAL:HG23	1:G:160:LEU:CD2	2.45	0.42	
1:G:433:ALA:O	1:G:434:PRO:C	2.58	0.42	
1:G:508:VAL:CG1	1:G:509:LYS:N	2.83	0.42	
1:H:433:ALA:O	1:H:434:PRO:C	2.58	0.42	
1:A:161:LEU:N	1:A:161:LEU:CD1	2.82	0.42	
1:B:161:LEU:N	1:B:161:LEU:CD1	2.82	0.42	
1:E:88:LEU:CD2	1:F:58:MET:HE2	2.47	0.42	
1:F:72:GLY:O	1:F:73:ALA:C	2.57	0.42	
1:F:195:LEU:HD11	1:F:200:TRP:CH2	2.55	0.42	
1:F:284:LYS:HB3	1:F:311:TYR:CE2	2.54	0.42	
1:G:529:VAL:HG12	1:H:58:MET:SD	2.60	0.42	
1:I:256:GLU:O	1:I:258:PRO:CG	2.68	0.42	
1:A:106:THR:O	1:A:107:ALA:C	2.58	0.42	
1:B:106:THR:O	1:B:107:ALA:C	2.58	0.42	
1:B:132:ILE:HD12	1:B:521:THR:HB	2.01	0.42	
1:B:289:LYS:HB2	1:B:289:LYS:HE3	1.86	0.42	
1:B:505:PRO:O	1:B:507:LEU:N	2.52	0.42	
1:C:291:LEU:O	1:C:294:GLY:N	2.53	0.42	
1:C:505:PRO:O	1:C:507:LEU:N	2.52	0.42	
1:D:268:ASP:HB3	1:D:269:PRO:HD2	2.02	0.42	
1:E:46:LEU:N	1:E:46:LEU:CD1	2.82	0.42	
1:E:264:ILE:CG1	1:E:265:ARG:O	2.66	0.42	
1:E:484:TRP:HA	1:E:484:TRP:HE3	1.85	0.42	
1:F:298:ILE:O	1:F:298:ILE:HG23	2.20	0.42	
1:F:528:ASP:O	1:G:57:LYS:HA	2.19	0.42	
1:H:132:ILE:HD12	1:H:521:THR:HB	2.01	0.42	
1:H:140:GLU:OE2	1:H:140:GLU:HA	2.20	0.42	
1:A:118:ALA:O	1:A:122:LEU:CD2	2.67	0.42	
1:B:46:LEU:O	1:B:49:THR:N	2.43	0.42	
1:B:484:TRP:HA	1:B:484:TRP:HE3	1.85	0.42	
1:C:264:ILE:HD12	1:C:265:ARG:HH22	1.84	0.42	
1:D:155:ILE:O	1:D:155:ILE:HG12	2.19	0.42	
1:E:128:PRO:CG	1:F:55:MET:HE1	2.48	0.42	
1:E:195:LEU:HD11	1:E:200:TRP:CH2	2.55	0.42	
1:E:459:ILE:O	1:E:462:ALA:HB3	2.19	0.42	
1:G:132:ILE:HD12	1:G:521:THR:HB	2.01	0.42	
1:H:134:GLY:HA3	1:H:443:ALA:CB	2.49	0.42	
1:I:59:LEU:HD13	1:I:78:LYS:HB2	2.00	0.42	
1:I:249:ILE:CD1	1:I:346:ILE:HD11	2.50	0.42	
1:I:459:ILE:O	1:I:462:ALA:HB3	2.19	0.42	



	A L O	Interatomic	Clash		
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
1:I:505:PRO:O	1:I:507:LEU:N	2.52	0.42		
1:I:506:ALA:O	1:I:510:MET:HB2	2.20	0.42		
1:A:195:LEU:HD11	1:A:200:TRP:CH2	2.55	0.42		
1:A:268:ASP:HB3	1:A:269:PRO:HD2	2.02	0.42		
1:A:321:ARG:HB3	1:A:322:ARG:H	1.56	0.42		
1:B:264:ILE:HD12	1:B:265:ARG:HH22	1.84	0.42		
1:B:298:ILE:O	1:B:298:ILE:HG23	2.19	0.42		
1:B:433:ALA:O	1:B:434:PRO:C	2.58	0.42		
1:C:506:ALA:O	1:C:510:MET:HB2	2.20	0.42		
1:D:132:ILE:HD12	1:D:521:THR:HB	2.01	0.42		
1:D:161:LEU:N	1:D:161:LEU:CD1	2.82	0.42		
1:D:195:LEU:HD11	1:D:200:TRP:CH2	2.55	0.42		
1:D:433:ALA:O	1:D:434:PRO:C	2.58	0.42		
1:F:39:VAL:HG11	1:F:115:VAL:HG21	2.00	0.42		
1:F:506:ALA:O	1:F:510:MET:HB2	2.20	0.42		
1:G:176:GLY:O	1:G:177:ALA:C	2.59	0.42		
1:G:268:ASP:HB3	1:G:269:PRO:HD2	2.02	0.42		
1:I:118:ALA:O	1:I:122:LEU:CD2	2.67	0.42		
1:A:317:VAL:HG12	1:A:318:LEU:N	2.35	0.41		
1:A:484:TRP:HA	1:A:484:TRP:HE3	1.85	0.41		
1:B:140:GLU:HA	1:B:140:GLU:OE2	2.20	0.41		
1:B:209:ILE:CB	1:B:399:ARG:HH22	2.28	0.41		
1:B:506:ALA:O	1:B:510:MET:HB2	2.20	0.41		
1:D:256:GLU:O	1:D:258:PRO:CG	2.68	0.41		
1:D:284:LYS:HB3	1:D:311:TYR:CE2	2.54	0.41		
1:D:298:ILE:O	1:D:298:ILE:HG23	2.20	0.41		
1:D:415:ILE:HG23	1:D:506:ALA:CB	2.48	0.41		
1:F:146:ILE:HB	1:F:510:MET:HE3	2.00	0.41		
1:F:433:ALA:O	1:F:434:PRO:C	2.58	0.41		
1:F:505:PRO:O	1:F:507:LEU:N	2.53	0.41		
1:G:195:LEU:HD11	1:G:200:TRP:CH2	2.55	0.41		
1:G:493:GLN:HA	1:G:494:PRO:HD3	1.90	0.41		
1:H:72:GLY:O	1:H:73:ALA:C	2.57	0.41		
1:H:176:GLY:O	1:H:177:ALA:C	2.59	0.41		
1:H:195:LEU:HD11	1:H:195:LEU:HD11 1:H:200:TRP:CH2		0.41		
1:A:176:GLY:O	1:A:177:ALA:C	2.59	0.41		
1:B:176:GLY:O	1:B:177:ALA:C	2.59	0.41		
1:B:268:ASP:HB3	1:B:269:PRO:HD2	2.02	0.41		
1:D:359:GLU:HA	1:D:367:MET:O	2.20	0.41		
1:E:249:ILE:CD1	1:E:346:ILE:HD11	2.50	0.41		
1:E:317:VAL:HG12	1:E:318:LEU:N	2.35	0.41		



