

# Full wwPDB X-ray Structure Validation Report (i)

### Aug 17, 2020 – 11:32 AM BST

PDB ID	:	1MX9
$\operatorname{Title}$	:	Crystal Structure of Human Liver Carboxylesterase in complexed with nalox-
		one methiodide, a heroin analogue
Authors	:	Bencharit, S.; Morton, C.L.; Xue, Y.; Potter, P.M.; Redinbo, M.R.
Deposited on	:	2002-10-01
Resolution	:	2.90  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

The 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)	:	NOT EXECUTED
$\mathrm{EDS}$	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of	chain
1	А	548	54%	41% ••
1	В	548	61%	33% • •
1	С	548	59%	34% • •
1	D	548	62%	33% • •
1	Е	548	55%	38% ••
1	F	548	57%	37% • •
1	G	548	53%	41% ••
1	Н	548	57%	38% •••



Continued from previous page...

Mol	Chain	Length	Quality of chain						
1	Ι	548	49%	43% • •					
1	J	548	56%	38% • •					
1	K	548	53%	42% •••					
1	L	548	54%	40% • •					

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	J	479	-	-	Х	-
3	NLX	А	1	Х	-	Х	-
3	NLX	В	2	Х	-	Х	-
3	NLX	С	3	Х	-	Х	-
3	NLX	D	4	Х	-	Х	-
3	NLX	Е	5	Х	-	Х	-
3	NLX	F	6	Х	-	Х	-
3	NLX	G	1	X	-	Х	-
3	NLX	Н	2	Х	-	Х	-
3	NLX	Ι	3	Х	-	Х	-
3	NLX	J	4	Х	-	Х	-
3	NLX	K	5	Х	-	Х	-
3	NLX	L	6	X	-	Х	-



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 51134 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	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	520	Total	С	Ν	Ο	S	0	0	0
	A	002	4130	2662	685	763	20	0	0	0
1	D	520	Total	С	Ν	Ο	S	Ο	0	0
	D	002	4130	2662	685	763	20	0	0	0
1	C	521	Total	С	Ν	Ο	S	0	0	0
		001	4124	2659	684	761	20	0	0	0
1	п	522	Total	С	Ν	Ο	S	0	0	0
	D	000	4135	2665	686	764	20	0	0	0
1	F	521	Total	С	Ν	Ο	S	0	0	0
		001	4124	2659	684	761	20	0	0	0
1	Б	591	Total	С	Ν	Ο	S	0	0	0
	Г	001	4124	2659	684	761	20		0	0
1	C	520	Total	С	Ν	0	S	0	0	0
	G	552	4130	2662	685	763	20	0	0	0
1	Ц	531	Total	С	Ν	0	S	0	0	0
1	11	001	4124	2659	684	761	20	0	0	0
1	т	521	Total	С	Ν	Ο	S	0	0	0
1	L	001	4124	2659	684	761	20	0	0	0
1	т	539	Total	С	Ν	Ο	S	0	0	0
1	1	002	4130	2662	685	763	20	0	0	0
1	K	531	Total	С	Ν	Ο	S	0	0	0
		001	4124	2659	684	761	20	U	U	U
1	T	531	Total	С	Ν	0	S	0	0	0
		001	4124	2659	684	761	20	0	0	0

• Molecule 1 is a protein called liver Carboxylesterase I.

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	GLN	deletion	UNP P23141
В	?	-	GLN	deletion	UNP P23141
С	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
Е	?	-	GLN	deletion	UNP P23141



Chain	Residue	Modelled	Actual	Comment	Reference					
F	?	-	GLN	deletion	UNP P23141					
G	?	-	GLN	deletion	UNP P23141					
Н	?	-	GLN	deletion	UNP P23141					
Ι	?	-	GLN	deletion	UNP P23141					
J	?	-	GLN	deletion	UNP P23141					
K	?	-	GLN	deletion	UNP P23141					
L	?	-	GLN	deletion	UNP P23141					

• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf									
2	А	1	Total	С	N	0 ž	0	0									
			14	8	1	9											
2	Δ	1	Total	$\mathbf{C}$	Ν	Ο	0	0									
2	11	L L	14	8	1	5	0	0									
0	р	1	Total	С	Ν	Ο	0	0									
	D	D	D	D	D	D	D	D	D	D	L	14	8	1	5	0	U
0	C	1	Total	С	Ν	0	0	0									
	U	L	14	8	1	5	0	0									
0	п	1	Total	С	Ν	0	0	0									
		L	14	8	1	5	0	0									
0	Г	1	Total	С	Ν	0	0	0									
			14	8	1	5		U									
0	Б	1	Total	С	Ν	0	0	0									
	Г		14	8	1	5		U									



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
0	С	1	Total	С	Ν	Ο	0	0
	G	L	14	8	1	5	0	0
0	Ц	1	Total	С	Ν	Ο	0	0
	2 H		14	8	1	5	0	0
9	Т	1	Total	С	Ν	Ο	0	0
		T	14	8	1	5		0
9	т	1	Total	С	Ν	Ο	0	0
	J	I	14	8	1	5	0	0
9	K	1	Total	С	Ν	Ο	0	0
	IX	I	14	8	1	5	0	0
9	т	1	Total	С	Ν	Ο	0	0
			14	8	1	5		0

• Molecule 3 is (5A,17R)-4,5-EPOXY-3,14-DIHYDROXY-17-METHYL-6-OXO-17-(2-PROP ENYL)-MORPHINANIUM (three-letter code: NLX) (formula: C<sub>20</sub>H<sub>24</sub>NO<sub>4</sub>).



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	
3	2 1	1	Total	С	Ν	Ο	0	0	
0	л	L	25	20	1	4	0	0	
3	В	1	Total	С	Ν	Ο	0	0	
J	D	T	25	20	1	4	0	0	
3	C	C 1	Total	С	Ν	Ο	0	0	
0	U	1	25	20	1	4	0	0	
3	П	1	Total	С	Ν	Ο	0	0	
0				20	1	4	0	0	
3	F	1	Total	С	Ν	Ο	0	0	
		L	25	20	1	4	0	0	



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	Б	1	Total C N O	0	0	
J	Г	L	25  20  1  4	0	0	
2	С	1	Total C N O	0	0	
0	G	I	25  20  1  4	0	0	
2	Ц	1	Total C N O	0	0	
5	11	T	25  20  1  4	0	0	
3	Т	1	Total C N O	0	0	
5	1	T	25  20  1  4	0	0	
3	Т	1	Total C N O	0	0	
5	บ	T	25  20  1  4	0	0	
3	K	1	Total C N O	0	0	
5	17	T	25  20  1  4	0	0	
3	T.	1	Total C N O	0	0	
3	L		25 20 1 4	0	0	

Continued from previous page...

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	87	Total         O           87         87	0	0
4	В	120	Total O 120 120	0	0
4	С	98	Total O 98 98	0	0
4	D	119	Total O 119 119	0	0
4	Е	112	Total O 112 112	0	0
4	F	91	Total O 91 91	0	0
4	G	69	Total O 69 69	0	0
4	Н	95	Total O 95 95	0	0
4	Ι	80	Total O 80 80	0	0
4	J	110	Total O 110 110	0	0
4	K	73	Total O 73 73	0	0
4	L	75	Total O 75 75	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.



• Molecule 1: liver Carboxylesterase I











BANK



### PRO GLN THR HIS HIS ILE GLU CLU

• Molecule 1: liver Carboxylesterase I









• Molecule 1: liver Carboxylesterase I







 $\bullet$  Molecule 1: liver Carboxyl esterase I

Chain J:

38%



• Molecule 1: liver Carboxylesterase I



| ia                 | in  | L  | :   |   |   |   |  
   
   
   
  |  |  |  |  |  | 54  | 1%  |   
   |   
   
  |  
   
   
   |   |   |   |   
   
  |  |  |   |   |  
   
  |   |  
   
  |   |  
  | 4  
   
  | 0%  |  |   
  |   |  |       |   |   | •  | •     |  |                |                |       |
|--------------------|---|--|---|---|---|---
--
--
--
---|--|--
--|--|--|---|---|---
--
--
--
--
--
--|---|---|---
--
--
--|--|--|---|---
--
---
---
--
---|---
--
---
--
---|---|--
--|---
--|-------|---|---|--|-------|--|----------------|----------------|-------|
| SER                | 56022                                     | F0025<br>P6024   | V6025   |   | V6029   | H6030   | G6031<br>K6032   
   
   
   
  | V6033  | L6034  |  | F6037  | L6040  | E6041   |   | A6048   
   | L   
   
  | L6051  
   
   
   | P6054   | -   | 16060   |   
   
  | H6064  | P6067  |   | P6073   | V6077  
   
  | K6078   |  
   
  | Y6083   | F000 <del>1</del><br>P6085   
  | M6086  
   
  | C6087   | D6090  | P6091   
  | K6092   |  | 16096 | L6097   | 26098   | E0039  | R6104 | K6105  | E6106<br>We107 | I6108          | P6109 |
| L6112              | S6113<br>F6114                            | D6115  | 10101   | 16121<br>Y6122  | T6123   | P6124   | A0125  
   
   
   
  | L6127  | T6128  | K6129  | K6130  | L6133  | P6134   | V6135   | M6136   
   | V6137   
   
  | W6138  
   
   
   | H6140   | <b>G6141</b>  | G6142   | G6143   
   
  | L6144<br>M6145   | -  | A6149   | T C T   | 46156<br>A6156   
   
  |   | E6161  
   
  | N6162<br>V6162  | 0101   
  | 06169  
   
  | Y6170   | T / TON  | 16174   
  | W6175   | F6177  |       | D6182   | E6183<br>UG 1 64  | 0104<br>C6105  | B6186 | G6187  | N6188          | 06194          | -     |
| N6204              | 16205<br>46206                            | 86207  |   |   | I6217   | F6218   | 66219<br>E6220   
   
   
   
  | S6221  | A6222  | G6223  | 66224<br>F6005   | S6226  | V6227   |   | 86233   
   | P6234   
   
  | L6235  
   
   
   | A0230<br>K6237  | N6238   |   | H6241   
   
  | R6242<br>A6243   | I6244  | S6245   | E6246   | 16251  
   
  | T6252   | <mark>S6253</mark>   
   
  | V6254<br>TROFF  | V6256  
  | K6257  
   
  | K6258   | 02239<br>D6260   | V6261   
  | K6262<br>D6763  | 16264  | A6265 | E6266   | 06267   | 00701  | T6271 |  | T6278          | 802/9<br>A6280 | -     |
| L6286              | K6280                                     | T6290  | E6291   | E6292   |   | T6297   | K6302  
   
   
   
  | F6303  | L6304  |  | D6311  | F0312<br>R6313   |   | 06316   | P6317   
   | L6318   
   
  | L6319  
   
   
   | V6322   | I6323   | D6324   | G6325   
   
  | M6326<br>L6327   |  | <mark>Е6333</mark>                                      |   |  
   
  | R6339   |  
   
  | H6342   | M6347  
  | V6348  
   
  | 66349<br>16850  | 16351<br>N6351   |   
  | F6355   | WG357  | L6358 | 16359   | P6360   | 10201  |       | Y6366  | P6367          | 66371          | Q6372 |
| <mark>q6375</mark> | 46378                                     | O / COH  | L6382   | WD 383  | Y6386   | P6387   | K6393  
   
   
   
  | E6394  | L6395  | I6396  |  | E6401  |   | D6409   | T6410   
   | V6411   
   
  | K6412  
   
   
   | K6414 K6414   | D6415   | L6416   | F6417   
   
  | D6419  | L6420  |   | F6426   | V6428  
   
  | P6429   |  
   
  | I6432<br>Ve433  | A6434  
  | R6435  
   
  |   | LO <sup>409</sup>  | T6444   
  | Y6445<br>Me446  | 76447  |       | R6452   | P6453   | CE AEC   | 00700 | M6459  | K6460          | T6463          | V6464 |
| H6468              | FG471                                     | 16472  | TC ATE  | VD4/0   | A6478   | P6479   | r6480<br>16481   
   
   
   
  |  | <mark>G6484</mark>   | A6485  | S6486<br>F6487   |  | L6492   | S6493   |   
   | V6496   
   
  | M6497  
   
   
   | F6499   | W6500   | A6501   |   
   
  |  | P6509  |   | W6517   | Y6520  
   
  |   | K6523  
   
  | E6524<br>CEEDE  | Y6526  
  | L6527  
   
  | 06528   | 10329<br>G6530   | A6531   
  | N6532<br>Tef32  | 10333<br>06534   | A6535 | A6536   | 06537<br>V6530  | 16530  | K6540 | D6541  | 112 E / /      | A6545          | F6546 |
| N6549              | L6550                                     | K6553  | TYS   | VAL.  | GLU   | LYS   | PRO  
   
   
   