	A L O	Interatomic	Clash overlap (Å)		
Atom-1	Atom-2	distance (Å)			
1:E:525:ARG:HG2	1:E:525:ARG:NH1	2.31	0.41		
1:F:459:ILE:O	1:F:462:ALA:HB3	2.19	0.41		
1:G:264:ILE:HD12	1:G:265:ARG:HH22	1.84	0.41		
1:G:284:LYS:HB3	1:G:311:TYR:CE2	2.54	0.41		
1:H:484:TRP:HA	1:H:484:TRP:HE3	1.85	0.41		
1:I:176:GLY:O	1:I:177:ALA:C	2.59	0.41		
1:I:433:ALA:O	1:I:434:PRO:C	2.58	0.41		
1:E:140:GLU:HA	1:E:140:GLU:OE2	2.20	0.41		
1:E:268:ASP:HB3	1:E:269:PRO:HD2	2.02	0.41		
1:E:298:ILE:O	1:E:298:ILE:HG23	2.20	0.41		
1:E:506:ALA:O	1:E:510:MET:HB2	2.20	0.41		
1:E:525:ARG:HG3	1:F:56:ASP:CB	2.46	0.41		
1:G:298:ILE:O	1:G:298:ILE:HG23	2.20	0.41		
1:I:106:THR:O	1:I:107:ALA:C	2.58	0.41		
1:A:48:SER:O	1:A:55:MET:HB2	2.21	0.41		
1:A:249:ILE:CD1	1:A:346:ILE:HD11	2.50	0.41		
1:A:359:GLU:HA	1:A:367:MET:O	2.20	0.41		
1:C:132:ILE:HD12	1:C:521:THR:HB	2.01	0.41		
1:C:140:GLU:OE2	1:C:140:GLU:HA	2.20	0.41		
1:D:176:GLY:O	1:D:177:ALA:C	2.59	0.41		
1:D:264:ILE:HD12	1:D:265:ARG:HH22	1.84	0.41		
1:E:48:SER:O	1:E:55:MET:HB2	2.20	0.41		
1:E:89:LEU:CD2	1:E:108:VAL:HG23	2.44	0.41		
1:F:81:LEU:HD22	1:F:86:ALA:HB1	2.01	0.41		
1:F:249:ILE:CD1	1:F:346:ILE:HD11	2.50	0.41		
1:F:359:GLU:HA	1:F:367:MET:O	2.20	0.41		
1:G:106:THR:O	1:G:107:ALA:C	2.58	0.41		
1:G:260:LEU:CD1	1:G:260:LEU:C	2.81	0.41		
1:G:359:GLU:HA	1:G:367:MET:O	2.20	0.41		
1:H:46:LEU:N	1:H:46:LEU:CD1	2.82	0.41		
1:H:268:ASP:HB3	1:H:269:PRO:HD2	2.01	0.41		
1:I:359:GLU:HA	1:I:367:MET:O	2.20	0.41		
1:I:454:LEU:HD12	1:I:454:LEU:HA	1.91	0.41		
1:I:508:VAL:CG1	1:I:509:LYS:N	2.83	0.41		
1:A:46:LEU:N	1:A:46:LEU:CD1	2.82	0.41		
1:A:58:MET:CE	1:I:88:LEU:HD22	2.50	0.41		
1:A:194:GLU:O	1:A:200:TRP:HA	2.21	0.41		
1:C:249:ILE:CD1	1:C:346:ILE:HD11	2.50	0.41		
1:C:359:GLU:HA	1:C:367:MET:O	2.20	0.41		
1:D:530:VAL:O	1:E:59:LEU:HA	2.19	0.41		
1:F:106:THR:O	1:F:107:ALA:C	2.58	0.41		



	to ac pagem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:F:134:GLY:HA3	1:F:443:ALA:CB	2.49	0.41		
1:G:48:SER:O	1:G:55:MET:HB2	2.21	0.41		
1:G:415:ILE:HG23	1:G:506:ALA:CB	2.48	0.41		
1:I:46:LEU:N	1:I:46:LEU:CD1	2.82	0.41		
1:I:195:LEU:HD11	1:I:200:TRP:CH2	2.55	0.41		
1:A:264:ILE:CG1	1:A:265:ARG:O	2.66	0.41		
1:B:291:LEU:O	1:B:294:GLY:N	2.53	0.41		
1:B:504:GLU:HA	1:B:505:PRO:HD3	1.90	0.41		
1:C:256:GLU:O	1:C:258:PRO:CG	2.68	0.41		
1:D:454:LEU:HD12	1:D:454:LEU:HA	1.91	0.41		
1:E:194:GLU:O	1:E:200:TRP:HA	2.21	0.41		
1:E:230:LYS:NZ	1:E:321:ARG:HH12	2.18	0.41		
1:E:415:ILE:HG23	1:E:506:ALA:CB	2.48	0.41		
1:G:194:GLU:O	1:G:200:TRP:HA	2.21	0.41		
1:H:506:ALA:O	1:H:510:MET:HB2	2.20	0.41		
1:H:522:LEU:HD11	1:I:68:ILE:HD12	2.03	0.41		
1:A:508:VAL:CG1	1:A:509:LYS:N	2.83	0.41		
1:B:493:GLN:HA	1:B:494:PRO:HD3	1.90	0.41		
1:C:81:LEU:HD13	1:C:87:LYS:HG2	2.03	0.41		
1:C:317:VAL:HG12	1:C:318:LEU:N	2.35	0.41		
1:C:321:ARG:HB3	1:C:322:ARG:H	1.56	0.41		
1:D:48:SER:O	1:D:55:MET:HB2	2.21	0.41		
1:F:291:LEU:O	1:F:294:GLY:N	2.53	0.41		
1:I:46:LEU:O	1:I:49:THR:N	2.43	0.41		
1:A:88:LEU:HD22	1:B:58:MET:CE	2.51	0.41		
1:A:253:LEU:HG	1:A:253:LEU:O	2.21	0.41		
1:A:291:LEU:O	1:A:294:GLY:N	2.53	0.41		
1:A:506:ALA:O	1:A:510:MET:HB2	2.20	0.41		
1:B:81:LEU:HD12	1:B:81:LEU:N	2.28	0.41		
1:B:249:ILE:O	1:B:300:CYS:HB2	2.21	0.41		
1:B:317:VAL:HG12	1:B:318:LEU:N	2.35	0.41		
1:C:253:LEU:HG	1:C:253:LEU:O	2.21	0.41		
1:D:317:VAL:HG12	1:D:318:LEU:N	2.35	0.41		
1:E:454:LEU:HD12	1:E:454:LEU:HA	1.91	0.41		
1:H:81:LEU:HD22	1:H:86:ALA:HB1	2.01	0.41		
1:H:259:GLU:O	1:H:262:ALA:O	2.39	0.41		
1:I:48:SER:O	1:I:55:MET:HB2	2.21	0.41		
1:I:81:LEU:HD13	1:I:87:LYS:HG2	2.03	0.41		
1:I:140:GLU:HA	1:I:140:GLU:OE2	2.20	0.41		
1:I:317:VAL:HG12	1:I:318:LEU:N	2.35	0.41		
1:A:46:LEU:O	1:A:49:THR:N	2.43	0.41		



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:389:ARG:HH12	1:I:88:LEU:CD1	2.31	0.41		
1:A:525:ARG:HG2	1:A:525:ARG:NH1	2.31	0.41		
1:B:46:LEU:N	1:B:46:LEU:CD1	2.82	0.41		
1:B:48:SER:O	1:B:55:MET:HB2	2.21	0.41		
1:B:195:LEU:HD11	1:B:200:TRP:CH2	2.55	0.41		
1:C:176:GLY:O	1:C:177:ALA:C	2.59	0.41		
1:C:195:LEU:HD11	1:C:200:TRP:CH2	2.55	0.41		
1:C:433:ALA:O	1:C:434:PRO:C	2.58	0.41		
1:D:81:LEU:HD13	1:D:87:LYS:HG2	2.03	0.41		
1:D:253:LEU:O	1:D:253:LEU:HG	2.21	0.41		
1:D:436:VAL:CG2	1:D:441:GLN:HA	2.51	0.41		
1:D:506:ALA:O	1:D:510:MET:HB2	2.20	0.41		
1:E:176:GLY:O	1:E:177:ALA:C	2.59	0.41		
1:E:359:GLU:HA	1:E:367:MET:O	2.20	0.41		
1:E:433:ALA:O	1:E:434:PRO:C	2.58	0.41		
1:F:176:GLY:O	1:F:177:ALA:C	2.59	0.41		
1:F:253:LEU:O	1:F:253:LEU:HG	2.21	0.41		
1:F:268:ASP:HB3	1:F:269:PRO:HD2	2.02	0.41		
1:F:317:VAL:HG12	1:F:318:LEU:N	2.35	0.41		
1:G:94:LYS:O	1:G:96:GLN:N	2.48	0.41		
1:G:140:GLU:HA	1:G:140:GLU:OE2	2.20	0.41		
1:G:249:ILE:CD1	1:G:346:ILE:HD11	2.50	0.41		
1:G:506:ALA:O	1:G:510:MET:HB2	2.20	0.41		
1:H:249:ILE:CD1	1:H:346:ILE:HD11	2.50	0.41		
1:H:291:LEU:O	1:H:294:GLY:N	2.53	0.41		
1:H:359:GLU:HA	1:H:367:MET:O	2.20	0.41		
1:I:484:TRP:HA	1:I:484:TRP:HE3	1.85	0.41		
1:A:140:GLU:OE2	1:A:140:GLU:HA	2.20	0.41		
1:A:166:MET:CE	1:A:179:GLU:HG2	2.51	0.41		
1:A:246:ILE:HA	1:A:297:VAL:CG1	2.51	0.41		
1:B:194:GLU:O	1:B:200:TRP:HA	2.21	0.41		
1:C:155:ILE:O	1:C:155:ILE:HG12	2.19	0.41		
1:C:259:GLU:O	1:C:262:ALA:O	2.39	0.41		
1:D:484:TRP:HA	1:D:484:TRP:HE3	1.85	0.41		
1:E:436:VAL:CG2	1:E:441:GLN:HA	2.51	0.41		
1:F:194:GLU:O	1:F:200:TRP:HA	2.21	0.41		
1:F:246:ILE:HA	1:F:297:VAL:CG1	2.51	0.41		
1:G:249:ILE:O	1:G:300:CYS:HB2	2.21	0.41		
1:H:194:GLU:O	1:H:200:TRP:HA	2.21	0.41		
1:I:245:LYS:H	1:I:296:ASN:ND2	2.07	0.41		
1:I:253:LEU:HG	1:I:253:LEU:O	2.21	0.41		



	A 4 O	Interatomic	Clash		
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
1:I:321:ARG:HB3	1:I:322:ARG:H	1.56	0.41		
1:I:436:VAL:CG2	1:I:441:GLN:HA	2.51	0.41		
1:A:147:GLN:C	1:A:149:LEU:H	2.25	0.40		
1:B:253:LEU:HG	1:B:253:LEU:O	2.21	0.40		
1:C:66:ILE:CD1	1:C:66:ILE:N	2.76	0.40		
1:D:249:ILE:CD1	1:D:346:ILE:HD11	2.50	0.40		
1:D:531:SER:HB3	1:E:60:VAL:HB	2.04	0.40		
1:G:253:LEU:HG	1:G:253:LEU:O	2.21	0.40		
1:G:436:VAL:CG2	1:G:441:GLN:HA	2.52	0.40		
1:H:253:LEU:HG	1:H:253:LEU:O	2.21	0.40		
1:H:351:LEU:HD23	1:H:351:LEU:N	2.26	0.40		
1:H:436:VAL:CG2	1:H:441:GLN:HA	2.51	0.40		
1:I:194:GLU:O	1:I:200:TRP:HA	2.21	0.40		
1:B:81:LEU:HD13	1:B:87:LYS:HG2	2.03	0.40		
1:B:147:GLN:C	1:B:149:LEU:H	2.25	0.40		
1:B:153:VAL:HG23	L:HG23 1:B:160:LEU:CD2		0.40		
1:C:230:LYS:NZ	1:C:321:ARG:HH12	2.18	0.40		
1:C:410:LYS:HB3	1:C:410:LYS:HE2	1.89	0.40		
1:C:508:VAL:CG1	1:C:509:LYS:N	2.83	0.40		
1:D:194:GLU:O	1:D:200:TRP:HA	2.21	0.40		
1:E:166:MET:CE	1:E:179:GLU:HG2	2.51	0.40		
1:E:259:GLU:O	1:E:262:ALA:O	2.39	0.40		
1:F:48:SER:O	1:F:55:MET:HB2	2.21	0.40		
1:F:140:GLU:OE2	U:OE2 1:F:140:GLU:HA 2.20		0.40		
1:F:166:MET:CE	1:F:179:GLU:HG2	2.51	0.40		
1:F:423:ILE:HG12	1:F:473:LEU:HD11	2.03	0.40		
1:G:317:VAL:HG12	1:G:318:LEU:N	2.35	0.40		
1:H:246:ILE:HA	1:H:297:VAL:CG1	2.51	0.40		
1:H:256:GLU:O	1:H:258:PRO:CG	2.68	0.40		
1:I:264:ILE:CG1	1:I:265:ARG:O	2.67	0.40		
1:I:473:LEU:C	1:I:475:SER:N	2.75	0.40		
1:A:84:PRO:HB2	1:B:58:MET:SD	2.61	0.40		
1:A:259:GLU:O	1:A:262:ALA:O	2.39	0.40		
1:A:410:LYS:HE2	1:A:410:LYS:HB3	1.89	0.40		
1:B:246:ILE:HA	1:B:246:ILE:HA 1:B:297:VAL:CG1		0.40		
1:B:508:VAL:CG1	1:B:509:LYS:N	2.83	0.40		
1:C:249:ILE:O	1:C:300:CYS:HB2	2.21	0.40		
1:D:147:GLN:C	1:D:149:LEU:H	2.25	0.40		
1:D:166:MET:CE	1:D:179:GLU:HG2	2.51	0.40		
1:D:246:ILE:HA	1:D:297:VAL:CG1	2.51	0.40		
1:E:166:MET:HE2	1:E:178:ARG:HG2	2.03	0.40		