  | GLN  | THR  | GLU  | STH  | GLU  | LEU   |   |   
   |   
   
  |  
   
   
   |   |   |   |   
   
  |  |  |   |   |  
   
  |   |  
   
  |   |  
  |  
   
  |   |  |   
  |   |  |       |   |   |  |       |  |                |                |       |
|                    | N6549 H6468 Q6375 L6286 N6204 L6112 SER E | N6549         #6468         Q6375         L6286         N6204         L6112         SER           L6550         1         16205         56113         5602         10           L6550         1         1         1         1         10         10         10 | N6549         #6468         06375         L6286         N6204         L6112         SER         SER           L6550         E6471         A6378         K2289         J6205         56113         S6022         UI         UI           R6471         A6378         K2289         J6206         B6114         P6023         UI         V< | N6549         #6468         Q6375         L6286         N6204         L6112         SER           L6550         B6471         A6378         K6209         B6471         A6378         S6022         S6024         S6024 | N6549         #6468         Q6375         L6286         N6204         L6112         SER           L6560         B6471         A6378         K6209         M6204         L6112         SER           K6563         E471         A6378         K6209         M6206         B6114         P6023           K6563         L6472         L6372         E2291         B6114         P6023           LX         V6475         M6333         E2291         V6216         V6025           VAL         V6475         M6333         E2291         V6216         V6122         V6025 | N6549         #6468         06375         L6286         N6204         L6112         SER           L6560         B6471         A6378         L6205         56113         S622         S612           K653         B6471         A6378         K6289         A6376         B6471         A6378         S602         S613         S6022         S613         S6022         S613         S6022         S613         S6022         S6023         S6023         S6023         S6023         S6024         S6024 | N6549         #6468         06375         L6286         N6204         L6112         SER           L6560         E6471         .6378         16205         56133         56023         56133         56023           K6553         L6471         .6578         .6209         .6206         56133         56023         56133         56023           LYN         V6475         .6382         E6291         .6206         E6291         V6026         56023         56023           LA         V6475         .6833         E6291         .66216         16121         V6026         16122         V6026         16122         V6026         16122         V6026         16122         V6026         16121         V6026         16123         V6026         16123         V6026         16123         16123         16123 <t< th=""><th>N6549         #6468         06375         L6286         N6204         L6112         SER           L6550         E6471         .6578         16205         56113         SER           L6550         E6471         .6578         16205         56113         SER           L7         L6112         .6579         .16205         56113         S6022           L7         L6382         E6299         .16205         E6114         P6024           ALA         V6475         .6633         E6291         16121         V6026           ALA         V6475         .6833         E6291         16121         V6026           L1         .7         .7         16121         V6026           L3         .7         .7         16121         V6026           L3         .7         .7         .7         16124         V6026           L4</th><th>N6549         H6463         06375         L6286         N6204         L6112         SBR           L6660         B6472         L6206         N6204         L6112         SBR           L6650         B6471         A6378         K6289         M6206         S113         SBR           L145         B6471         A6378         K6289         M6206         S113         SBR           L15         L6472         L6382         E6291         U6116         P6023           L15         L6472         L6382         E6291         U6116         P6024           VAL         W6478         K6536         E6291         U6116         P6024           VAL         M6478         K6302         E6291         U6217         U6026           VAL         M6478         K6302         E6291         U6217         U6026           L641         K6302         E6239         T6217         U6020         U6026           PM0         F6480         K6302         E6219         M6126         U6031           L641         K6302         E6219         M6126         U6031         U6031           F0303         F6303         F6303         F6303         F63</th><th>N6549         H6468         06375         L6286         N6204         L6112         SBR           L6660         B6472         L6376         L6205         S6113         SBR           L6651         B471         A6378         K6289         M6206         S6113         SBR           L14         A6378         K6289         M6206         S6113         SBR         F9022           L14         L6302         E6291         U6115         L6302         B6126         F0024           L1A         U472         L6382         E6291         U6216         B6124         F0024           L1A         U475         U6835         E6291         U6216         U6124         F0024           L1A         U475         U6836         E6291         U6216         U6024         F0024           L1A         U475         U6836         T6217         U6029         F0024         F0026           L1A         E6393         T6217         U6123         F0029         F0026         F0024           L1A         E6393         T6216         H6123         H6029         F0026         F0024           L1A         E6393         E6203         F02126         F002</th><th>N6549         H6468         06375         L6286         N6204         L6112         SBR           L6650         E6471         6637         L6205         56113         SB7         SB7           L6550         E4472         6375         L6205         56113         SB7         SB7           L6550         E4472         6375         L6205         S6113         SB022         SB022           LNS         E4472         6375         L6305         E6291         H6115         P6024           LNS         V417         6332         E6291         H6126         V6125         V6025           LN         V4476         H6305         E6291         V6125         V6026         V6026           LN         V6479         H6305         E6291         V6121         V6026         V6026           LN         V41         K6533         E6292         V6122         V6026         V6026           PND         F6491         K6303         E6203         H6124         V6026         K6033           PND         F6495         E6303         E6203         E6303         E6303         E6303         E6030           L10         E6303         E6303</th><th>N6549         H6468         06375         L6286         N6204         L6112         SBR           L6650         B6471         6375         L6205         5113         SB7         L6112         SB7           L6650         B6471         6375         L6325         5113         SB7         B6205         S113         SB7           L1X         K6553         L6472         6383         K6206         B6115         P6023           L1X         V4         B630         L6472         B630         L6112         V6025           L1X         V6476         M6383         E6291         N6125         V6026         N6025           L1X         V6476         M6383         E6292         V6125         V6026         N6025           L1X         V6476         M6383         E6292         V6126         V6026         V6026           L1X         V6476         M6383         E6292         V6126         V6026         V6026           L1X         V6476         M6383         E6292         V6126         V6026         V6026           L1X         V6484         V6386         L6121         V6026         V6026         V6026           L1X</th><th>N6549         #6468         06375         L6286         N6204         L6112         SER           L6550         B6471         A6378         L6205         B6114         B6372         S6022         S6113         S6022         S6022</th><th>Nice46         He468         Q6375         L6286         N6204         L6112         SER           L6660         B6472         L6378         Q6375         L6206         N6204         L6112         SER           L6660         B6471         A6378         K6583         L6472         S604         L6113         SER           L1NS         L6472         L6382         L6376         L6116         P6024         P6024           L1NS         U4475         K6583         L6382         E6293         U6206         B6114         P6024           L1NS         U4476         K6583         L6392         K6289         M6126         P6024         P6024           L1NS         U4476         K6386         T5297         U6217         U6029         P6024         P6026           L1A         U4478         K6393         E6239         U6217         U6029         P6024         P6026           PNO         F6490         F6333         F6230         L6127         U6029         L6034           THR        
G6484         L6393         F6030         B6212         L6127         U6034           THR         G6484         L6396         L6312         L6127</th><th>Nice46         Nic566         Nic504         Nic506         Nic506&lt;</th><th>Ni6549         IR6468         06375         L6286         N6204         L6112         SBR           L6650         B6471         6378         L6205         16205         5113         SBR           L6550         B6471         6378         L6372         16305         5113         SBR           L15         B6471         6378         K6583         L6472         6306         9113         56022           L15         L6472         6338         E6291         16205         8113         56026           L15         VAL         W6476         16636         16216         16121         96024           L15         W6476         N633         E6291         16217         96026         96030           L14         NAL         N6478         16321         16217         96036         96030           PNO         E6491         K6333         K6126         16217         96030         16213         96036           PNO         E6491         K6333         K6126         16124         96030         16126           PNO         E6491         K6333         K6126         16124         96030         16126           L111         K6126<th>N6549         H6468         06375         L6286         N6204         L6112         SBR 71         L6112           L6650         B6471         6375         L6205         86471         6375         56204         16112         58672         58672           L6550         B6471         A6375         L6382         E6291         16205         51113         56022         58022           L1X         VAL         V6475         16382         E6291         16205         56113         70023         56022           L1X         V6476         166383         16205         16121         V6026         56113         56022         56073         56073         56073         56073         56073         56073         56073         56073         56073         56073         56073         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         <t< th=""><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th>Nice46         Nice46         Nice304         Nice304</th><th>Ni6549         IR6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6113         SBR           L1X5         L6472         L6378         K6533         L6472         N6206         S113         S6022           L1X5         L6472         L6332         L6326         N6206         S113         S6022           L1X5         N6476         N636         E6293         N6206         S613         S6027           L1X5         N6476         N636         E6293         N6126         N6126         S6024           L1X         N6476         N636         E6293         N6126         N6026         S6027           L1X         N6476         N6366         L6332         L6326         N6126         N6026           L1X         N4478         N6316         L6333         L6217         N6128         N6023           L1X         R6448         L6336         L6336         L6126         N6026         L6033           L1X         R6448         L6336         L6128         L6033         L6036         L6034           L1X         L6432         <td< th=""><th>Nice46         Nice46         Nice47         Statt         S</th><th>Ni6440         B6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6115         SB113         SBR           L1         B6471         6378         K6533         L6472         6378         K6024         S6113         SBR           L1         W476         K6533         L6472         K6333         E6299         K6115         W6026         S6113         S6024         S62</th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th>Nice46         Nice46         Nice47         Senta         <th< th=""><th>Inee46         Inee46         Inee47         Inee44         Inee44&lt;</th><th>Michola         Michola         <t< th=""><th>Inteledent         Inteledent         Inteled</th><th>Michola         Michola         <t< th=""><th>Michael         Michael         <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<></th></t<></th></t<></th></th<></th></td<></th></t<></th></th></t<> | N6549         #6468         06375         L6286         N6204         L6112         SER           L6550         E6471         .6578         16205         56113         SER           L6550         E6471         .6578         16205         56113         SER           L7         L6112         .6579         .16205         56113         S6022           L7         L6382         E6299         .16205         E6114         P6024           ALA         V6475        
.6633         E6291         16121         V6026           ALA         V6475         .6833         E6291         16121         V6026           L1         .7         .7         16121         V6026           L3         .7         .7         16121         V6026           L3         .7         .7         .7         16124         V6026           L4 | N6549         H6463         06375         L6286         N6204         L6112         SBR           L6660         B6472         L6206         N6204         L6112         SBR           L6650         B6471         A6378         K6289         M6206         S113         SBR           L145         B6471         A6378         K6289         M6206         S113         SBR           L15         L6472         L6382         E6291         U6116         P6023           L15         L6472         L6382         E6291         U6116         P6024           VAL         W6478         K6536         E6291         U6116         P6024           VAL         M6478         K6302         E6291         U6217         U6026           VAL         M6478         K6302         E6291         U6217         U6026           L641         K6302         E6239         T6217         U6020         U6026           PM0         F6480         K6302         E6219         M6126         U6031           L641         K6302         E6219         M6126         U6031         U6031           F0303         F6303         F6303         F6303         F63 | N6549         H6468         06375         L6286         N6204         L6112         SBR           L6660         B6472         L6376         L6205         S6113         SBR           L6651         B471         A6378         K6289         M6206         S6113         SBR           L14         A6378         K6289         M6206         S6113         SBR         F9022           L14         L6302         E6291         U6115         L6302         B6126         F0024           L1A         U472         L6382         E6291         U6216         B6124         F0024           L1A         U475         U6835         E6291         U6216         U6124         F0024           L1A         U475         U6836         E6291         U6216         U6024         F0024           L1A         U475         U6836         T6217         U6029         F0024         F0026           L1A         E6393         T6217         U6123         F0029         F0026         F0024           L1A         E6393         T6216         H6123         H6029         F0026         F0024           L1A         E6393         E6203         F02126         F002 | N6549         H6468         06375         L6286         N6204         L6112         SBR           L6650         E6471         6637         L6205         56113         SB7         SB7           L6550         E4472         6375         L6205         56113         SB7         SB7           L6550         E4472         6375         L6205         S6113         SB022         SB022           LNS         E4472         6375         L6305         E6291         H6115         P6024           LNS         V417         6332         E6291         H6126         V6125         V6025           LN         V4476         H6305         E6291         V6125         V6026         V6026           LN         V6479         H6305         E6291         V6121         V6026         V6026           LN         V41         K6533         E6292         V6122         V6026         V6026           PND         F6491         K6303         E6203         H6124         V6026         K6033           PND         F6495         E6303         E6203         E6303         E6303         E6303         E6030           L10         E6303         E6303 | N6549         H6468         06375         L6286         N6204         L6112         SBR           L6650         B6471         6375         L6205         5113         SB7         L6112         SB7           L6650         B6471         6375         L6325         5113         SB7         B6205         S113         SB7           L1X         K6553         L6472         6383         K6206         B6115         P6023           L1X         V4         B630         L6472         B630         L6112         V6025           L1X         V6476         M6383         E6291         N6125         V6026         N6025           L1X         V6476         M6383         E6292         V6125         V6026         N6025           L1X         V6476         M6383         E6292         V6126         V6026         V6026           L1X         V6476         M6383         E6292         V6126         V6026         V6026           L1X         V6476         M6383         E6292         V6126         V6026         V6026           L1X         V6484         V6386         L6121         V6026         V6026         V6026           L1X | N6549         #6468         06375         L6286         N6204         L6112         SER           L6550         B6471         A6378         L6205         B6114         B6372         S6022         S6113         S6022         S6022 | Nice46         He468         Q6375         L6286         N6204         L6112         SER           L6660         B6472         L6378         Q6375         L6206         N6204         L6112         SER           L6660         B6471         A6378         K6583         L6472         S604         L6113         SER           L1NS         L6472         L6382         L6376         L6116         P6024         P6024           L1NS         U4475         K6583         L6382         E6293         U6206         B6114         P6024           L1NS         U4476         K6583         L6392         K6289         M6126         P6024         P6024           L1NS         U4476         K6386         T5297         U6217         U6029         P6024         P6026           L1A         U4478         K6393         E6239         U6217         U6029         P6024         P6026           PNO         F6490         F6333         F6230         L6127         U6029         L6034           THR         G6484         L6393         F6030         B6212         L6127         U6034           THR         G6484         L6396         L6312         L6127 | Nice46         Nic566         Nic504         Nic506         Nic506< | Ni6549         IR6468         06375         L6286         N6204         L6112         SBR           L6650         B6471         6378         L6205         16205         5113         SBR           L6550         B6471         6378         L6372         16305         5113         SBR           L15         B6471         6378         K6583         L6472         6306         9113         56022           L15         L6472         6338         E6291         16205         8113         56026           L15         VAL         W6476         16636         16216         16121         96024           L15         W6476         N633         E6291         16217         96026         96030           L14         NAL         N6478         16321         16217         96036         96030           PNO         E6491         K6333         K6126         16217         96030         16213         96036           PNO         E6491         K6333         K6126         16124         96030         16126           PNO         E6491         K6333         K6126         16124         96030         16126           L111         K6126 <th>N6549         H6468         06375         L6286         N6204         L6112         SBR 71         L6112           L6650         B6471         6375         L6205         86471         6375         56204         16112         58672         58672           L6550         B6471         A6375         L6382         E6291         16205         51113         56022         58022           L1X         VAL         V6475         16382         E6291         16205         56113         70023         56022           L1X         V6476         166383         16205         16121         V6026         56113         56022         56073         56073         56073         56073         56073         56073         56073         56073         56073         56073         56073         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         <t< th=""><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th>Nice46         Nice46         Nice304         Nice304</th><th>Ni6549         IR6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6113         SBR           L1X5         L6472         L6378         K6533         L6472         N6206         S113         S6022           L1X5         L6472         L6332         L6326         N6206         S113         S6022           L1X5         N6476         N636         E6293         N6206         S613         S6027           L1X5         N6476         N636         E6293         N6126         N6126         S6024           L1X         N6476         N636         E6293         N6126         N6026         S6027           L1X         N6476         N6366         L6332         L6326         N6126         N6026           L1X         N4478         N6316         L6333         L6217         N6128         N6023           L1X         R6448         L6336         L6336         L6126         N6026         L6033           L1X         R6448         L6336         L6128         L6033         L6036         L6034           L1X         L6432         <td< th=""><th>Nice46         Nice46         Nice47         Statt        
S</th><th>Ni6440         B6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6115         SB113         SBR           L1         B6471         6378         K6533         L6472         6378         K6024         S6113         SBR           L1         W476         K6533         L6472         K6333         E6299         K6115         W6026         S6113         S6024         S62</th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th>Nice46         Nice46         Nice47         Senta         <th< th=""><th>Inee46         Inee46         Inee47         Inee44         Inee44&lt;</th><th>Michola         Michola         <t< th=""><th>Inteledent         Inteledent         Inteled</th><th>Michola         Michola         <t< th=""><th>Michael         Michael         <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<></th></t<></th></t<></th></th<></th></td<></th></t<></th> | N6549         H6468         06375         L6286         N6204         L6112         SBR 71         L6112           L6650         B6471         6375         L6205         86471         6375         56204         16112         58672         58672           L6550         B6471         A6375         L6382         E6291         16205         51113         56022         58022           L1X         VAL         V6475         16382         E6291         16205         56113         70023         56022           L1X         V6476         166383         16205         16121         V6026         56113         56022         56073         56073         56073         56073         56073         56073         56073         56073         56073         56073         56073         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033         56026         56033 <t< th=""><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th>Nice46         Nice46         Nice304         Nice304</th><th>Ni6549         IR6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6113         SBR           L1X5         L6472         L6378         K6533         L6472         N6206         S113         S6022           L1X5         L6472         L6332         L6326         N6206         S113         S6022           L1X5         N6476         N636         E6293         N6206         S613         S6027           L1X5         N6476         N636         E6293         N6126         N6126         S6024           L1X         N6476         N636         E6293         N6126         N6026         S6027           L1X         N6476         N6366         L6332         L6326         N6126         N6026           L1X         N4478         N6316         L6333         L6217         N6128         N6023           L1X         R6448         L6336         L6336         L6126         N6026         L6033           L1X         R6448         L6336         L6128         L6033         L6036         L6034           L1X         L6432         <td< th=""><th>Nice46         Nice46         Nice47         Statt         S</th><th>Ni6440         B6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6115         SB113         SBR           L1         B6471         6378         K6533         L6472         6378         K6024         S6113         SBR           L1         W476         K6533         L6472         K6333         E6299         K6115         W6026         S6113         S6024         S62</th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th>Nice46         Nice46         Nice47         Senta         <th< th=""><th>Inee46         Inee46         Inee47         Inee44         Inee44&lt;</th><th>Michola         Michola         <t< th=""><th>Inteledent         Inteledent         Inteled</th><th>Michola         Michola         <t< th=""><th>Michael         Michael         <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10        
161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<></th></t<></th></t<></th></th<></th></td<></th></t<> | $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | Nice46         Nice46         Nice304         Nice304 | Ni6549         IR6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6113         SBR           L1X5         L6472         L6378         K6533         L6472         N6206         S113         S6022           L1X5         L6472         L6332         L6326         N6206         S113         S6022           L1X5         N6476         N636         E6293         N6206         S613         S6027           L1X5         N6476         N636         E6293         N6126         N6126         S6024           L1X         N6476         N636         E6293         N6126         N6026         S6027           L1X         N6476         N6366         L6332         L6326         N6126         N6026           L1X         N4478         N6316         L6333         L6217         N6128         N6023           L1X         R6448         L6336         L6336         L6126         N6026         L6033           L1X         R6448         L6336         L6128         L6033         L6036         L6034           L1X         L6432 <td< th=""><th>Nice46         Nice46         Nice47         Statt         S</th><th>Ni6440         B6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6115         SB113         SBR           L1         B6471         6378         K6533         L6472         6378         K6024         S6113         SBR           L1         W476         K6533         L6472         K6333         E6299         K6115         W6026         S6113         S6024         S62</th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th><math display="block"> \begin{array}{c c c c c c c c c c c c c c c c c c c </math></th><th>Nice46         Nice46         Nice47         Senta         <th< th=""><th>Inee46         Inee46         Inee47         Inee44         Inee44&lt;</th><th>Michola         Michola         <t< th=""><th>Inteledent         Inteledent         Inteled</th><th>Michola         Michola         <t< th=""><th>Michael         Michael         <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06        
165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<></th></t<></th></t<></th></th<></th></td<> | Nice46         Nice47         Statt         S | Ni6440         B6468         06375         L6206         N6204         L6112         SBR           L6650         B6471         6378         L6206         N6204         N6115         SB113         SBR           L1         B6471         6378         K6533         L6472         6378         K6024         S6113         SBR           L1         W476         K6533         L6472         K6333         E6299         K6115         W6026         S6113         S6024         S62 | $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | Nice46         Nice47         Senta         Senta <th< th=""><th>Inee46         Inee46         Inee47         Inee44         Inee44&lt;</th><th>Michola         Michola         <t< th=""><th>Inteledent         Inteledent         Inteled</th><th>Michola         Michola         <t< th=""><th>Michael         Michael         <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<></th></t<></th></t<></th></th<> | Inee46         Inee47         Inee44         Inee44< | Michola         Michola <t< th=""><th>Inteledent         Inteledent         Inteled</th><th>Michola         Michola         <t< th=""><th>Michael         Michael         <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06       
 165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<></th></t<></th></t<> | Inteledent         Inteled | Michola         Michola <t< th=""><th>Michael         Michael         <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<></th></t<> | Michael         Michael <t< th=""><th>Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         16</th><th>Unicade         Medical         Magnetical         Medical         Medical</th><th>Internation         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (6)<br/>(11)         Ref (7)<br/>(11)         Ref (7)<br/>(11)<!--</th--><th>Increase         Resolution         Resolutio</th><th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th><th></th><th>Interval         165/06         165/0</th><th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th><th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th><th></th><th>Main         File         Models         Models</th><th></th><th></th><th></th></th></t<> | Internation         165-10         165/10         165/10         165/10         165/10         165/10         161/10         161/10        
161/10         16 | Unicade         Medical         Magnetical         Medical         Medical | Internation         Ref (6)<br>(11)         Ref (6)<br>(11)         Ref (6)<br>(11)         Ref (6)<br>(11)         Ref (7)<br>(11)         Ref (7)<br>(11) </th <th>Increase         Resolution         Resolutio</th> <th>Internation         1000000         10000000         100000000         100000000000000000000000000000000</th> <th></th> <th>Interval         165/06         165/0</th> <th><math display="block"> \begin{array}{ c c c c c c c c c c c c c c c c c c c</math></th> <th>Line         Line         <thlin< th="">         Line         Line         L</thlin<></th> <th></th> <th>Main         File         Models         Models</th> <th></th> <th></th> <th></th> | Increase         Resolution         Resolutio | Internation         1000000         10000000         100000000         100000000000000000000000000000000 |       | Interval         165/06         165/0 | $ \begin{array}{ c c c c c c c c c c c c c c c c c c c$ | Line         Line <thlin< th="">         Line         Line         L</thlin<> |       | Main         File         Models         Models |                |                |       |



### 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants	91.17Å 120.71Å 177.02Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.28^{\circ}$ $89.32^{\circ}$ $99.22^{\circ}$	Depositor
Resolution (Å)	29.82 - 2.90	Depositor
% Data completeness	95.7 (29.82-2.90)	Depositor
(in resolution range)	50.1 (25.02 2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
$R, R_{free}$	0.214 , $0.280$	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51134	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP



## 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: NLX, NAG

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					
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5				
1	А	0.38	0/4236	0.62	0/5754				
1	В	0.41	0/4236	0.66	2/5754~(0.0%)				
1	С	0.42	0/4230	0.65	2/5746~(0.0%)				
1	D	0.41	0/4241	0.63	0/5761				
1	Ε	0.40	0/4230	0.64	1/5746~(0.0%)				
1	F	0.38	0/4230	0.62	0/5746				
1	G	0.36	0/4236	0.60	0/5754				
1	Н	0.39	0/4230	0.63	0/5746				
1	Ι	0.36	0/4230	0.61	0/5746				
1	J	0.39	0/4236	0.62	0/5754				
1	K	0.36	0/4230	0.60	0/5746				
1	L	0.37	0/4230	0.63	1/5746~(0.0%)				
All	All	0.39	0/50795	0.63	6/68999~(0.0%)				

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ε	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	3420	LEU	CA-CB-CG	5.80	128.63	115.30
1	С	3388	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	В	2339	ARG	N-CA-C	5.37	125.50	111.00
1	В	2075	SER	N-CA-C	5.33	125.41	111.00



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	L	6140	HIS	N-CA-C	5.01	124.53	111.00
1	Е	5075	SER	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group		
1	Ε	5118	TYR	Sidechain		

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4130	0	4132	231	0
1	В	4130	0	4132	182	0
1	С	4124	0	4127	180	0
1	D	4135	0	4134	165	0
1	Е	4124	0	4127	200	0
1	F	4124	0	4127	192	0
1	G	4130	0	4132	237	0
1	Н	4124	0	4127	194	0
1	Ι	4124	0	4127	232	0
1	J	4130	0	4134	216	0
1	Κ	4124	0	4127	226	0
1	L	4124	0	4127	244	0
2	А	28	0	26	3	0
2	В	14	0	13	4	0
2	С	14	0	13	0	0
2	D	14	0	13	4	0
2	Ε	14	0	13	2	0
2	F	14	0	13	0	0
2	G	14	0	13	4	0
2	Н	14	0	13	1	0
2	Ι	14	0	13	1	0
2	J	14	0	13	7	0
2	K	14	0	13	1	0
2	L	14	0	13	0	0



1MX9
------

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	25	0	23	20	0
3	В	25	0	23	21	0
3	С	25	0	19	27	0
3	D	25	0	24	15	0
3	Е	25	0	24	18	0
3	F	25	0	21	23	0
3	G	25	0	23	12	0
3	Н	25	0	23	30	0
3	Ι	25	0	24	19	0
3	J	25	0	24	20	0
3	K	25	0	24	18	0
3	L	25	0	24	23	0
4	А	87	0	0	9	0
4	В	120	0	0	12	0
4	С	98	0	0	10	0
4	D	119	0	0	9	0
4	Е	112	0	0	16	0
4	F	91	0	0	8	0
4	G	69	0	0	10	0
4	Н	95	0	0	10	0
4	Ι	80	0	0	10	0
4	J	110	0	0	8	0
4	K	73	0	0	11	0
4	L	75	0	0	15	0
All	All	51134	0	49998	2453	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2453) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:NLX:N1	3:C:3:NLX:C9	1.69	1.56
3:C:3:NLX:C9	3:C:3:NLX:C14	1.78	1.55
1:D:4343:THR:HB	1:D:4442:ALA:HB2	1.17	1.13
1:H:2304:LEU:HB3	3:H:2:NLX:H201	1.28	1.11
1:C:3364:MET:CE	3:C:3:NLX:H181	1.83	1.08
1:A:1251:LEU:HD11	1:A:1336:GLN:HE22	1.18	1.08
1:D:4359:ILE:HG23	3:D:4:NLX:H82	1.39	1.04
1:H:2363:LEU:HB3	3:H:2:NLX:H181	1.36	1.03
1:F:6097:LEU:HD22	3:F:6:NLX:H192	1.39	1.03



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:4363:LEU:HB3	3:D:4:NLX:H181	1.43	1.01
1:G:1134:PRO:HG2	1:G:1163:VAL:HG12	1.44	1.00
1:B:2373:LEU:HD21	1:B:2378:ALA:HB2	1.43	0.99
1:A:1498:LYS:HD2	1:A:1514:LEU:HD11	1.45	0.98
1:K:5258:LYS:H	1:K:5258:LYS:HD2	1.26	0.97
1:A:1025:VAL:HG22	1:A:1034:LEU:HD23	1.45	0.97
1:B:2234:PRO:HA	1:B:2237:LYS:HE2	1.48	0.96
3:C:3:NLX:C9	3:C:3:NLX:C16	2.44	0.95
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.00	0.95
1:C:3242:ARG:HH11	1:C:3242:ARG:HG2	1.29	0.94
1:J:4216:THR:HG23	1:J:4242:ARG:HB2	1.50	0.94
1:G:1215:VAL:H	1:G:1241:HIS:HD2	1.14	0.94
1:C:3364:MET:HE1	3:C:3:NLX:H181	1.47	0.93
1:B:2359:ILE:HG12	3:B:2:NLX:H71	1.51	0.92
1:I:3490:ILE:HG22	1:I:3494:LYS:HD2	1.49	0.92
1:K:5237:LYS:HA	1:K:5237:LYS:HE2	1.49	0.92
1:E:5363:LEU:CB	3:E:5:NLX:H201	1.99	0.92
1:H:2359:ILE:HG23	3:H:2:NLX:H82	1.49	0.92
1:J:4363:LEU:HD13	3:J:4:NLX:H181	1.52	0.92
1:E:5304:LEU:HD13	3:E:5:NLX:H181	1.52	0.92
1:B:2091:PRO:HG3	1:B:2112:LEU:HD11	1.51	0.91
1:D:4215:VAL:H	1:D:4241:HIS:HD2	1.14	0.91
1:G:1079:ASN:HB2	2:G:179:NAG:H82	1.50	0.91
1:A:1414:LYS:HZ2	1:F:6370:GLU:HA	1.36	0.91
1:I:3290:THR:OG1	1:I:3293:GLU:HG3	1.71	0.90
1:D:4134:PRO:HG2	1:D:4163:VAL:HG12	1.52	0.90
1:L:6363:LEU:HD13	3:L:6:NLX:H203	1.54	0.90
1:L:6134:PRO:HG2	1:L:6163:VAL:HG12	1.53	0.90
1:L:6215:VAL:H	1:L:6241:HIS:HD2	1.18	0.89
1:E:5363:LEU:HB3	3:E:5:NLX:H201	1.51	0.89
1:H:2404:LEU:HB3	1:H:2413:LYS:HG3	1.53	0.89
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.53	0.89
1:C:3143:GLY:HA3	3:C:3:NLX:H152	1.52	0.89
1:G:1302:LYS:HG3	1:L:6092:LYS:NZ	1.88	0.88
1:A:1215:VAL:H	1:A:1241:HIS:HD2	1.14	0.88
1:E:5404:LEU:HB3	1:E:5413:LYS:HG2	1.54	0.88
1:B:2359:ILE:HG23	3:B:2:NLX:H82	1.56	0.87
1:G:1302:LYS:HG3	1:L:6092:LYS:HZ3	1.38	0.87
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.57	0.86
1:G:1396:ILE:HB	1:G:1397:PRO:HD3	1.56	0.86
1:H:2304:LEU:CB	3:H:2:NLX:H201	2.05	0.86