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:258:PRO:CG	1:E:279:GLU:OE2	2.56	0.40	
1:F:259:GLU:O	1:F:262:ALA:O	2.39	0.40	
1:G:246:ILE:HA	1:G:297:VAL:CG1	2.52	0.40	
1:G:264:ILE:CG1	1:G:265:ARG:O	2.66	0.40	
1:G:484:TRP:HA	1:G:484:TRP:HE3	1.85	0.40	
1:H:48:SER:O	1:H:55:MET:HB2	2.21	0.40	
1:A:258:PRO:CG	1:A:279:GLU:OE2	2.56	0.40	
1:D:140:GLU:OE2	1:D:140:GLU:HA	2.20	0.40	
1:D:423:ILE:HG12	1:D:473:LEU:HD11	2.03	0.40	
1:E:106:THR:O	1:E:107:ALA:C	2.58	0.40	
1:E:246:ILE:HA	1:E:297:VAL:CG1	2.51	0.40	
1:F:94:LYS:O	1:F:96:GLN:N	2.48	0.40	
1:F:436:VAL:CG2	1:F:441:GLN:HA	2.51	0.40	
1:G:209:ILE:CB	1:G:399:ARG:HH22	2.28	0.40	
1:H:454:LEU:HA	1:H:454:LEU:HD12	1.91	0.40	
1:I:153:VAL:HG23	1:I:160:LEU:CD2	2.45	0.40	
1:B:359:GLU:HA	1:B:367:MET:O	2.20	0.40	
1:B:473:LEU:C	1:B:475:SER:N	2.75	0.40	
1:C:89:LEU:CD2	1:C:108:VAL:HG23	2.44	0.40	
1:D:249:ILE:O	1:D:300:CYS:HB2	2.21	0.40	
1:D:259:GLU:O	1:D:262:ALA:O	2.39	0.40	
1:D:347:SER:C	1:D:349:GLN:N	2.75	0.40	
1:G:238:PRO:O	1:G:318:LEU:HD13	2.22	0.40	
1:G:259:GLU:O	1:G:262:ALA:O	2.39	0.40	
1:G:423:ILE:HG12	1:G:473:LEU:HD11	2.03	0.40	
1:G:473:LEU:C	1:G:475:SER:N	2.75	0.40	
1:H:317:VAL:HG12	1:H:318:LEU:N	2.35	0.40	

All (28) 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	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:272:MET:CE	1:B:275:PHE:CD1[2_656]	1.14	1.06
1:E:273:GLN:NE2	1:H:276:LEU:CD1[2_656]	1.28	0.92
1:C:435:GLN:NE2	1:H:478:GLU:O[1_556]	1.36	0.84
1:B:264:ILE:O	1:B:266:ILE:O[2_656]	1.37	0.83
1:D:183:ASP:OD2	1:H:159:ASP:OD1[1_556]	1.39	0.81
1:B:156:ASN:ND2	1:E:193:ALA:CB[4_546]	1.41	0.79
1:D:183:ASP:OD2	1:H:159:ASP:CG[1_556]	1.49	0.71
1:E:266:ILE:O	1:H:264:ILE:O[2_656]	1.56	0.64



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:289:LYS:NZ	1:G:281:ASN:OD1[2_656]	1.67	0.53	
1:B:193:ALA:CB	$1:E:156:ASN:ND2[4_546]$	1.71	0.49	
1:B:198:ASP:O	$1:E:198:ASP:CB[4_546]$	1.73	0.47	
1:F:156:ASN:ND2	$1:I:156:ASN:ND2[4_555]$	1.79	0.41	
1:E:276:LEU:CD1	1:H:272:MET:CB[2_656]	1.84	0.36	
1:C:435:GLN:NE2	1:H:478:GLU:C[1_556]	1.87	0.33	
1:B:198:ASP:CB	$1:E:198:ASP:O[4_546]$	2.00	0.20	
1:B:198:ASP:OD1	$1:E:198:ASP:OD1[4_546]$	2.02	0.18	
1:A:281:ASN:OD1	1:B:289:LYS:NZ[2_656]	2.05	0.15	
1:E:285:GLU:OE2	1:G:281:ASN:O[2_656]	2.05	0.15	
1:B:156:ASN:ND2	1:E:193:ALA:CA[4_546]	2.06	0.14	
1:D:266:ILE:O	1:I:264:ILE:O[2_656]	2.07	0.13	
1:B:200:TRP:CZ2	$1:E:200:TRP:CZ2[4_546]$	2.08	0.12	
1:D:183:ASP:OD2	$1:H:159:ASP:CB[1_556]$	2.10	0.10	
1:D:289:LYS:NZ	$1:H:281:ASN:OD1[2_656]$	2.11	0.09	
1:A:266:ILE:O	$1:C:264:ILE:O[2_656]$	2.12	0.08	
1:D:273:GLN:NE2	1:I:276:LEU:CD1[2_656]	2.12	0.08	
1:B:272:MET:CE	1:B:275:PHE:CE1[2_656]	2.14	0.06	
1:C:137:LYS:CD	$1:H:481:ASN:OD1[1_556]$	2.18	0.02	
1:C:137:LYS:CG	1:H:481:ASN:OD1[1_556]	2.19	0.01	

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	Perc	centiles
1	А	503/553~(91%)	396~(79%)	89~(18%)	18 (4%)	3	29
1	В	503/553~(91%)	397~(79%)	88 (18%)	18 (4%)	3	29
1	С	503/553~(91%)	397~(79%)	88 (18%)	18 (4%)	3	29
1	D	503/553~(91%)	396 (79%)	89~(18%)	18 (4%)	3	29
1	Ε	503/553~(91%)	397~(79%)	88 (18%)	18 (4%)	3	29
1	F	503/553~(91%)	397 (79%)	88 (18%)	18 (4%)	3	29



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Р	erc	entile	es
1	G	503/553~(91%)	396 (79%)	89 (18%)	18 (4%)		3	29	
1	Н	503/553~(91%)	396 (79%)	89 (18%)	18 (4%)		3	29	
1	Ι	503/553~(91%)	396 (79%)	89 (18%)	18 (4%)		3	29	
All	All	4527/4977 (91%)	3568 (79%)	797 (18%)	162 (4%)		3	29	

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All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	96	GLN
1	А	99	GLU
1	А	213	ALA
1	А	321	ARG
1	В	96	GLN
1	В	99	GLU
1	В	213	ALA
1	В	321	ARG
1	С	96	GLN
1	С	99	GLU
1	С	213	ALA
1	С	321	ARG
1	D	96	GLN
1	D	99	GLU
1	D	213	ALA
1	D	321	ARG
1	Е	96	GLN
1	Е	99	GLU
1	Е	213	ALA
1	Е	321	ARG
1	F	96	GLN
1	F	99	GLU
1	F	213	ALA
1	F	321	ARG
1	G	96	GLN
1	G	99	GLU
1	G	213	ALA
1	G	321	ARG
1	Н	96	GLN
1	Н	99	GLU
1	Н	213	ALA
1	Н	321	ARG
1	I	96	GLN



Mol	Chain	Res	Type
1	Ι	99	GLU
1	Ι	213	ALA
1	Ι	321	ARG
1	А	30	GLU
1	А	100	THR
1	А	177	ALA
1	А	198	ASP
1	В	30	GLU
1	В	100	THR
1	В	177	ALA
1	В	198	ASP
1	С	30	GLU
1	С	100	THR
1	С	177	ALA
1	С	198	ASP
1	D	30	GLU
1	D	100	THR
1	D	177	ALA
1	D	198	ASP
1	Е	30	GLU
1	Е	100	THR
1	Е	177	ALA
1	Е	198	ASP
1	F	30	GLU
1	F	100	THR
1	F	177	ALA
1	F	198	ASP
1	G	30	GLU
1	G	100	THR
1	G	177	ALA
1	G	198	ASP
1	Н	30	GLU
1	Н	100	THR
1	H	177	ALA
1	Н	198	ASP
1	I	30	GLU
1	Ι	100	THR
1	Ι	177	ALA
1	I	198	ASP
1	A	377	LYS
1	A	438	GLY
1	В	377	LYS



Mol	Chain	Res	Type
1	В	438	GLY
1	С	377	LYS
1	С	438	GLY
1	D	377	LYS
1	D	438	GLY
1	Е	377	LYS
1	Е	438	GLY
1	F	377	LYS
1	F	438	GLY
1	G	377	LYS
1	G	438	GLY
1	Н	377	LYS
1	Н	438	GLY
1	Ι	377	LYS
1	Ι	438	GLY
1	А	149	LEU
1	А	174	VAL
1	А	196	ARG
1	В	149	LEU
1	В	174	VAL
1	С	149	LEU
1	С	174	VAL
1	С	196	ARG
1	D	149	LEU
1	D	174	VAL
1	Е	149	LEU
1	Е	174	VAL
1	Е	196	ARG
1	F	149	LEU
1	F	174	VAL
1	F	196	ARG
1	G	149	LEU
1	G	174	VAL
1	G	196	ARG
1	Н	149	LEU
1	H	174	VAL
1	Н	196	ARG
1	Ι	149	LEU
1	Ι	174	VAL
1	Ι	196	ARG
1	А	348	GLU
1	А	376	PRO



Mol	Chain	Res	Type
1	А	480	GLU
1	В	196	ARG
1	В	348	GLU
1	В	376	PRO
1	В	480	GLU
1	С	348	GLU
1	С	376	PRO
1	С	480	GLU
1	D	196	ARG
1	D	348	GLU
1	D	376	PRO
1	D	480	GLU
1	Е	348	GLU
1	Е	376	PRO
1	Е	480	GLU
1	F	348	GLU
1	F	376	PRO
1	F	480	GLU
1	G	348	GLU
1	G	376	PRO
1	G	480	GLU
1	Н	348	GLU
1	Н	376	PRO
1	Н	480	GLU
1	Ι	348	GLU
1	Ι	376	PRO
1	Ι	480	GLU
1	А	215	GLY
1	В	215	GLY
1	С	215	GLY
1	D	215	GLY
1	Е	215	GLY
1	F	215	GLY
1	G	215	GLY
1	Н	215	GLY
1	I	215	GLY
1	В	340	VAL
1	Ι	340	VAL
1	A	340	VAL
1	С	340	VAL
1	D	340	VAL
1	Е	340	VAL



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Mol	Chain	Res	Type
1	F	340	VAL
1	G	340	VAL
1	Н	340	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	410/447~(92%)	386~(94%)	24~(6%)	19	51
1	В	410/447~(92%)	386~(94%)	24~(6%)	19	51
1	С	410/447~(92%)	386~(94%)	24~(6%)	19	51
1	D	410/447~(92%)	386~(94%)	24~(6%)	19	51
1	Ε	410/447~(92%)	386~(94%)	24~(6%)	19	51
1	F	410/447~(92%)	386~(94%)	24~(6%)	19	51
1	G	410/447~(92%)	386~(94%)	24~(6%)	19	51
1	Н	410/447~(92%)	386 (94%)	24 (6%)	19	51
1	Ι	410/447~(92%)	386 (94%)	24 (6%)	19	51
All	All	3690/4023~(92%)	3474 (94%)	216 (6%)	19	51

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	33	ARG
1	А	66	ILE
1	А	80	ASP
1	А	81	LEU
1	А	82	GLN
1	А	98	GLU
1	А	129	THR
1	А	162	ARG
1	А	178	ARG
1	А	179	GLU
1	A	212	LYS



Mol	Chain	Res	Type
1	А	255	VAL
1	А	256	GLU
1	А	263	GLU
1	А	264	ILE
1	А	265	ARG
1	А	299	ILE
1	А	321	ARG
1	А	324	LYS
1	А	361	LYS
1	А	374	LYS
1	А	393	GLU
1	А	404	THR
1	А	415	ILE
1	В	33	ARG
1	В	66	ILE
1	В	80	ASP
1	В	81	LEU
1	В	82	GLN
1	В	98	GLU
1	В	129	THR
1	В	162	ARG
1	В	178	ARG
1	В	179	GLU
1	В	212	LYS
1	В	255	VAL
1	В	256	GLU
1	В	263	GLU
1	В	264	ILE
1	В	265	ARG
1	В	299	ILE
1	В	321	ARG
1	В	324	LYS
1	В	361	LYS
1	В	374	LYS
1	В	393	GLU
1	В	404	THR
1	В	415	ILE
1	С	33	ARG
1	С	66	ILE
1	C	80	ASP
1	С	81	LEU
1	С	82	GLN



Mol	Chain	Res	Type
1	С	98	GLU
1	С	129	THR
1	С	162	ARG
1	С	178	ARG
1	С	179	GLU
1	С	212	LYS
1	С	255	VAL
1	С	256	GLU
1	С	263	GLU
1	С	264	ILE
1	С	265	ARG
1	С	299	ILE
1	С	321	ARG
1	С	324	LYS
1	С	361	LYS
1	С	374	LYS
1	С	393	GLU
1	С	404	THR
1	С	415	ILE
1	D	33	ARG
1	D	66	ILE
1	D	80	ASP
1	D	81	LEU
1	D	82	GLN
1	D	98	GLU
1	D	129	THR
1	D	162	ARG
1	D	178	ARG
1	D	179	GLU
1	D	212	LYS
1	D	255	VAL
1	D	256	GLU
1	D	263	GLU
1	D	264	ILE
1	D	265	ARG
1	D	299	ILE
1	D	321	ARG
1	D	324	LYS
1	D	361	LYS
1	D	374	LYS
1	D	393	GLU
1	D	404	THR



Mol	Chain	Res	Type
1	D	415	ILE
1	Е	33	ARG
1	Е	66	ILE
1	Е	80	ASP
1	Е	81	LEU
1	Е	82	GLN
1	Е	98	GLU
1	Е	129	THR
1	Е	162	ARG
1	Е	178	ARG
1	Е	179	GLU
1	Е	212	LYS
1	Е	255	VAL
1	Е	256	GLU
1	Е	263	GLU
1	Е	264	ILE
1	Е	265	ARG
1	Е	299	ILE
1	Е	321	ARG
1	Ε	324	LYS
1	Ε	361	LYS
1	Е	374	LYS
1	Ε	393	GLU
1	Ε	404	THR
1	Е	415	ILE
1	F	33	ARG
1	F	66	ILE
1	F	80	ASP
1	F	81	LEU
1	F	82	GLN
1	F	98	GLU
1	F	129	THR
1	F	162	ARG
1	F	178	ARG
1	F	179	GLU
1	F	212	LYS
1	F	255	VAL
1	F	256	GLU
1	F	263	GLU
1	F	264	ILE
1	F	265	ARG
1	F	299	ILE



Mol	Chain	Res	Type
1	F	321	ARG
1	F	324	LYS
1	F	361	LYS
1	F	374	LYS
1	F	393	GLU
1	F	404	THR
1	F	415	ILE
1	G	33	ARG
1	G	66	ILE
1	G	80	ASP
1	G	81	LEU
1	G	82	GLN
1	G	98	GLU
1	G	129	THR
1	G	162	ARG
1	G	178	ARG
1	G	179	GLU
1	G	212	LYS
1	G	255	VAL
1	G	256	GLU
1	G	263	GLU
1	G	264	ILE
1	G	265	ARG
1	G	299	ILE
1	G	321	ARG
1	G	324	LYS
1	G	361	LYS
1	G	374	LYS
1	G	393	GLU
1	G	404	THR
1	G	415	ILE
1	H	33	ARG
1	Н	66	ILE
1	H	80	ASP
1	Н	81	LEU
1	Н	82	GLN
1	Н	98	GLU
1	Н	129	THR
1	Н	162	ARG
1	Н	178	ARG
1	Н	179	GLU
1	Н	212	LYS