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:5091:PRO:HG3	1:E:5112:LEU:HD11	1.57	0.86
1:K:5234:PRO:HA	1:K:5237:LYS:HE3	1.57	0.85
1:C:3215:VAL:H	1:C:3241:HIS:CD2	1.91	0.85
1:G:1404:LEU:HD13	1:G:1413:LYS:HG2	1.58	0.85
1:E:5304:LEU:HD22	3:E:5:NLX:H102	1.59	0.85
1:H:2134:PRO:HG2	1:H:2163:VAL:HG12	1.57	0.85
1:L:6235:LEU:HD12	1:L:6327:LEU:HD12	1.58	0.85
1:K:5371:GLY:HA2	1:K:5414:LYS:HD3	1.57	0.85
1:F:6134:PRO:HG2	1:F:6163:VAL:HG12	1.59	0.84
1:K:5304:LEU:HD13	3:K:5:NLX:H181	1.59	0.84
1:B:2318:LEU:HG	3:B:2:NLX:H171	1.58	0.84
1:K:5221:SER:OG	3:K:5:NLX:H71	1.78	0.84
1:E:5490:ILE:O	1:E:5494:LYS:HG3	1.76	0.84
1:K:5221:SER:OG	1:K:5222:ALA:N	2.09	0.84
1:D:4292:GLU:O	1:D:4296:GLU:HG3	1.78	0.83
1:G:1304:LEU:HG	3:G:1:NLX:H203	1.60	0.83
1:D:4304:LEU:CG	3:D:4:NLX:H201	2.08	0.83
1:L:6215:VAL:H	1:L:6241:HIS:CD2	1.96	0.83
1:C:3257:LYS:HD3	4:C:7152:HOH:O	1.78	0.82
1:J:4468:HIS:NE2	3:J:4:NLX:H21	1.94	0.82
1:A:1353:GLN:NE2	1:A:1465:ILE:H	1.77	0.82
1:F:6034:LEU:HD12	1:F:6079:ASN:ND2	1.93	0.82
1:A:1414:LYS:NZ	1:F:6370:GLU:HA	1.93	0.82
1:H:2263:PRO:O	1:H:2267:GLN:HG3	1.79	0.82
1:I:3370:GLU:HG3	1:J:4461:PRO:HG3	1.59	0.82
1:A:1461:PRO:HG2	1:A:1464:VAL:HG23	1.62	0.82
1:L:6023:PRO:HB2	1:L:6034:LEU:HD21	1.61	0.82
1:D:4242:ARG:HG2	1:D:4242:ARG:HH11	1.44	0.82
1:D:4304:LEU:CB	3:D:4:NLX:H201	2.10	0.82
1:C:3318:LEU:HD11	3:C:3:NLX:H151	1.60	0.81
1:H:2363:LEU:HD13	3:H:2:NLX:H101	1.62	0.81
1:A:1331:THR:OG1	1:A:1334:GLU:HG2	1.79	0.81
1:H:2221:SER:HB3	3:H:2:NLX:O1	1.81	0.81
1:L:6105:LYS:HD3	1:L:6106:GLU:HG3	1.60	0.81
1:C:3088:THR:HA	1:C:3112:LEU:HD22	1.62	0.81
1:E:5304:LEU:HD21	1:E:5318:LEU:HD21	1.62	0.81
1:K:5115:ASP:OD2	1:L:6280:ALA:HB3	1.81	0.81
1:F:6254:VAL:HG21	3:F:6:NLX:O1	1.80	0.81
1:C:3343:THR:HB	1:C:3442:ALA:HB2	1.62	0.80
1:F:6363:LEU:HD13	3:F:6:NLX:H171	1.62	0.80
1:K:5363:LEU:CB	3:K:5:NLX:H201	2.12	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:3364:MET:SD	3:C:3:NLX:H181	2.22	0.80
1:A:1304:LEU:HB3	3:A:1:NLX:H203	1.63	0.80
1:K:5083:TYR:CE2	1:K:5108:ILE:HD13	2.16	0.79
1:G:1382:LEU:HD22	1:G:1420:LEU:HD21	1.62	0.79
1:F:6331:THR:OG1	1:F:6334:GLU:HG3	1.81	0.79
1:A:1092:LYS:HE3	4:A:8088:HOH:O	1.83	0.79
1:A:1375:GLN:HE22	1:A:1400:THR:HG22	1.47	0.79
1:F:6215:VAL:H	1:F:6241:HIS:HD2	1.28	0.79
1:K:5235:LEU:HD12	1:K:5327:LEU:HD12	1.65	0.79
1:K:5215:VAL:H	1:K:5241:HIS:HD2	1.28	0.79
1:E:5407:THR:HG21	1:E:5412:LYS:HB2	1.65	0.79
1:A:1363:LEU:HD13	3:A:1:NLX:H101	1.63	0.78
1:I:3371:GLY:O	1:I:3411:VAL:HA	1.82	0.78
1:A:1376:LYS:HD3	1:F:6462:LYS:HE2	1.62	0.78
1:L:6258:LYS:H	1:L:6258:LYS:HD3	1.45	0.78
1:B:2079:ASN:HD22	2:B:279:NAG:H82	1.49	0.78
1:I:3318:LEU:HG	3:I:3:NLX:C19	2.12	0.78
1:K:5134:PRO:HG2	1:K:5163:VAL:HG12	1.62	0.78
1:B:2079:ASN:ND2	2:B:279:NAG:H82	1.99	0.78
1:B:2317:PRO:HB2	3:B:2:NLX:H192	1.64	0.78
1:J:4428:VAL:HB	1:J:4429:PRO:HD3	1.64	0.78
1:F:6216:THR:HG23	1:F:6242:ARG:HB2	1.66	0.78
1:G:1104:ARG:NH1	1:G:1153:ASP:HB2	1.99	0.77
1:J:4338:GLU:HG3	1:J:4338:GLU:O	1.83	0.77
1:F:6290:THR:HG23	1:F:6293:GLU:OE1	1.85	0.77
1:A:1363:LEU:HD22	3:A:1:NLX:H181	1.64	0.77
1:L:6304:LEU:HD22	3:L:6:NLX:H172	1.64	0.77
1:I:3234:PRO:O	1:I:3237:LYS:HG2	1.85	0.77
1:J:4132:ARG:HH12	1:J:4206:ALA:CB	1.98	0.77
1:J:4215:VAL:H	1:J:4241:HIS:HD2	1.33	0.77
1:L:6114:GLU:OE1	1:L:6291:GLU:HB2	1.84	0.77
1:B:2220:GLU:OE1	1:B:2221:SER:HB2	1.84	0.77
1:B:2359:ILE:HG12	3:B:2:NLX:C7	2.14	0.77
1:C:3268:ILE:HD11	1:C:3319:LEU:HD11	1.67	0.77
1:A:1079:ASN:ND2	2:A:179:NAG:H2	2.00	0.77
1:D:4359:ILE:HD13	3:D:4:NLX:H71	1.67	0.76
1:F:6097:LEU:HD22	3:F:6:NLX:C19	2.13	0.76
1:K:5395:LEU:HB3	1:K:5550:LEU:HD21	1.66	0.76
1:D:4304:LEU:HG	3:D:4:NLX:H201	1.67	0.76
1:L:6304:LEU:HD22	3:L:6:NLX:H102	1.67	0.76
1:G:1290:THR:OG1	1:G:1293:GLU:HG3	1.86	0.76



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:I:3512:GLU:H	1:I:3512:GLU:CD	1.86	0.76
1:D:4471:GLU:O	1:D:4475:VAL:HG23	1.85	0.76
1:D:4538:LYS:HD3	1:D:4541:ASP:OD1	1.86	0.76
1:E:5142:GLY:HA2	3:E:5:NLX:H82	1.67	0.76
1:G:1228:SER:O	1:G:1231:VAL:HG12	1.85	0.76
1:L:6142:GLY:HA2	3:L:6:NLX:H82	1.69	0.75
1:D:4349:GLY:HA3	1:D:4447:TYR:CZ	2.20	0.75
1:I:3428:VAL:HB	1:I:3429:PRO:HD3	1.68	0.75
1:H:2304:LEU:HB3	3:H:2:NLX:C20	2.13	0.75
1:B:2359:ILE:HG13	4:B:7392:HOH:O	1.85	0.75
1:F:6215:VAL:H	1:F:6241:HIS:CD2	2.04	0.75
1:H:2220:GLU:HG2	1:H:2472:LEU:HD21	1.68	0.75
1:H:2215:VAL:H	1:H:2241:HIS:HD2	1.34	0.75
1:I:3353:GLN:NE2	1:I:3465:ILE:H	1.85	0.75
1:F:6452:ARG:HB2	1:F:6465:ILE:HG12	1.69	0.75
1:K:5382:LEU:HD11	1:K:5391:ILE:HD12	1.69	0.75
1:K:5304:LEU:HD22	3:K:5:NLX:H102	1.69	0.75
1:J:4059:PRO:HD3	1:J:4117:LEU:HD12	1.69	0.74
3:C:3:NLX:C17	3:C:3:NLX:C9	2.64	0.74
1:C:3215:VAL:N	1:C:3241:HIS:HD2	1.81	0.74
1:D:4242:ARG:HG2	1:D:4242:ARG:NH1	2.01	0.74
1:H:2176:GLY:HA2	1:H:2189:TRP:HB2	1.69	0.74
1:B:2318:LEU:CG	3:B:2:NLX:H171	2.18	0.74
1:C:3371:GLY:O	1:C:3411:VAL:HA	1.88	0.74
1:F:6257:LYS:HA	1:F:6257:LYS:HE3	1.70	0.74
1:H:2371:GLY:HA2	1:H:2414:LYS:HD3	1.68	0.74
1:B:2372:GLN:O	1:B:2410:THR:HB	1.87	0.74
1:A:1090:ASP:HB3	1:A:1093:ALA:HB3	1.67	0.74
1:B:2234:PRO:O	1:B:2237:LYS:HG2	1.87	0.73
1:F:6242:ARG:HH11	1:F:6242:ARG:HG2	1.54	0.73
1:H:2370:GLU:HG3	1:K:5461:PRO:HG3	1.69	0.73
1:G:1363:LEU:HB3	3:G:1:NLX:H181	1.71	0.73
1:C:3242:ARG:HG2	1:C:3242:ARG:NH1	2.01	0.73
1:I:3498:LYS:HB3	1:I:3514:LEU:HD11	1.70	0.73
1:F:6353:GLN:NE2	1:F:6465:ILE:H	1.86	0.73
1:G:1428:VAL:HB	1:G:1429:PRO:HD3	1.70	0.73
1:J:4304:LEU:HG	3:J:4:NLX:H203	1.70	0.73
1:J:4251:LEU:HD11	1:J:4336:GLN:HE22	1.52	0.73
1:B:2359:ILE:HB	1:B:2360:PRO:CD	2.19	0.73
1:I:3142:GLY:HA2	3:I:3:NLX:H71	1.70	0.73
1:K:5363:LEU:HB2	3:K:5:NLX:H201	1.70	0.73



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:4359:ILE:HB	1:D:4360:PRO:HD3	1.71	0.73
1:D:4304:LEU:HB3	3:D:4:NLX:H201	1.69	0.73
1:G:1215:VAL:H	1:G:1241:HIS:CD2	2.02	0.73
1:F:6235:LEU:HD12	1:F:6327:LEU:HD12	1.70	0.72
1:H:2420:LEU:O	1:H:2424:VAL:HG23	1.89	0.72
1:L:6358:LEU:HG	1:L:6363:LEU:HD12	1.71	0.72
1:B:2371:GLY:HA2	1:B:2414:LYS:HD3	1.71	0.72
1:B:2304:LEU:HA	3:B:2:NLX:H191	1.71	0.72
1:C:3143:GLY:HA3	3:C:3:NLX:C15	2.18	0.72
1:E:5235:LEU:HD12	1:E:5327:LEU:HA	1.70	0.72
1:F:6097:LEU:CD2	3:F:6:NLX:H192	2.18	0.72
1:K:5396:ILE:HB	1:K:5397:PRO:HD3	1.69	0.72
1:J:4260:ASP:OD2	1:J:4263:PRO:HD3	1.89	0.72
1:D:4363:LEU:HB3	3:D:4:NLX:C18	2.18	0.72
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.25	0.72
1:K:5353:GLN:NE2	1:K:5465:ILE:H	1.87	0.72
1:L:6030:HIS:HB3	1:L:6073:PRO:HA	1.69	0.72
1:F:6359:ILE:HB	1:F:6360:PRO:HD3	1.71	0.72
1:A:1095:GLN:O	1:A:1099:GLU:HG3	1.90	0.72
1:E:5308:LEU:HD21	1:E:5367:PRO:HG3	1.70	0.72
1:C:3249:VAL:HG23	1:C:3251:LEU:H	1.55	0.72
1:D:4354:GLU:O	1:D:4468:HIS:HB2	1.90	0.72
1:E:5308:LEU:HD21	1:E:5367:PRO:CG	2.20	0.71
1:A:1237:LYS:HG2	1:A:1238:ASN:ND2	2.05	0.71
3:C:3:NLX:C9	3:C:3:NLX:C20	2.68	0.71
1:E:5491:ARG:HG2	4:E:7516:HOH:O	1.89	0.71
1:H:2048:ALA:HB3	1:H:2123:THR:HG23	1.72	0.71
1:H:2227:VAL:O	1:H:2231:VAL:HG23	1.91	0.71
1:L:6255:LEU:HD23	1:L:6318:LEU:HD13	1.73	0.71
1:A:1104:ARG:CZ	1:A:1153:ASP:HB2	2.20	0.71
1:F:6034:LEU:HD12	1:F:6079:ASN:HD22	1.53	0.71
1:B:2355:PHE:CE2	1:B:2359:ILE:HG21	2.25	0.71
1:G:1104:ARG:HB3	1:G:1104:ARG:HH11	1.55	0.71
1:A:1527:LEU:HD11	1:A:1533:THR:CG2	2.19	0.71
1:B:2353:GLN:NE2	1:B:2465:ILE:H	1.88	0.71
1:K:5359:ILE:HG23	3:K:5:NLX:H152	1.71	0.71
1:A:1319:LEU:H	1:A:1319:LEU:HD12	1.56	0.70
1:E:5255:LEU:HD23	1:E:5318:LEU:HD13	1.74	0.70
1:H:2121:ILE:HD13	1:H:2166:VAL:HG22	1.73	0.70
1:E:5304:LEU:HB3	3:E:5:NLX:C18	2.21	0.70
1:K:5024:PRO:HD3	1:K:5037:PHE:CD1	2.27	0.70



	• • • • •	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1313:ARG:HG2	1:A:1386:TYR:CE2	2.27	0.70
1:D:4508:ASN:HD21	1:D:4510:ASN:HB2	1.57	0.70
1:H:2158:ALA:HB2	1:H:2165:VAL:HG23	1.72	0.70
1:C:3319:LEU:HA	4:C:7152:HOH:O	1.92	0.70
4:B:7643:HOH:O	1:E:5092:LYS:HD2	1.91	0.70
1:E:5363:LEU:HB2	3:E:5:NLX:H201	1.74	0.70
1:H:2359:ILE:HD13	3:H:2:NLX:H71	1.72	0.70
1:L:6029:VAL:HG23	1:L:6204:ASN:OD1	1.92	0.70
1:L:6550:LEU:HA	1:L:6553:LYS:NZ	2.05	0.70
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.04	0.69
1:D:4428:VAL:HB	1:D:4429:PRO:HD3	1.73	0.69
1:D:4161:GLU:OE2	1:D:4498:LYS:HA	1.92	0.69
1:E:5089:GLN:HB2	1:E:5146:VAL:HG12	1.72	0.69
1:I:3215:VAL:H	1:I:3241:HIS:HD2	1.38	0.69
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.27	0.69
1:B:2079:ASN:ND2	2:B:279:NAG:C1	2.55	0.69
1:G:1023:PRO:HB2	1:G:1034:LEU:HD21	1.74	0.69
1:K:5082:SER:HB2	4:K:7929:HOH:O	1.92	0.69
1:L:6373:LEU:HB2	1:L:6414:LYS:HB3	1.75	0.69
1:D:4343:THR:HA	4:D:7962:HOH:O	1.92	0.69
1:G:1404:LEU:HB3	1:G:1413:LYS:HG3	1.74	0.69
1:I:3491:ARG:HA	1:I:3494:LYS:HD3	1.74	0.69
1:G:1385:SER:O	1:G:1389:VAL:HG22	1.93	0.69
1:H:2258:LYS:HD2	4:H:7424:HOH:O	1.92	0.69
1:I:3242:ARG:HH11	1:I:3242:ARG:HG2	1.58	0.69
1:L:6262:LYS:O	1:L:6266:GLU:HG2	1.93	0.69
1:B:2227:VAL:O	1:B:2231:VAL:HG23	1.91	0.69
1:L:6260:ASP:HA	4:L:7557:HOH:O	1.93	0.69
1:L:6359:ILE:HB	1:L:6360:PRO:HD3	1.73	0.69
1:C:3404:LEU:HD22	1:C:3413:LYS:O	1.92	0.69
1:E:5264:LEU:HD13	1:E:5316:GLN:HG3	1.73	0.69
1:F:6395:LEU:HB3	1:F:6550:LEU:HD21	1.73	0.69
1:L:6215:VAL:N	1:L:6241:HIS:HD2	1.91	0.69
1:L:6257:LYS:HE2	1:L:6316:GLN:NE2	2.08	0.69
1:L:6355:PHE:CE1	1:L:6360:PRO:HG3	2.27	0.69
1:C:3132:ARG:HB3	1:C:3211:ASN:HB2	1.74	0.69
1:G:1429:PRO:O	1:G:1433:VAL:HG23	1.92	0.69
1:I:3217:ILE:O	1:I:3217:ILE:HG13	1.92	0.69
1:K:5420:LEU:HD12	1:K:5547:TRP:HZ2	1.58	0.69
1:A:1527:LEU:HD11	1:A:1533:THR:HG22	1.74	0.69
1:C:3057:LYS:HD3	1:C:3063:LEU:HD11	1.75	0.69



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:1304:LEU:CD1	1:G:1318:LEU:HD23	2.23	0.69
1:C:3370:GLU:HG3	1:D:4461:PRO:HG3	1.73	0.68
3:C:3:NLX:C14	3:C:3:NLX:C10	2.71	0.68
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.74	0.68
1:C:3527:LEU:HD11	1:C:3533:THR:HG22	1.75	0.68
1:L:6371:GLY:O	1:L:6411:VAL:HA	1.94	0.68
1:C:3236:ALA:HA	1:C:3239:LEU:HD12	1.76	0.68
1:G:1156:ALA:HB3	4:G:7720:HOH:O	1.91	0.68
1:H:2460:LYS:HG2	4:H:7161:HOH:O	1.94	0.68
1:K:5456:SER:HB3	1:K:5460:LYS:HD3	1.75	0.68
1:C:3290:THR:OG1	1:C:3293:GLU:HG3	1.94	0.68
1:J:4334:GLU:O	1:J:4338:GLU:HG2	1.92	0.68
1:L:6550:LEU:HA	1:L:6553:LYS:HZ3	1.56	0.68
1:G:1391:ILE:HA	4:G:8113:HOH:O	1.92	0.68
1:H:2221:SER:CB	3:H:2:NLX:O1	2.42	0.68
1:K:5351:ASN:HB3	1:K:5466:GLY:O	1.94	0.68
1:D:4260:ASP:OD1	1:D:4263:PRO:HD3	1.94	0.68
1:F:6024:PRO:HG3	1:F:6037:PHE:CE1	2.28	0.68
1:H:2363:LEU:HD13	3:H:2:NLX:C10	2.23	0.68
1:I:3088:THR:HG22	1:I:3295:LEU:HD13	1.76	0.68
1:G:1417:PHE:O	1:G:1420:LEU:HB3	1.95	0.67
1:B:2486:SER:O	1:B:2490:ILE:HG13	1.94	0.67
1:J:4525:GLY:HA2	1:J:4537:GLN:HG2	1.76	0.67
1:L:6271:THR:HG22	1:L:6297:THR:HG23	1.76	0.67
1:L:6545:ALA:O	1:L:6548:THR:HG22	1.95	0.67
1:A:1372:GLN:HB2	1:A:1410:THR:HG22	1.75	0.67
1:A:1385:SER:O	1:A:1389:VAL:HG22	1.95	0.67
1:B:2174:ILE:HG13	4:B:7012:HOH:O	1.95	0.67
1:F:6174:ILE:HG13	4:F:7076:HOH:O	1.95	0.67
1:F:6353:GLN:HE22	1:F:6465:ILE:H	1.40	0.67
1:F:6220:GLU:HG2	1:F:6472:LEU:HD21	1.77	0.67
1:H:2386:TYR:N	1:H:2387:PRO:HD2	2.09	0.67
1:L:6254:VAL:HG22	1:L:6318:LEU:HD12	1.75	0.67
1:A:1376:LYS:HD3	1:F:6462:LYS:CE	2.24	0.67
1:F:6043:PHE:HA	4:F:7849:HOH:O	1.94	0.67
1:K:5498:LYS:HG2	1:K:5502:ASN:HD21	1.60	0.67
1:L:6087:CYS:HB3	4:L:7703:HOH:O	1.95	0.67
1:A:1363:LEU:CD2	3:A:1:NLX:H181	2.25	0.67
1:D:4358:LEU:O	1:D:4363:LEU:HD12	1.95	0.67
1:J:4303:PHE:CZ	1:J:4319:LEU:HD21	2.29	0.67
1:K:5290:THR:OG1	1:K:5293:GLU:HG3	1.95	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:F:6097:LEU:HB2	3:F:6:NLX:H192	1.77	0.67
1:I:3317:PRO:HG2	3:I:3:NLX:C19	2.25	0.67
1:I:3324:ASP:OD1	1:I:3326:MET:HB2	1.94	0.67
1:J:4215:VAL:H	1:J:4241:HIS:CD2	2.11	0.67
1:H:2186:ARG:HB3	1:H:2324:ASP:HB2	1.77	0.67
1:C:3227:VAL:O	1:C:3231:VAL:HG23	1.94	0.67
1:E:5125:ALA:HB1	1:E:5131:ASN:ND2	2.10	0.67
1:E:5242:ARG:HH11	1:E:5242:ARG:HG3	1.61	0.66
1:L:6429:PRO:O	1:L:6433:VAL:HG23	1.95	0.66
1:A:1363:LEU:HD13	3:A:1:NLX:C10	2.24	0.66
1:B:2304:LEU:HA	3:B:2:NLX:C19	2.25	0.66
1:H:2083:TYR:CE2	1:H:2108:ILE:HD13	2.31	0.66
1:A:1363:LEU:HB3	3:A:1:NLX:H181	1.77	0.66
1:B:2371:GLY:HA3	1:E:5371:GLY:HA3	1.77	0.66
1:D:4409:ASP:HB3	1:D:4412:LYS:HB2	1.78	0.66
1:G:1142:GLY:HA2	3:G:1:NLX:H152	1.76	0.66
1:G:1146:VAL:HG21	3:G:1:NLX:H162	1.77	0.66
1:K:5221:SER:HB2	3:K:5:NLX:O3	1.95	0.66
1:L:6141:GLY:N	4:L:7115:HOH:O	2.22	0.66
1:E:5145:MET:HB2	1:E:5304:LEU:HD11	1.76	0.66
1:F:6411:VAL:HG23	4:F:7705:HOH:O	1.94	0.66
1:F:6414:LYS:HD2	1:F:6415:ASP:N	2.11	0.66
1:H:2498:LYS:HG2	1:H:2514:LEU:HD11	1.76	0.66
1:J:4132:ARG:HH12	1:J:4206:ALA:HB1	1.59	0.66
1:L:6216:THR:HG23	1:L:6242:ARG:HB2	1.78	0.66
1:C:3498:LYS:HB3	1:C:3514:LEU:HD11	1.75	0.66
1:E:5409:ASP:OD2	1:E:5411:VAL:HB	1.96	0.66
1:F:6143:GLY:N	3:F:6:NLX:H82	2.11	0.66
1:F:6258:LYS:O	1:F:6258:LYS:HE2	1.95	0.66
1:I:3412:LYS:O	1:I:3416:LEU:HG	1.95	0.66
1:J:4221:SER:OG	1:J:4222:ALA:N	2.28	0.66
1:J:4396:ILE:HB	1:J:4397:PRO:HD3	1.77	0.66
1:L:6083:TYR:CE2	1:L:6108:ILE:HD13	2.31	0.66
1:L:6375:GLN:HE22	1:L:6401:GLU:HA	1.61	0.66
1:L:6395:LEU:HD22	1:L:6550:LEU:HD11	1.77	0.66
1:J:4191:HIS:O	1:J:4195:VAL:HG23	1.95	0.66
1:A:1232:LEU:HD23	1:A:1341:PHE:HB3	1.78	0.66
1:C:3407:THR:HG21	1:C:3412:LYS:NZ	2.11	0.66
1:D:4303:PHE:O	1:D:4304:LEU:HB2	1.95	0.66
1:E:5304:LEU:HD21	1:E:5318:LEU:CD2	2.26	0.66
1:G:1146:VAL:CG2	3:G:1:NLX:H162	2.26	0.66



		Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	overlap (Å)
1:J:4364:MET:SD	3:J:4:NLX:H72	2.35	0.66
1:K:5104:ARG:NH1	1:K:5153:ASP:HB2	2.10	0.66
1:L:6024:PRO:HA	4:L:7722:HOH:O	1.96	0.66
1:A:1428:VAL:HB	1:A:1429:PRO:HD3	1.78	0.65
1:E:5134:PRO:HG2	1:E:5163:VAL:HG12	1.78	0.65
1:G:1220:GLU:HA	1:G:1246:GLU:O	1.97	0.65
1:K:5218:PHE:HB2	1:K:5244:ILE:HB	1.77	0.65
1:A:1358:LEU:HG	1:A:1363:LEU:CD1	2.26	0.65
1:E:5371:GLY:O	1:E:5414:LYS:HD3	1.97	0.65
3:F:6:NLX:O4	4:F:7502:HOH:O	2.13	0.65
1:I:3398:GLU:HG3	4:I:8065:HOH:O	1.95	0.65
1:J:4237:LYS:HE2	1:J:4238:ASN:HD21	1.59	0.65
1:E:5395:LEU:HB3	1:E:5550:LEU:HD11	1.78	0.65
1:G:1363:LEU:HD13	3:G:1:NLX:H102	1.78	0.65
1:J:4304:LEU:HG	3:J:4:NLX:C20	2.26	0.65
1:D:4257:LYS:HZ1	1:D:4316:GLN:HG3	1.60	0.65
1:D:4395:LEU:HD13	1:D:4550:LEU:HG	1.78	0.65
1:I:3125:ALA:HB2	1:I:3133:LEU:HD11	1.79	0.65
1:I:3447:TYR:HB3	1:I:3517:TRP:CZ2	2.31	0.65
1:G:1276:THR:HG22	1:G:1282:MET:SD	2.36	0.65
1:J:4549:ASN:HB2	4:J:8096:HOH:O	1.95	0.65
1:E:5149:ALA:HB1	1:E:5167:THR:HB	1.79	0.65
1:J:4104:ARG:NH1	1:J:4153:ASP:HB2	2.12	0.65
1:L:6139:ILE:HG22	4:L:7115:HOH:O	1.96	0.65
1:A:1086:MET:HE2	1:A:1110:LEU:HD12	1.77	0.65
1:B:2359:ILE:HG23	3:B:2:NLX:C8	2.25	0.65
1:C:3357:TRP:O	1:C:3360:PRO:HD2	1.96	0.65
1:D:4330:LYS:HG3	1:D:4335:LEU:HG	1.78	0.65
1:E:5279:SER:HA	1:E:5282:MET:HE3	1.77	0.65
1:E:5290:THR:OG1	1:E:5293:GLU:HG3	1.95	0.65
1:I:3364:MET:SD	3:I:3:NLX:H162	2.37	0.65
1:J:4429:PRO:O	1:J:4433:VAL:HG23	1.97	0.65
1:L:6024:PRO:HG3	1:L:6037:PHE:CE1	2.31	0.65
1:A:1251:LEU:HD11	1:A:1336:GLN:NE2	2.02	0.65
1:H:2426:PHE:O	1:H:2429:PRO:HD2	1.97	0.65
1:J:4404:LEU:HD13	1:J:4413:LYS:HB3	1.77	0.65
1:G:1444:THR:O	1:G:1519:GLU:HG2	1.97	0.64
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.78	0.64
1:C:3313:ARG:HG2	1:C:3386:TYR:CE2	2.32	0.64
1:J:4427:GLY:O	1:J:4431:VAL:HG23	1.96	0.64
1:J:4461:PRO:HG2	1:J:4464:VAL:HG23	1.79	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1353:GLN:HE22	1:A:1465:ILE:H	1.45	0.64
1:E:5258:LYS:HD2	1:E:5258:LYS:O	1.97	0.64
1:F:6252:THR:HG23	1:F:6425:MET:O	1.96	0.64
1:F:6456:SER:HB3	1:F:6460:LYS:HD3	1.78	0.64
1:F:6343:THR:HB	1:F:6442:ALA:HB2	1.80	0.64
1:J:4227:VAL:O	1:J:4231:VAL:HG23	1.97	0.64
1:C:3296:GLU:HG2	1:D:4296:GLU:OE1	1.98	0.64
1:D:4079:ASN:HB2	2:D:479:NAG:H82	1.80	0.64
1:F:6221:SER:OG	3:F:6:NLX:H72	1.98	0.64
1:E:5464:VAL:C	1:E:5465:ILE:HD12	2.17	0.64
1:G:1218:PHE:CB	1:G:1244:ILE:HB	2.27	0.64
1:H:2090:ASP:HB3	1:H:2093:ALA:HB3	1.79	0.64
1:I:3296:GLU:O	1:I:3300:LYS:HG3	1.97	0.64
1:E:5486:SER:O	1:E:5490:ILE:HG13	1.98	0.64
1:E:5359:ILE:HG23	3:E:5:NLX:H152	1.80	0.64
1:F:6540:LYS:HD3	1:F:6543:GLU:OE1	1.97	0.64
1:I:3486:SER:O	1:I:3490:ILE:HG13	1.98	0.64
1:D:4251:LEU:HD21	1:D:4333:GLU:HG3	1.80	0.63
1:G:1435:ARG:NH1	1:G:1544:VAL:HG11	2.12	0.63
1:J:4098:SER:O	1:J:4102:THR:HG22	1.97	0.63
1:J:4130:LYS:HE2	1:J:4132:ARG:NE	2.13	0.63
1:K:5311:ASP:HB3	1:K:5314:GLU:HG2	1.80	0.63
1:L:6414:LYS:HE2	1:L:6415:ASP:OD2	1.97	0.63
1:I:3452:ARG:HB2	1:I:3465:ILE:HG12	1.79	0.63
1:A:1435:ARG:NH1	1:A:1544:VAL:HG11	2.14	0.63
1:F:6311:ASP:OD1	1:F:6313:ARG:HB2	1.98	0.63
1:G:1215:VAL:N	1:G:1241:HIS:HD2	1.91	0.63
1:G:1519:GLU:O	1:G:1521:ASN:N	2.31	0.63
1:E:5340:ASN:ND2	1:E:5342:HIS:H	1.96	0.63
1:F:6258:LYS:N	1:F:6258:LYS:HE2	2.13	0.63
1:G:1140:HIS:HD2	1:G:1141:GLY:O	1.81	0.63
1:A:1264:LEU:HG	1:A:1316:GLN:HG2	1.80	0.63
1:F:6258:LYS:H	1:F:6258:LYS:HE2	1.64	0.63
1:L:6051:LEU:HD13	1:L:6083:TYR:CE1	2.33	0.63
1:A:1216:THR:HG23	1:A:1242:ARG:HB2	1.80	0.63
1:D:4396:ILE:HB	1:D:4397:PRO:HD3	1.80	0.63
1:E:5215:VAL:H	1:E:5241:HIS:HD2	1.47	0.63
1:E:5523:LYS:O	1:E:5538:LYS:HE3	1.98	0.63
1:F:6478:ALA:HB3	1:F:6479:PRO:HD3	1.79	0.63
1:I:3142:GLY:CA	3:I:3:NLX:H71	2.29	0.63
1:K:5149:ALA:HB2	1:K:5169:GLN:HG3	1.80	0.63