Mol	Chain	Res	Type
1	Н	255	VAL
1	Н	256	GLU
1	Н	263	GLU
1	Н	264	ILE
1	Н	265	ARG
1	Н	299	ILE
1	Н	321	ARG
1	Н	324	LYS
1	Н	361	LYS
1	Н	374	LYS
1	Н	393	GLU
1	Н	404	THR
1	Н	415	ILE
1	Ι	33	ARG
1	Ι	66	ILE
1	Ι	80	ASP
1	Ι	81	LEU
1	Ι	82	GLN
1	Ι	98	GLU
1	Ι	129	THR
1	Ι	162	ARG
1	Ι	178	ARG
1	Ι	179	GLU
1	Ι	212	LYS
1	Ι	255	VAL
1	Ι	256	GLU
1	I	263	GLU
1	Ι	264	ILE
1	Ι	265	ARG
1	Ι	299	ILE
1	Ι	321	ARG
1	Ι	324	LYS
1	Ι	361	LYS
1	Ι	374	LYS
1	Ι	393	GLU
1	Ι	404	THR
1	Ι	415	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

	Cham	nes	Type
1	А	82	GLN



Mol	Chain	Res	Type	
1	А	83	HIS	
1	А	91	GLN	
1	А	96	GLN	
1	А	127	HIS	
1	А	147	GLN	
1	А	151	GLN	
1	А	208	GLN	
1	А	234	HIS	
1	А	281	ASN	
1	А	296	ASN	
1	А	441	GLN	
1	А	461	ASN	
1	А	477	HIS	
1	А	481	ASN	
1	А	511	ASN	
1	В	82	GLN	
1	В	83	HIS	
1	В	96	GLN	
1	В	127	HIS	
1	В	147	GLN	
1	В	151	GLN	
1	В	208	GLN	
1	В	234	HIS	
1	В	281	ASN	
1	В	296	ASN	
1	В	441	GLN	
1	В	461	ASN	
1	В	477	HIS	
1	В	481	ASN	
1	В	511	ASN	
1	С	82	GLN	
1	С	83	HIS	
1	С	91	GLN	
1	С	96	GLN	
1	С	127	HIS	
1	С	147	GLN	
1	С	151	GLN	
1	С	208	GLN	
1	С	234	HIS	
1	С	281	ASN	
1	С	296	ASN	
1	С	441	GLN	



Mol	Chain	Res	Type	
1	С	461	ASN	
1	С	477	HIS	
1	С	481	ASN	
1	С	511	ASN	
1	D	82	GLN	
1	D	83	HIS	
1	D	91	GLN	
1	D	96	GLN	
1	D	127	HIS	
1	D	147	GLN	
1	D	151	GLN	
1	D	208	GLN	
1	D	234	HIS	
1	D	281	ASN	
1	D	296	ASN	
1	D	441	GLN	
1	D	461	ASN	
1	D	477	HIS	
1	D	481	ASN	
1	D	511	ASN	
1	Е	82	GLN	
1	Е	83	HIS	
1	Е	96	GLN	
1	Е	127	HIS	
1	Е	147	GLN	
1	Е	151	GLN	
1	Е	208	GLN	
1	Е	234	HIS	
1	Е	281	ASN	
1	Е	296	ASN	
1	Ε	441	GLN	
1	Е	461	ASN	
1	Е	477	HIS	
1	E	481	ASN	
1	Е	511	ASN	
1	F	82	GLN	
1	F	83	HIS	
1	F	91	GLN	
1	F	96	GLN	
1	F	127	HIS	
1	F	147	GLN	
1	F	151	GLN	



Mol	Chain	Res	Type
1	F	208	GLN
1	F	234	HIS
1	F	281	ASN
1	F	296	ASN
1	F	441	GLN
1	F	461	ASN
1	F	477	HIS
1	F	481	ASN
1	F	511	ASN
1	G	82	GLN
1	G	83	HIS
1	G	91	GLN
1	G	96	GLN
1	G	127	HIS
1	G	147	GLN
1	G	151	GLN
1	G	208	GLN
1	G	234	HIS
1	G	281	ASN
1	G	296	ASN
1	G	441	GLN
1	G	461	ASN
1	G	477	HIS
1	G	481	ASN
1	G	511	ASN
1	Н	82	GLN
1	Н	83	HIS
1	Н	96	GLN
1	H	127	HIS
1	Н	147	GLN
1	Н	151	GLN
1	Н	208	GLN
1	Н	234	HIS
1	Н	281	ASN
1	Н	296	ASN
1	Н	441	GLN
1	Н	461	ASN
1	Н	477	HIS
1	Н	481	ASN
1	Н	511	ASN
1	I	82	GLN
1	Ι	83	HIS



Mol	Chain	Res	Type
1	Ι	91	GLN
1	Ι	96	GLN
1	Ι	127	HIS
1	Ι	147	GLN
1	Ι	151	GLN
1	Ι	208	GLN
1	Ι	234	HIS
1	Ι	281	ASN
1	Ι	296	ASN
1	Ι	441	GLN
1	Ι	461	ASN
1	Ι	477	HIS
1	Ι	481	ASN
1	Ι	511	ASN

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)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	В	ond ang	les
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	ADP	С	800	-	24,29,29	1.47	2 (8%)	$29,\!45,\!45$	2.12	7 (24%)
2	ADP	Е	800	-	24,29,29	1.49	2 (8%)	$29,\!45,\!45$	2.12	7 (24%)
2	ADP	F	800	-	24,29,29	1.48	2 (8%)	$29,\!45,\!45$	2.11	7 (24%)
2	ADP	А	800	-	24,29,29	1.48	2 (8%)	$29,\!45,\!45$	2.12	7 (24%)
2	ADP	D	800	-	24,29,29	1.49	2 (8%)	$29,\!45,\!45$	2.12	7 (24%)
2	ADP	В	800	-	24,29,29	1.48	2 (8%)	$29,\!45,\!45$	2.11	7 (24%)
2	ADP	Ι	800	-	24,29,29	1.48	2 (8%)	$29,\!45,\!45$	2.12	7 (24%)
2	ADP	G	800	-	24,29,29	1.49	2 (8%)	29,45,45	2.12	7 (24%)
2	ADP	Н	800	-	24,29,29	1.49	2 (8%)	29,45,45	2.12	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	С	800	-	-	2/12/32/32	0/3/3/3
2	ADP	Е	800	-	-	2/12/32/32	0/3/3/3
2	ADP	F	800	-	-	2/12/32/32	0/3/3/3
2	ADP	А	800	-	-	2/12/32/32	0/3/3/3
2	ADP	D	800	-	-	2/12/32/32	0/3/3/3
2	ADP	В	800	-	-	2/12/32/32	0/3/3/3
2	ADP	Ι	800	-	-	2/12/32/32	0/3/3/3
2	ADP	G	800	-	-	2/12/32/32	0/3/3/3
2	ADP	Н	800	-	-	2/12/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ε	800	ADP	C2'-C1'	-5.59	1.45	1.53
2	G	800	ADP	C2'-C1'	-5.59	1.45	1.53
2	D	800	ADP	C2'-C1'	-5.58	1.45	1.53
2	Н	800	ADP	C2'-C1'	-5.57	1.45	1.53
2	В	800	ADP	C2'-C1'	-5.57	1.45	1.53
2	А	800	ADP	C2'-C1'	-5.56	1.45	1.53
2	F	800	ADP	C2'-C1'	-5.54	1.45	1.53
2	Ι	800	ADP	C2'-C1'	-5.54	1.45	1.53
2	С	800	ADP	C2'-C1'	-5.52	1.45	1.53


Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	Ι	800	ADP	C5-C4	2.50	1.47	1.40
2	D	800	ADP	C5-C4	2.49	1.47	1.40
2	С	800	ADP	C5-C4	2.48	1.47	1.40
2	Н	800	ADP	C5-C4	2.48	1.47	1.40
2	А	800	ADP	C5-C4	2.47	1.47	1.40
2	G	800	ADP	C5-C4	2.47	1.47	1.40
2	F	800	ADP	C5-C4	2.46	1.47	1.40
2	В	800	ADP	C5-C4	2.46	1.47	1.40
2	Е	800	ADP	C5-C4	2.46	1.47	1.40

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All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	800	ADP	C3'-C2'-C1'	5.49	109.24	100.98
2	G	800	ADP	C3'-C2'-C1'	5.48	109.23	100.98
2	А	800	ADP	C3'-C2'-C1'	5.47	109.22	100.98
2	Ι	800	ADP	C3'-C2'-C1'	5.47	109.21	100.98
2	Н	800	ADP	C3'-C2'-C1'	5.47	109.21	100.98
2	D	800	ADP	C3'-C2'-C1'	5.47	109.21	100.98
2	С	800	ADP	C3'-C2'-C1'	5.46	109.20	100.98
2	F	800	ADP	C3'-C2'-C1'	5.45	109.19	100.98
2	В	800	ADP	C3'-C2'-C1'	5.45	109.19	100.98
2	D	800	ADP	O2'-C2'-C3'	4.67	126.92	111.82
2	С	800	ADP	O2'-C2'-C3'	4.66	126.91	111.82
2	Е	800	ADP	O2'-C2'-C3'	4.66	126.90	111.82
2	А	800	ADP	O2'-C2'-C3'	4.66	126.89	111.82
2	В	800	ADP	O2'-C2'-C3'	4.66	126.89	111.82
2	Н	800	ADP	O2'-C2'-C3'	4.66	126.89	111.82
2	F	800	ADP	O2'-C2'-C3'	4.65	126.88	111.82
2	G	800	ADP	O2'-C2'-C3'	4.65	126.86	111.82
2	Ι	800	ADP	O2'-C2'-C3'	4.65	126.86	111.82
2	С	800	ADP	O3'-C3'-C4'	-4.54	97.92	111.05
2	Н	800	ADP	O3'-C3'-C4'	-4.54	97.94	111.05
2	Е	800	ADP	O3'-C3'-C4'	-4.54	97.94	111.05
2	G	800	ADP	O3'-C3'-C4'	-4.53	97.94	111.05
2	А	800	ADP	O3'-C3'-C4'	-4.53	97.95	111.05
2	Ι	800	ADP	O3'-C3'-C4'	-4.52	97.97	111.05
2	В	800	ADP	O3'-C3'-C4'	-4.52	97.98	111.05
2	F	800	ADP	O3'-C3'-C4'	-4.52	97.98	111.05
2	D	800	ADP	O3'-C3'-C4'	-4.51	98.00	111.05
2	D	800	ADP	N3-C2-N1	-3.31	123.50	128.68
2	F	800	ADP	N3-C2-N1	-3.28	123.56	128.68



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Ι	800	ADP	N3-C2-N1	-3.27	123.56	128.68
2	А	800	ADP	N3-C2-N1	-3.27	123.57	128.68
2	Е	800	ADP	N3-C2-N1	-3.27	123.57	128.68
2	G	800	ADP	N3-C2-N1	-3.26	123.58	128.68
2	Н	800	ADP	N3-C2-N1	-3.25	123.60	128.68
2	С	800	ADP	N3-C2-N1	-3.24	123.61	128.68
2	В	800	ADP	N3-C2-N1	-3.24	123.61	128.68
2	Е	800	ADP	O4'-C1'-C2'	-3.20	102.26	106.93
2	Ι	800	ADP	O4'-C1'-C2'	-3.19	102.26	106.93
2	А	800	ADP	O4'-C1'-C2'	-3.19	102.26	106.93
2	D	800	ADP	O4'-C1'-C2'	-3.18	102.27	106.93
2	С	800	ADP	O4'-C1'-C2'	-3.18	102.28	106.93
2	Н	800	ADP	O4'-C1'-C2'	-3.18	102.28	106.93
2	В	800	ADP	O4'-C1'-C2'	-3.18	102.28	106.93
2	F	800	ADP	O4'-C1'-C2'	-3.18	102.28	106.93
2	G	800	ADP	O4'-C1'-C2'	-3.18	102.28	106.93
2	С	800	ADP	C4-C5-N7	-2.88	106.40	109.40
2	Ι	800	ADP	C4-C5-N7	-2.87	106.41	109.40
2	Н	800	ADP	C4-C5-N7	-2.87	106.41	109.40
2	D	800	ADP	C4-C5-N7	-2.85	106.43	109.40
2	А	800	ADP	C4-C5-N7	-2.84	106.44	109.40
2	G	800	ADP	C4-C5-N7	-2.84	106.44	109.40
2	В	800	ADP	C4-C5-N7	-2.83	106.45	109.40
2	Ε	800	ADP	C4-C5-N7	-2.82	106.45	109.40
2	F	800	ADP	C4-C5-N7	-2.82	106.45	109.40
2	D	800	ADP	PA-O3A-PB	-2.76	123.34	132.83
2	Ι	800	ADP	PA-O3A-PB	-2.76	123.36	132.83
2	Н	800	ADP	PA-O3A-PB	-2.76	123.36	132.83
2	G	800	ADP	PA-O3A-PB	-2.76	123.37	132.83
2	А	800	ADP	PA-O3A-PB	-2.75	123.38	132.83
2	В	800	ADP	PA-O3A-PB	-2.75	123.39	132.83
2	F	800	ADP	PA-O3A-PB	-2.75	123.40	132.83
2	Е	800	ADP	PA-O3A-PB	-2.75	123.41	132.83
2	С	800	ADP	PA-O3A-PB	-2.73	123.46	132.83

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There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	800	ADP	PB-O3A-PA-O5'
2	В	800	ADP	PB-O3A-PA-O5'
2	С	800	ADP	PB-O3A-PA-O5'



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Mol	Chain	Res	Type	Atoms
2	D	800	ADP	PB-O3A-PA-O5'
2	Е	800	ADP	PB-O3A-PA-O5'
2	F	800	ADP	PB-O3A-PA-O5'
2	G	800	ADP	PB-O3A-PA-O5'
2	Н	800	ADP	PB-O3A-PA-O5'
2	Ι	800	ADP	PB-O3A-PA-O5'
2	А	800	ADP	PB-O3A-PA-O1A
2	В	800	ADP	PB-O3A-PA-O1A
2	С	800	ADP	PB-O3A-PA-O1A
2	D	800	ADP	PB-O3A-PA-O1A
2	Е	800	ADP	PB-O3A-PA-O1A
2	F	800	ADP	PB-O3A-PA-O1A
2	G	800	ADP	PB-O3A-PA-O1A
2	Н	800	ADP	PB-O3A-PA-O1A
2	Ι	800	ADP	PB-O3A-PA-O1A

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There are no ring outliers.