	t i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:5526:TYR:HD2	1:K:5537:GLN:O	1.81	0.63
1:A:1304:LEU:CD1	1:A:1318:LEU:HD23	2.29	0.63
1:B:2149:ALA:HB2	1:B:2169:GLN:HG3	1.80	0.63
1:E:5351:ASN:OD1	1:E:5449:PHE:HB3	1.98	0.63
1:G:1279:SER:O	1:G:1283:VAL:HG23	1.98	0.63
1:D:4126:ASP:H	1:D:4131:ASN:ND2	1.96	0.63
1:F:6138:TRP:CZ3	1:F:6219:GLY:HA2	2.34	0.63
1:H:2235:LEU:HD12	1:H:2327:LEU:HA	1.80	0.63
1:H:2526:TYR:CE1	1:H:2539:LEU:HD13	2.34	0.63
1:J:4079:ASN:HD21	2:J:479:NAG:H5	1.63	0.63
1:D:4461:PRO:HG2	1:D:4464:VAL:HG23	1.80	0.63
1:G:1409:ASP:HB3	1:G:1412:LYS:HB2	1.80	0.63
1:J:4407:THR:HG21	1:J:4412:LYS:HD2	1.81	0.63
1:K:5324:ASP:OD1	1:K:5326:MET:HB2	1.99	0.63
1:G:1092:LYS:NZ	1:L:6302:LYS:HB2	2.13	0.63
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.14	0.62
1:A:1363:LEU:CD1	3:A:1:NLX:H101	2.28	0.62
3:C:3:NLX:C13	3:C:3:NLX:C9	2.76	0.62
1:D:4423:ASP:OD1	1:D:4540:LYS:HE2	1.99	0.62
1:K:5467:ASP:OD1	1:K:5468:HIS:N	2.30	0.62
1:L:6523:LYS:HB3	1:L:6537:GLN:OE1	1.98	0.62
1:C:3351:ASN:ND2	1:C:3449:PHE:HB3	2.14	0.62
1:E:5188:ASN:O	1:E:5192:LEU:HG	1.99	0.62
1:I:3220:GLU:HG2	4:I:7760:HOH:O	1.99	0.62
1:J:4354:GLU:O	1:J:4468:HIS:HB2	1.99	0.62
1:E:5089:GLN:OE1	1:E:5146:VAL:HB	1.99	0.62
1:D:4145:MET:HG3	1:D:4304:LEU:HD11	1.80	0.62
1:A:1359:ILE:HG23	3:A:1:NLX:H71	1.82	0.62
1:C:3324:ASP:OD1	1:C:3326:MET:HB2	1.98	0.62
1:E:5311:ASP:O	1:E:5314:GLU:HG2	1.99	0.62
1:F:6097:LEU:HD13	3:F:6:NLX:H191	1.82	0.62
1:H:2463:THR:HG23	4:H:7113:HOH:O	1.98	0.62
3:C:3:NLX:H102	3:C:3:NLX:C20	2.30	0.62
1:I:3234:PRO:O	1:I:3237:LYS:HE3	1.98	0.62
1:J:4034:LEU:CD1	2:J:479:NAG:H82	2.30	0.62
1:K:5464:VAL:C	1:K:5465:ILE:HD12	2.20	0.62
1:I:3358:LEU:O	1:I:3363:LEU:HD12	1.99	0.62
1:A:1030:HIS:HB3	1:A:1073:PRO:HA	1.81	0.62
1:F:6304:LEU:HD22	3:F:6:NLX:H101	1.81	0.62
1:G:1471:GLU:O	1:G:1475:VAL:HG23	1.99	0.62
1:H:2304:LEU:HD13	3:H:2:NLX:H171	1.80	0.62



	at pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:5403:TYR:O	1:K:5416:LEU:HD13	1.99	0.62
1:F:6097:LEU:HD11	1:F:6101:PHE:CE2	2.35	0.62
1:K:5220:GLU:O	1:K:5221:SER:HB3	1.99	0.62
1:L:6363:LEU:HB3	3:L:6:NLX:H201	1.79	0.62
1:G:1417:PHE:CD1	1:G:1420:LEU:HD23	2.34	0.62
1:I:3381:LEU:HD23	1:J:4459:MET:HG2	1.82	0.62
1:A:1086:MET:HE2	1:A:1110:LEU:HB2	1.82	0.61
1:A:1279:SER:O	1:A:1283:VAL:HG23	2.00	0.61
1:J:4251:LEU:HD11	1:J:4336:GLN:NE2	2.14	0.61
1:K:5428:VAL:HB	1:K:5429:PRO:HD3	1.81	0.61
1:A:1308:LEU:HD11	1:A:1367:PRO:HG3	1.82	0.61
1:A:1409:ASP:HB3	1:A:1412:LYS:HB2	1.82	0.61
1:D:4349:GLY:HA3	1:D:4447:TYR:CE1	2.35	0.61
1:G:1395:LEU:HB3	1:G:1550:LEU:HD11	1.83	0.61
1:I:3302:LYS:HD2	1:J:4092:LYS:HD2	1.80	0.61
1:B:2024:PRO:HG3	1:B:2037:PHE:CE1	2.35	0.61
1:C:3268:ILE:HG12	1:C:3301:MET:HE2	1.81	0.61
1:F:6144:LEU:HB3	1:F:6177:PHE:CE2	2.35	0.61
1:G:1373:LEU:O	1:G:1413:LYS:HD2	1.99	0.61
1:L:6447:TYR:CD2	1:L:6447:TYR:C	2.74	0.61
1:A:1423:ASP:O	1:A:1428:VAL:HG23	2.01	0.61
1:F:6140:HIS:HD2	1:F:6141:GLY:O	1.83	0.61
1:H:2264:LEU:HD22	1:H:2316:GLN:HE21	1.63	0.61
1:J:4032:LYS:HB2	1:J:4077:VAL:HA	1.82	0.61
1:J:4386:TYR:N	1:J:4387:PRO:HD2	2.16	0.61
1:A:1114:GLU:HG3	1:A:1291:GLU:OE2	2.00	0.61
1:B:2174:ILE:CD1	1:B:2298:THR:HG22	2.29	0.61
3:D:4:NLX:O4	3:D:4:NLX:H203	2.00	0.61
1:G:1303:PHE:HB3	1:G:1304:LEU:HD22	1.81	0.61
1:I:3258:LYS:H	1:I:3258:LYS:HE2	1.65	0.61
1:J:4231:VAL:O	1:J:4341:PHE:HB2	1.99	0.61
1:K:5104:ARG:CZ	1:K:5153:ASP:HB2	2.30	0.61
1:K:5218:PHE:CB	1:K:5244:ILE:HB	2.30	0.61
1:G:1302:LYS:CG	1:L:6092:LYS:NZ	2.63	0.61
1:L:6257:LYS:HE2	1:L:6316:GLN:CD	2.21	0.61
1:G:1357:TRP:CE3	1:G:1460:LYS:HD3	2.35	0.61
1:G:1452:ARG:HB2	1:G:1465:ILE:HG13	1.83	0.61
1:I:3144:LEU:HD12	1:I:3320:GLY:HA2	1.82	0.61
1:J:4074:TRP:CE2	1:J:4078:LYS:HE2	2.36	0.61
1:J:4081:THR:OG1	2:J:479:NAG:H5	2.00	0.61
1:L:6363:LEU:HB3	3:L:6:NLX:H162	1.82	0.61



	• • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2104:ARG:HG2	1:B:2104:ARG:HH11	1.66	0.61
1:B:2498:LYS:HG2	1:B:2514:LEU:HD11	1.82	0.61
1:C:3364:MET:SD	3:C:3:NLX:C18	2.87	0.61
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.63	0.61
1:C:3495:MET:HG3	1:C:3514:LEU:HD22	1.82	0.61
1:I:3352:LYS:HE3	1:I:3450:GLN:NE2	2.15	0.61
1:K:5258:LYS:HD2	1:K:5258:LYS:N	2.03	0.61
1:G:1355:PHE:CE1	1:G:1360:PRO:HG3	2.35	0.61
1:I:3363:LEU:HD13	4:I:7519:HOH:O	2.01	0.61
1:B:2024:PRO:HG3	1:B:2037:PHE:CZ	2.36	0.61
1:L:6024:PRO:HG3	1:L:6037:PHE:CZ	2.36	0.61
1:B:2464:VAL:CG2	1:E:5370:GLU:HG3	2.31	0.61
1:E:5524:GLU:OE2	1:E:5538:LYS:HD3	2.01	0.61
1:F:6047:VAL:HG21	1:F:6155:LEU:HD23	1.83	0.61
1:F:6527:LEU:HD11	1:F:6533:THR:HG22	1.82	0.61
1:A:1371:GLY:O	1:A:1414:LYS:HD3	2.00	0.60
1:D:4421:ILE:HG22	1:D:4425:MET:HE2	1.83	0.60
1:G:1452:ARG:HG2	1:G:1452:ARG:HH11	1.66	0.60
1:J:4023:PRO:HB2	1:J:4034:LEU:HD21	1.82	0.60
1:J:4302:LYS:NZ	1:J:4302:LYS:HB3	2.16	0.60
1:K:5366:TYR:HB3	1:K:5368:LEU:HD13	1.81	0.60
1:F:6417:PHE:O	1:F:6420:LEU:HB3	2.02	0.60
1:G:1456:SER:HB3	1:G:1460:LYS:HE3	1.82	0.60
1:K:5284:HIS:O	1:K:5288:GLN:HG3	2.00	0.60
1:A:1257:LYS:HD2	1:A:1320:GLY:H	1.66	0.60
1:A:1304:LEU:HB3	3:A:1:NLX:C20	2.31	0.60
1:E:5353:GLN:NE2	1:E:5465:ILE:H	1.99	0.60
1:F:6097:LEU:HD11	1:F:6101:PHE:CD2	2.36	0.60
1:F:6324:ASP:OD1	1:F:6326:MET:N	2.32	0.60
1:K:5304:LEU:HD22	3:K:5:NLX:C10	2.32	0.60
1:L:6478:ALA:HB3	1:L:6479:PRO:HD3	1.82	0.60
1:E:5266:GLU:O	1:E:5270:ILE:HG13	2.00	0.60
1:E:5452:ARG:NE	1:E:5462:LYS:HA	2.16	0.60
1:L:6104:ARG:HH11	1:L:6104:ARG:HG2	1.64	0.60
1:A:1145:MET:HB2	1:A:1304:LEU:HD21	1.83	0.60
1:A:1244:ILE:HG12	1:A:1347:MET:HB3	1.84	0.60
1:E:5330:LYS:HB3	1:E:5334:GLU:OE2	2.01	0.60
1:F:6355:PHE:CE1	1:F:6360:PRO:HG3	2.36	0.60
1:G:1064:ARG:NH1	1:G:1294:LEU:HD11	2.15	0.60
1:L:6428:VAL:HB	1:L:6429:PRO:HD3	1.83	0.60
1:E:5292:GLU:O	1:E:5296:GLU:HG3	2.02	0.60



	t i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:6083:TYR:CE2	1:F:6108:ILE:HD13	2.37	0.60
1:G:1308:LEU:HD21	1:G:1367:PRO:CG	2.32	0.60
1:K:5487:GLU:O	1:K:5491:ARG:HG3	2.02	0.60
1:L:6086:MET:HG3	1:L:6112:LEU:HD23	1.82	0.60
1:L:6174:ILE:HG13	4:L:7009:HOH:O	2.01	0.60
1:E:5487:GLU:O	1:E:5491:ARG:HG3	2.01	0.60
1:I:3284:HIS:O	1:I:3288:GLN:HG2	2.02	0.60
1:I:3395:LEU:HB3	1:I:3550:LEU:HD11	1.84	0.60
1:H:2257:LYS:HE3	1:H:2316:GLN:HE22	1.66	0.60
1:I:3352:LYS:HG3	1:I:3353:GLN:HG3	1.82	0.60
1:J:4468:HIS:CD2	3:J:4:NLX:H21	2.36	0.60
1:K:5341:PHE:HD2	1:K:5341:PHE:H	1.50	0.60
1:L:6538:LYS:HB3	1:L:6541:ASP:HB2	1.82	0.60
1:C:3332:PRO:O	1:C:3336:GLN:HG3	2.02	0.60
1:H:2536:ALA:O	1:H:2537:GLN:HG3	2.01	0.60
1:L:6086:MET:CE	1:L:6110:LEU:HB2	2.31	0.60
1:L:6324:ASP:OD1	1:L:6326:MET:HB2	2.02	0.60
1:L:6409:ASP:HB3	1:L:6412:LYS:HB2	1.82	0.60
1:B:2402:LYS:HG2	1:B:2546:PHE:CE1	2.37	0.60
1:F:6136:MET:HB3	1:F:6218:PHE:CE1	2.37	0.60
1:F:6351:ASN:HB3	1:F:6466:GLY:O	2.02	0.60
1:I:3464:VAL:CG2	1:J:4370:GLU:HG3	2.32	0.60
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.37	0.59
1:B:2216:THR:HG23	1:B:2242:ARG:CB	2.32	0.59
1:B:2255:LEU:HD23	1:B:2318:LEU:CD1	2.33	0.59
1:D:4025:VAL:HG22	1:D:4034:LEU:HD23	1.82	0.59
1:E:5104:ARG:HD2	4:E:7316:HOH:O	2.01	0.59
1:F:6029:VAL:HG13	4:F:7744:HOH:O	2.02	0.59
1:K:5091:PRO:HG3	1:K:5112:LEU:HD21	1.84	0.59
1:L:6262:LYS:HB3	1:L:6263:PRO:HD3	1.82	0.59
1:L:6145:MET:HE1	1:L:6303:PHE:CD1	2.38	0.59
1:F:6186:ARG:HD3	1:F:6324:ASP:O	2.02	0.59
1:F:6220:GLU:HA	1:F:6246:GLU:O	2.03	0.59
1:I:3180:THR:HG23	1:I:3185:SER:HB3	1.84	0.59
1:J:4134:PRO:HG2	1:J:4163:VAL:HG12	1.83	0.59
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.84	0.59
1:A:1477:GLY:HA2	1:A:1493:SER:OG	2.03	0.59
1:B:2317:PRO:HB2	3:B:2:NLX:C19	2.31	0.59
1:H:2370:GLU:C	1:H:2372:GLN:H	2.03	0.59
1:I:3064:ARG:HD3	1:I:3065:PHE:CZ	2.37	0.59
1:I:3538:LYS:HE2	1:I:3541:ASP:OD1	2.02	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:L:6493:SER:O	1:L:6497:MET:HG3	2.01	0.59
1:B:2104:ARG:HG2	1:B:2104:ARG:NH1	2.17	0.59
1:B:2512:GLU:HB3	4:B:7018:HOH:O	2.01	0.59
1:D:4260:ASP:OD1	1:D:4262:LYS:HB3	2.01	0.59
1:E:5396:ILE:HB	1:E:5397:PRO:HD3	1.84	0.59
1:H:2379:MET:HG2	1:H:2396:ILE:HG22	1.83	0.59
1:E:5125:ALA:HB1	1:E:5131:ASN:HD22	1.66	0.59
1:E:5375:GLN:NE2	1:E:5400:THR:HG22	2.18	0.59
1:A:1381:LEU:HD21	1:F:6459:MET:HB3	1.85	0.59
1:I:3462:LYS:NZ	1:J:4376:LYS:NZ	2.50	0.59
1:K:5119:LEU:O	1:K:5119:LEU:HD12	2.02	0.59
1:L:6048:ALA:HB3	1:L:6123:THR:HG23	1.85	0.59
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.65	0.59
1:F:6149:ALA:HB2	1:F:6169:GLN:HG3	1.84	0.59
1:I:3478:ALA:N	1:I:3479:PRO:CD	2.66	0.59
1:J:4027:ASP:OD1	1:J:4032:LYS:HD3	2.03	0.59
1:K:5395:LEU:HD21	1:K:5553:LYS:HB2	1.83	0.59
1:L:6233:SER:O	1:L:6342:HIS:NE2	2.34	0.59
1:A:1372:GLN:C	1:A:1373:LEU:HD12	2.23	0.59
1:C:3251:LEU:HD12	1:C:3433:VAL:HG23	1.83	0.59
1:D:4038:VAL:HG21	1:D:4049:ILE:HD12	1.85	0.59
1:I:3526:TYR:CE2	1:I:3539:LEU:HB2	2.37	0.59
1:L:6420:LEU:CD1	1:L:6547:TRP:CZ2	2.85	0.59
1:A:1372:GLN:HE21	1:A:1410:THR:HG21	1.67	0.59
1:B:2174:ILE:HG13	1:B:2298:THR:HG22	1.85	0.59
1:F:6135:VAL:HG21	1:F:6205:ILE:HG12	1.85	0.59
1:F:6242:ARG:NH1	1:F:6242:ARG:HG2	2.15	0.59
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.18	0.59
1:B:2348:VAL:O	1:B:2446:MET:HA	2.02	0.59
1:D:4421:ILE:HG22	1:D:4425:MET:CE	2.33	0.58
1:F:6550:LEU:O	1:F:6553:LYS:HB2	2.03	0.58
1:H:2456:SER:HB2	1:H:2460:LYS:HD3	1.85	0.58
1:J:4304:LEU:HB3	3:J:4:NLX:H203	1.85	0.58
1:K:5447:TYR:HA	1:K:5527:LEU:O	2.03	0.58
1:L:6105:LYS:HD3	1:L:6106:GLU:CG	2.33	0.58
1:A:1309:GLN:NE2	1:A:1310:GLY:N	2.51	0.58
1:C:3456:SER:HB3	1:C:3460:LYS:HD3	1.85	0.58
3:C:3:NLX:C10	3:C:3:NLX:C20	2.82	0.58
1:G:1313:ARG:HG3	1:G:1313:ARG:HH11	1.67	0.58
1:K:5339:ARG:O	1:K:5339:ARG:HG3	2.02	0.58
1:E:5491:ARG:HD2	4:E:7007:HOH:O	2.03	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:F:6132:ARG:HB3	1:F:6211:ASN:HB2	1.85	0.58
1:G:1218:PHE:HB3	1:G:1244:ILE:HB	1.84	0.58
1:H:2143:GLY:HA3	3:H:2:NLX:H152	1.85	0.58
1:K:5264:LEU:HD13	1:K:5316:GLN:HG3	1.84	0.58
1:G:1339:ARG:HH12	1:G:1436:ASN:HD22	1.50	0.58
1:I:3132:ARG:HB3	1:I:3211:ASN:HB2	1.86	0.58
1:I:3218:PHE:H	1:I:3218:PHE:HD1	1.50	0.58
1:I:3501:ALA:O	1:I:3505:ARG:HG2	2.04	0.58
1:C:3296:GLU:O	1:C:3300:LYS:HG3	2.04	0.58
1:C:3309:GLN:HG3	1:D:4096:LEU:HD13	1.83	0.58
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	1.86	0.58
1:E:5048:ALA:HB3	1:E:5123:THR:HG23	1.84	0.58
1:G:1379:MET:SD	1:G:1397:PRO:HG3	2.44	0.58
1:K:5026:VAL:HG12	1:K:5027:ASP:N	2.17	0.58
1:K:5389:VAL:O	1:K:5390:CYS:HB2	2.03	0.58
1:L:6375:GLN:HE21	1:L:6400:THR:HG22	1.68	0.58
1:B:2528:GLN:O	1:B:2533:THR:HA	2.04	0.58
1:F:6215:VAL:N	1:F:6241:HIS:HD2	1.99	0.58
1:J:4348:VAL:O	1:J:4446:MET:HA	2.04	0.58
1:D:4104:ARG:HD2	4:D:7709:HOH:O	2.01	0.58
1:D:4249:VAL:HB	1:D:4433:VAL:HG21	1.85	0.58
1:J:4220:GLU:HG3	1:J:4472:LEU:HD21	1.86	0.58
1:L:6264:LEU:HD22	1:L:6268:ILE:CD1	2.33	0.58
1:B:2390:CYS:HB3	4:B:7626:HOH:O	2.02	0.58
1:B:2359:ILE:CG1	3:B:2:NLX:H71	2.30	0.58
1:D:4262:LYS:HB3	1:D:4263:PRO:HD3	1.85	0.58
1:F:6334:GLU:O	1:F:6338:GLU:HG3	2.04	0.58
1:G:1435:ARG:O	1:G:1438:ARG:HB3	2.04	0.58
1:L:6026:VAL:CG1	1:L:6207:SER:HB3	2.34	0.58
1:L:6527:LEU:HD11	1:L:6533:THR:HG22	1.85	0.58
1:A:1319:LEU:HD12	1:A:1319:LEU:N	2.18	0.58
1:B:2040:LEU:HD13	1:B:2155:LEU:CD1	2.33	0.58
1:I:3318:LEU:HB2	4:I:7480:HOH:O	2.04	0.58
1:K:5133:LEU:HD22	1:K:5162:ASN:O	2.04	0.58
1:L:6104:ARG:NH1	1:L:6104:ARG:HG2	2.19	0.58
1:F:6306:LEU:HD21	1:F:6384:LYS:O	2.04	0.58
1:G:1252:THR:O	1:G:1254:VAL:N	2.36	0.58
1:J:4126:ASP:OD1	1:J:4128:THR:HG23	2.04	0.58
1:J:4333:GLU:CD	1:J:4333:GLU:H	2.07	0.58
1:L:6223:GLY:O	1:L:6227:VAL:HG23	2.04	0.58
1:C:3257:LYS:HE3	1:C:3322:VAL:CG1	2.33	0.57



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:F:6373:LEU:HD23	1:F:6414:LYS:HA	1.85	0.57
1:F:6435:ARG:O	1:F:6438:ARG:HB3	2.04	0.57
1:I:3456:SER:HB3	1:I:3460:LYS:HD3	1.84	0.57
1:J:4034:LEU:HD11	2:J:479:NAG:H82	1.86	0.57
1:A:1342:HIS:CD2	1:A:1342:HIS:N	2.70	0.57
1:C:3220:GLU:OE2	1:C:3221:SER:HB2	2.04	0.57
1:C:3318:LEU:HD21	3:C:3:NLX:H162	1.85	0.57
1:D:4301:MET:HG3	1:D:4303:PHE:CZ	2.39	0.57
1:B:2241:HIS:C	1:B:2242:ARG:HD2	2.24	0.57
1:E:5142:GLY:HA3	1:E:5146:VAL:O	2.04	0.57
1:E:5411:VAL:HA	4:E:7302:HOH:O	2.03	0.57
1:G:1308:LEU:HD21	1:G:1367:PRO:HG2	1.86	0.57
1:G:1521:ASN:HB2	1:G:1522:GLN:NE2	2.19	0.57
1:H:2372:GLN:NE2	1:H:2410:THR:OG1	2.37	0.57
1:J:4331:THR:HB	1:J:4333:GLU:OE1	2.04	0.57
1:K:5025:VAL:HG22	1:K:5034:LEU:HD23	1.86	0.57
1:L:6140:HIS:HD2	1:L:6141:GLY:O	1.87	0.57
1:D:4363:LEU:HD22	3:D:4:NLX:H102	1.86	0.57
1:G:1104:ARG:CB	1:G:1104:ARG:HH11	2.17	0.57
1:I:3364:MET:HG2	3:I:3:NLX:H201	1.85	0.57
1:I:3453:PRO:HD2	1:I:3470:ASP:OD2	2.04	0.57
1:J:4142:GLY:C	3:J:4:NLX:H152	2.24	0.57
1:J:4140:HIS:CD2	1:J:4147:GLY:HA3	2.40	0.57
1:J:4306:LEU:HD22	1:J:4366:TYR:CE1	2.39	0.57
1:K:5428:VAL:HG13	1:K:5544:VAL:HA	1.86	0.57
1:A:1227:VAL:O	1:A:1231:VAL:HG23	2.04	0.57
1:D:4456:SER:HB3	1:D:4460:LYS:HD3	1.87	0.57
1:H:2215:VAL:H	1:H:2241:HIS:CD2	2.18	0.57
1:J:4493:SER:HB2	4:J:7677:HOH:O	2.04	0.57
1:B:2371:GLY:CA	1:B:2414:LYS:HD3	2.34	0.57
1:C:3412:LYS:O	1:C:3416:LEU:HG	2.05	0.57
1:E:5262:LYS:HE2	1:E:5279:SER:OG	2.03	0.57
1:F:6024:PRO:HG3	1:F:6037:PHE:CZ	2.40	0.57
1:F:6095:GLN:O	1:F:6099:GLU:HG3	2.05	0.57
1:G:1064:ARG:HH11	1:G:1294:LEU:HD11	1.70	0.57
1:L:6420:LEU:HD13	1:L:6547:TRP:HZ2	1.69	0.57
1:H:2371:GLY:CA	1:H:2414:LYS:HD3	2.35	0.57
1:H:2426:PHE:C	1:H:2429:PRO:HD2	2.24	0.57
1:J:4232:LEU:HD23	1:J:4341:PHE:HB3	1.86	0.57
1:A:1358:LEU:HG	1:A:1363:LEU:HD12	1.85	0.57
1:E:5372:GLN:HA	4:E:7302:HOH:O	2.04	0.57



	at pagetti	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:F:6348:VAL:O	1:F:6446:MET:HA	2.04	0.57
1:C:3437:HIS:HD2	1:C:3444:THR:OG1	1.87	0.57
1:G:1371:GLY:O	1:G:1414:LYS:HD3	2.05	0.57
1:J:4349:GLY:HA3	1:J:4447:TYR:CZ	2.40	0.57
1:A:1140:HIS:HE1	4:A:7108:HOH:O	1.87	0.57
1:B:2220:GLU:OE2	1:B:2472:LEU:HD11	2.05	0.57
1:G:1527:LEU:HD11	1:G:1533:THR:HG22	1.87	0.57
1:L:6104:ARG:NE	1:L:6108:ILE:HD12	2.18	0.57
1:F:6467:ASP:N	1:F:6470:ASP:OD2	2.38	0.56
1:A:1132:ARG:HB3	1:A:1211:ASN:HB2	1.86	0.56
1:I:3229:VAL:HG13	1:I:3328:LEU:HD21	1.86	0.56
1:J:4404:LEU:N	1:J:4404:LEU:HD23	2.21	0.56
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.53	0.56
1:C:3138:TRP:CZ3	1:C:3219:GLY:HA2	2.39	0.56
1:C:3324:ASP:OD2	1:C:3327:LEU:HB3	2.05	0.56
1:D:4309:GLN:NE2	1:D:4309:GLN:C	2.59	0.56
1:E:5386:TYR:N	1:E:5387:PRO:HD2	2.20	0.56
1:F:6359:ILE:HG23	3:F:6:NLX:H152	1.87	0.56
1:K:5138:TRP:CZ3	1:K:5219:GLY:HA2	2.40	0.56
1:C:3401:GLU:OE2	1:C:3405:GLY:HA3	2.04	0.56
1:E:5190:GLY:O	1:E:5194:GLN:HG3	2.05	0.56
1:H:2396:ILE:HB	1:H:2397:PRO:HD3	1.86	0.56
1:I:3242:ARG:NH1	1:I:3242:ARG:HG2	2.20	0.56
1:I:3447:TYR:C	1:I:3447:TYR:CD2	2.78	0.56
1:K:5249:VAL:HB	1:K:5433:VAL:HG21	1.86	0.56
1:B:2132:ARG:HB3	1:B:2211:ASN:HB2	1.87	0.56
1:D:4335:LEU:O	1:D:4340:ASN:ND2	2.24	0.56
1:F:6350:ILE:C	1:F:6351:ASN:HD22	2.07	0.56
1:J:4215:VAL:N	1:J:4241:HIS:HD2	2.03	0.56
1:A:1304:LEU:CB	3:A:1:NLX:H203	2.34	0.56
1:E:5447:TYR:HA	1:E:5527:LEU:O	2.05	0.56
3:E:5:NLX:O4	3:E:5:NLX:H203	2.06	0.56
1:F:6359:ILE:HG12	3:F:6:NLX:H162	1.86	0.56
1:H:2370:GLU:HG3	1:K:5461:PRO:CG	2.35	0.56
1:I:3396:ILE:HB	1:I:3397:PRO:HD3	1.88	0.56
1:L:6357:TRP:O	1:L:6360:PRO:HD2	2.05	0.56
1:C:3237:LYS:HE2	1:C:3238:ASN:HD21	1.70	0.56
1:C:3332:PRO:HB2	1:C:3333:GLU:OE1	2.06	0.56
1:D:4057:LYS:HB3	1:D:4069:GLN:HB2	1.88	0.56
1:D:4311:ASP:HB3	1:D:4314:GLU:HG3	1.86	0.56
1:H:2304:LEU:HD13	3:H:2:NLX:H162	1.87	0.56