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	800	ADP	1	0
2	Е	800	ADP	1	0
2	F	800	ADP	1	0
2	А	800	ADP	1	0
2	D	800	ADP	1	0
2	В	800	ADP	1	0
2	Ι	800	ADP	1	0
2	G	800	ADP	1	0
2	Н	800	ADP	1	0

9 monomers are involved in 9 short contacts:

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 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	505/553~(91%)	0.10	13 (2%) 56	43	64, 126, 150, 150	0
1	В	505/553~(91%)	0.08	13 (2%) 56	43	64, 126, 150, 150	0
1	С	505/553~(91%)	0.16	17 (3%) 45	34	64, 126, 150, 150	0
1	D	505/553~(91%)	0.07	14 (2%) 53	40	64, 126, 150, 150	0
1	Ε	505/553~(91%)	0.23	26 (5%) 28	21	64, 126, 150, 150	0
1	F	505/553~(91%)	0.15	14 (2%) 53	40	64, 126, 150, 150	0
1	G	505/553~(91%)	0.20	22 (4%) 34	25	64, 126, 150, 150	0
1	Н	505/553~(91%)	0.09	11 (2%) 62	50	64, 126, 150, 150	0
1	Ι	505/553~(91%)	0.06	10 (1%) 65	53	64, 126, 150, 150	0
All	All	4545/4977~(91%)	0.13	140 (3%) 49	36	64, 127, 150, 150	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	ASP	6.9
1	Е	259	GLU	5.8
1	В	259	GLU	5.2
1	Н	267	ASN	5.1
1	F	259	GLU	5.0
1	С	259	GLU	4.8
1	А	259	GLU	4.3
1	F	267	ASN	4.3
1	С	261	ASP	4.2
1	F	63	LEU	4.1
1	G	259	GLU	4.0
1	F	261	ASP	4.0
1	Н	262	ALA	3.7
1	D	532	ALA	3.6
1	Н	265	ARG	3.5



Mol	Chain	Res	Type	RSRZ
1	Е	268	ASP	3.5
1	Н	264	ILE	3.5
1	D	267	ASN	3.4
1	G	532	ALA	3.4
1	В	261	ASP	3.4
1	Е	198	ASP	3.4
1	Е	267	ASN	3.3
1	Е	260	LEU	3.3
1	Е	154	SER	3.3
1	G	268	ASP	3.3
1	Ι	267	ASN	3.3
1	Е	157	ASP	3.3
1	С	267	ASN	3.2
1	Е	156	ASN	3.2
1	D	260	LEU	3.2
1	В	260	LEU	3.2
1	Е	262	ALA	3.1
1	G	194	GLU	3.1
1	Н	259	GLU	3.1
1	Е	263	GLU	3.1
1	G	481	ASN	3.1
1	D	259	GLU	3.1
1	С	374	LYS	3.0
1	F	260	LEU	3.0
1	F	162	ARG	3.0
1	E	261	ASP	3.0
1	B	156	ASN	2.9
1	C	353	TYR	2.9
1	F	65	ASP	2.9
1	B	198	ASP	2.9
1	B	268	ASP	2.8
1	G	260	LEU	2.8
1	G	261	ASP	2.8
1	A	261	ASP	2.8
1	G	266	ILE	2.8
1	C	262	ALA	2.8
1	Ā	366	LYS	2.7
1	G	531	SER	2.7
1	G	63	LEU	2.7
1	D	199	LYS	2.7
1	E	195	LEU	2.7
1	H	266	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	2.7
1	В	157	ASP	2.7
1	С	65	ASP	2.7
1	С	371	GLU	2.7
1	F	269	PRO	2.7
1	С	243	ASN	2.6
1	В	267	ASN	2.6
1	G	264	ILE	2.6
1	Н	261	ASP	2.6
1	А	371	GLU	2.5
1	Е	272	MET	2.5
1	А	197	GLY	2.5
1	Ι	265	ARG	2.5
1	А	374	LYS	2.5
1	D	268	ASP	2.5
1	В	262	ALA	2.5
1	Е	82	GLN	2.5
1	А	198	ASP	2.5
1	D	353	TYR	2.5
1	G	243	ASN	2.5
1	F	268	ASP	2.5
1	С	260	LEU	2.4
1	G	197	GLY	2.4
1	G	267	ASN	2.4
1	В	63	LEU	2.4
1	С	63	LEU	2.4
1	Н	243	ASN	2.4
1	F	226	ILE	2.4
1	С	357	ILE	2.4
1	Н	263	GLU	2.3
1	С	385	GLY	2.3
1	Ι	259	GLU	2.3
1	G	262	ALA	2.3
1	F	62	SER	2.3
1	A	532	ALA	2.3
1	F	532	ALA	2.3
1	С	62	SER	2.3
1	В	77	ASP	2.3
1	D	246	ILE	2.3
1	D	262	ALA	2.3
1	Е	65	ASP	2.3
1	G	196	ARG	2.3

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Mol	Chain	Res	Type	RSRZ	
1	Ε	317	VAL	2.3	
1	Ι	261	ASP	2.2	
1	Ι	242	GLU	2.2	
1	D	531	SER	2.2	
1	D	196	ARG	2.2	
1	Е	206	ASN	2.2	
1	Н	60	VAL	2.2	
1	А	481	ASN	2.2	
1	Е	531	SER	2.2	
1	С	242	GLU	2.2	
1	В	195	LEU	2.2	
1	А	353	TYR	2.2	
1	G	296	ASN	2.1	
1	Е	254	GLU	2.1	
1	Е	271	GLN	2.1	
1	А	194	GLU	2.1	
1	G	255	VAL	2.1	
1	G	269	PRO	2.1	
1	А	196	ARG	2.1	
1	А	267	ASN	2.1	
1	Е	61	ASP	2.1	
1	Ι	82	GLN	2.1	
1	G	265	ARG	2.1	
1	D	243	ASN	2.1	
1	G	156	ASN	2.1	
1	С	351	LEU	2.1	
1	Ι	262	ALA	2.1	
1	Ι	264	ILE	2.1	
1	Н	268	ASP	2.1	
1	Е	258	PRO	2.1	
1	F	227	VAL	2.1	
1	G	246	ILE	2.1	
1	С	356	LEU	2.1	
1	Е	240	ARG	2.0	
1	Е	266	ILE	2.0	
1	Е	77	ASP	2.0	
1	В	269	PRO	2.0	
1	Ι	260	LEU	2.0	
1	Е	243	ASN	2.0	
1	Ι	350	ASP	2.0	
1	F	531	SER	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	ADP	D	800	27/27	0.76	0.39	$150,\!150,\!150,\!150,\!150$	7
2	ADP	Е	800	27/27	0.77	0.34	$150,\!150,\!150,\!150,\!150$	7
2	ADP	G	800	27/27	0.78	0.37	150,150,150,150	7
2	ADP	С	800	27/27	0.79	0.34	$150,\!150,\!150,\!150$	7
2	ADP	А	800	27/27	0.80	0.35	$150,\!150,\!150,\!150,\!150$	7
2	ADP	В	800	27/27	0.80	0.33	150,150,150,150	7
2	ADP	Н	800	27/27	0.81	0.33	150, 150, 150, 150, 150	7
2	ADP	Ι	800	27/27	0.82	0.33	150,150,150,150	7
2	ADP	F	800	27/27	0.83	0.32	150,150,150,150	7

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





















6.5 Other polymers (i)

There are no such residues in this entry.