	at pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:4223:GLY:O	1:J:4226:SER:HB2	2.06	0.56
1:K:5125:ALA:HB2	1:K:5133:LEU:CD1	2.36	0.56
1:L:6054:PRO:HG3	1:L:6078:LYS:HE2	1.86	0.56
1:A:1236:ALA:HA	1:A:1239:LEU:HD12	1.87	0.56
1:A:1456:SER:HB3	1:A:1460:LYS:HD3	1.87	0.56
1:B:2218:PHE:CB	1:B:2244:ILE:HB	2.35	0.56
1:C:3234:PRO:O	1:C:3237:LYS:HG2	2.05	0.56
1:C:3532:ASN:HB3	1:C:3534:GLN:HE21	1.71	0.56
1:C:3359:ILE:HG23	3:C:3:NLX:H101	1.87	0.56
1:G:1104:ARG:HB3	1:G:1104:ARG:NH1	2.21	0.56
1:I:3462:LYS:HZ3	1:J:4376:LYS:HZ3	1.51	0.56
1:J:4107:ASN:HD22	1:J:4108:ILE:H	1.53	0.56
1:C:3144:LEU:HD13	1:C:3177:PHE:CE1	2.41	0.56
1:C:3350:ILE:O	1:C:3448:GLU:HA	2.06	0.56
1:G:1332:PRO:O	1:G:1336:GLN:HG2	2.05	0.56
1:I:3353:GLN:O	1:I:3467:ASP:HA	2.05	0.56
1:K:5039:SER:HB3	1:K:5046:PRO:HG3	1.87	0.56
1:B:2404:LEU:N	1:B:2404:LEU:HD23	2.21	0.56
1:C:3423:ASP:OD1	1:C:3540:LYS:HE3	2.06	0.56
1:D:4101:PHE:CZ	3:D:4:NLX:H21	2.41	0.56
1:G:1145:MET:CB	1:G:1304:LEU:HD21	2.36	0.56
1:L:6220:GLU:OE2	1:L:6221:SER:HB2	2.06	0.56
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.36	0.56
1:J:4135:VAL:HB	1:J:4215:VAL:HG22	1.88	0.56
1:J:4371:GLY:O	1:J:4414:LYS:HD3	2.06	0.56
1:K:5355:PHE:HB2	1:K:5422:ALA:HB2	1.88	0.56
1:L:6093:ALA:HB1	3:L:6:NLX:H192	1.87	0.56
1:A:1027:ASP:OD2	1:A:1032:LYS:HG2	2.04	0.55
1:K:5256:VAL:O	1:K:5258:LYS:HE3	2.06	0.55
1:L:6257:LYS:HB2	1:L:6322:VAL:HG12	1.88	0.55
1:C:3237:LYS:HE2	1:C:3238:ASN:ND2	2.21	0.55
1:I:3369:SER:HA	1:J:4368:LEU:O	2.06	0.55
1:A:1333:GLU:O	1:A:1337:ALA:HB2	2.06	0.55
1:B:2216:THR:HG23	1:B:2242:ARG:HB2	1.88	0.55
1:G:1097:LEU:HD11	1:G:1101:PHE:CE2	2.41	0.55
1:B:2297:THR:O	1:B:2301:MET:HG2	2.06	0.55
1:I:3088:THR:CG2	1:I:3295:LEU:HD13	2.35	0.55
1:I:3257:LYS:HE2	1:I:3316:GLN:NE2	2.21	0.55
1:I:3353:GLN:HE22	1:I:3465:ILE:H	1.54	0.55
1:K:5122:TYR:HE2	4:K:7094:HOH:O	1.88	0.55
1:L:6271:THR:CG2	1:L:6297:THR:HG23	2.35	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:L:6428:VAL:O	1:L:6432:ILE:HG13	2.06	0.55
1:L:6456:SER:HB3	1:L:6460:LYS:HD3	1.89	0.55
1:A:1363:LEU:HB3	3:A:1:NLX:H91	1.87	0.55
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.88	0.55
1:C:3434:ALA:HB2	1:C:3446:MET:HE3	1.88	0.55
1:E:5309:GLN:HG2	1:E:5310:GLY:N	2.20	0.55
1:H:2318:LEU:HD12	1:H:2318:LEU:C	2.25	0.55
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.89	0.55
1:C:3318:LEU:HD11	3:C:3:NLX:C15	2.32	0.55
1:F:6268:ILE:HG12	1:F:6301:MET:HE2	1.88	0.55
1:H:2486:SER:O	1:H:2490:ILE:HG13	2.07	0.55
1:A:1392:ALA:O	1:A:1396:ILE:HG12	2.07	0.55
1:B:2468:HIS:CD2	3:B:2:NLX:O3	2.60	0.55
1:F:6447:TYR:HB3	1:F:6517:TRP:CZ2	2.41	0.55
1:H:2423:ASP:OD2	1:H:2543:GLU:HG2	2.07	0.55
1:I:3447:TYR:HB3	1:I:3517:TRP:HZ2	1.71	0.55
1:J:4237:LYS:HG2	1:J:4238:ASN:ND2	2.22	0.55
1:J:4343:THR:HB	1:J:4442:ALA:HB2	1.89	0.55
1:K:5234:PRO:O	1:K:5237:LYS:HG2	2.06	0.55
1:B:2262:LYS:O	1:B:2266:GLU:HG3	2.07	0.55
1:I:3095:GLN:HG2	1:J:4309:GLN:OE1	2.07	0.55
1:J:4304:LEU:CG	3:J:4:NLX:H203	2.34	0.55
1:L:6099:GLU:HG3	1:L:6107:ASN:OD1	2.07	0.55
1:L:6142:GLY:HA2	3:L:6:NLX:C8	2.36	0.55
1:A:1221:SER:HA	1:A:1247:SER:O	2.07	0.55
1:D:4478:ALA:N	1:D:4479:PRO:CD	2.70	0.55
1:I:3173:GLY:HA3	4:I:7644:HOH:O	2.06	0.55
1:L:6144:LEU:HB3	1:L:6177:PHE:CE2	2.41	0.55
1:B:2130:LYS:HE3	1:B:2132:ARG:HG2	1.89	0.55
1:B:2180:THR:HG23	1:B:2185:SER:HB3	1.89	0.55
1:G:1197:ALA:O	1:G:1201:VAL:HG23	2.07	0.55
1:G:1313:ARG:HA	1:G:1386:TYR:CD2	2.42	0.55
1:G:1383:TRP:CH2	1:G:1393:LYS:HB2	2.41	0.55
1:H:2024:PRO:HD3	1:H:2037:PHE:CD1	2.41	0.55
1:I:3249:VAL:HG23	1:I:3251:LEU:H	1.72	0.55
1:J:4331:THR:OG1	1:J:4334:GLU:HG3	2.07	0.55
1:E:5437:HIS:HD2	1:E:5444:THR:OG1	1.90	0.54
1:F:6371:GLY:O	1:F:6414:LYS:HG2	2.06	0.54
1:G:1392:ALA:HB3	1:G:1395:LEU:HG	1.89	0.54
1:J:4478:ALA:N	1:J:4479:PRO:CD	2.70	0.54
1:K:5220:GLU:HG2	1:K:5472:LEU:HD21	1.90	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2354:GLU:HB2	1:B:2422:ALA:HB1	1.89	0.54
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.70	0.54
1:C:3447:TYR:C	1:C:3447:TYR:CD2	2.79	0.54
1:H:2222:ALA:CB	4:H:7211:HOH:O	2.55	0.54
1:H:2223:GLY:O	1:H:2227:VAL:HG23	2.07	0.54
1:H:2258:LYS:H	1:H:2258:LYS:HD2	1.70	0.54
1:D:4145:MET:HG3	1:D:4304:LEU:CD1	2.37	0.54
1:D:4318:LEU:C	1:D:4318:LEU:HD12	2.28	0.54
1:F:6104:ARG:O	1:F:6482:LYS:HE3	2.07	0.54
1:G:1323:ILE:HG13	1:G:1331:THR:HG22	1.89	0.54
1:L:6524:GLU:OE2	1:L:6538:LYS:HG2	2.06	0.54
1:D:4265:ALA:HB1	1:D:4282:MET:HE1	1.89	0.54
1:G:1086:MET:HE2	1:G:1148:ALA:HB2	1.90	0.54
1:I:3119:LEU:HD12	1:I:3119:LEU:O	2.06	0.54
1:K:5022:SER:N	4:K:7180:HOH:O	2.40	0.54
1:C:3329:LEU:HG	4:C:7056:HOH:O	2.06	0.54
1:E:5313:ARG:HG2	1:E:5386:TYR:CE2	2.43	0.54
1:F:6512:GLU:H	1:F:6512:GLU:CD	2.11	0.54
1:G:1313:ARG:HG2	1:G:1386:TYR:CE2	2.42	0.54
1:K:5112:LEU:N	1:K:5112:LEU:HD12	2.23	0.54
1:E:5105:LYS:HE2	1:E:5483:GLU:HG3	1.88	0.54
1:I:3491:ARG:HB3	1:I:3491:ARG:NH1	2.22	0.54
1:K:5149:ALA:CB	1:K:5169:GLN:HG3	2.38	0.54
1:K:5221:SER:O	1:K:5225:GLU:N	2.37	0.54
1:K:5505:ARG:NH1	4:K:7766:HOH:O	2.40	0.54
1:L:6395:LEU:HD22	1:L:6550:LEU:CD1	2.37	0.54
1:B:2237:LYS:HB2	4:B:7015:HOH:O	2.07	0.54
1:D:4244:ILE:HG12	1:D:4347:MET:HB3	1.90	0.54
1:I:3243:ALA:O	1:I:3346:TYR:HA	2.07	0.54
1:J:4420:LEU:CD1	1:J:4547:TRP:HZ2	2.21	0.54
1:K:5079:ASN:ND2	2:K:579:NAG:C1	2.71	0.54
1:A:1333:GLU:CD	1:A:1333:GLU:H	2.11	0.54
1:C:3089:GLN:OE1	1:C:3146:VAL:HB	2.07	0.54
1:D:4124:PRO:HD3	1:D:4158:ALA:HB1	1.89	0.54
1:D:4215:VAL:H	1:D:4241:HIS:CD2	2.07	0.54
1:E:5333:GLU:OE1	1:E:5333:GLU:N	2.33	0.54
1:F:6540:LYS:HA	1:F:6543:GLU:OE1	2.08	0.54
1:H:2363:LEU:CD1	3:H:2:NLX:H101	2.36	0.54
1:I:3278:THR:OG1	1:I:3281:VAL:HG23	2.07	0.54
1:L:6105:LYS:CD	1:L:6106:GLU:HG3	2.37	0.54
1:G:1304:LEU:CD1	1:G:1318:LEU:HB3	2.38	0.54



	A + 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:H:2316:GLN:OE1	1:H:2317:PRO:HD2	2.07	0.54
1:F:6264:LEU:O	1:F:6264:LEU:HD22	2.07	0.54
1:F:6257:LYS:HB2	1:F:6322:VAL:HG12	1.90	0.54
1:H:2420:LEU:HD12	1:H:2547:TRP:HZ2	1.73	0.54
1:I:3218:PHE:HB3	1:I:3244:ILE:HB	1.90	0.54
1:I:3420:LEU:HD13	1:I:3547:TRP:CZ2	2.43	0.54
1:J:4456:SER:HB3	1:J:4460:LYS:HD3	1.90	0.54
1:A:1131:ASN:O	1:A:1132:ARG:HG2	2.07	0.53
1:A:1134:PRO:CG	1:A:1163:VAL:HG12	2.32	0.53
1:A:1079:ASN:HD22	2:A:179:NAG:H2	1.74	0.53
1:C:3404:LEU:O	1:C:3406:GLY:N	2.41	0.53
1:K:5394:GLU:HG3	1:K:5395:LEU:HG	1.91	0.53
1:L:6177:PHE:HB2	1:L:6319:LEU:HD22	1.90	0.53
1:A:1318:LEU:O	1:A:1318:LEU:HD12	2.08	0.53
1:C:3404:LEU:C	1:C:3406:GLY:H	2.11	0.53
1:D:4091:PRO:HB3	1:D:4112:LEU:HD11	1.90	0.53
1:D:4386:TYR:N	1:D:4387:PRO:HD2	2.23	0.53
1:H:2456:SER:HB2	1:H:2460:LYS:CD	2.39	0.53
1:I:3428:VAL:O	1:I:3432:ILE:HG13	2.08	0.53
1:J:4264:LEU:CD1	1:J:4316:GLN:HG2	2.38	0.53
1:G:1092:LYS:HZ1	1:L:6302:LYS:HB2	1.73	0.53
1:C:3370:GLU:HG3	1:D:4461:PRO:CG	2.39	0.53
1:D:4132:ARG:HB3	1:D:4211:ASN:HB2	1.91	0.53
1:E:5252:THR:HG22	1:E:5252:THR:O	2.08	0.53
1:G:1435:ARG:HH12	1:G:1544:VAL:HG11	1.73	0.53
1:H:2540:LYS:O	1:H:2544:VAL:HG23	2.09	0.53
1:K:5357:TRP:O	1:K:5361:MET:HB2	2.08	0.53
1:L:6358:LEU:HG	1:L:6363:LEU:CD1	2.38	0.53
1:A:1260:ASP:OD2	1:A:1263:PRO:HD3	2.08	0.53
1:F:6271:THR:HG22	1:F:6297:THR:HG23	1.90	0.53
1:G:1026:VAL:CG1	1:G:1027:ASP:N	2.71	0.53
1:G:1132:ARG:HB3	1:G:1211:ASN:HB2	1.89	0.53
1:H:2104:ARG:HG2	1:H:2104:ARG:HH11	1.73	0.53
1:H:2216:THR:HG23	1:H:2242:ARG:HB2	1.90	0.53
1:I:3217:ILE:CD1	1:I:3227:VAL:HG13	2.38	0.53
1:L:6359:ILE:HD11	1:L:6468:HIS:ND1	2.23	0.53
1:E:5126:ASP:H	1:E:5131:ASN:ND2	2.07	0.53
1:E:5355:PHE:HD1	1:E:5418:LEU:HD22	1.73	0.53
1:E:5480:PHE:HZ	1:E:5494:LYS:HG2	1.72	0.53
1:G:1303:PHE:HB2	4:G:7512:HOH:O	2.07	0.53
1:L:6130:LYS:H	1:L:6130:LYS:HE3	1.74	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1392:ALA:HB1	1:A:1394:GLU:OE2	2.08	0.53
1:B:2112:LEU:O	1:B:2113:SER:HB2	2.07	0.53
1:D:4131:ASN:O	1:D:4132:ARG:NH1	2.42	0.53
1:D:4251:LEU:CD2	1:D:4333:GLU:HG3	2.39	0.53
1:F:6537:GLN:O	1:F:6538:LYS:HB2	2.08	0.53
1:I:3343:THR:HG22	1:I:3442:ALA:HB2	1.91	0.53
1:I:3462:LYS:HZ3	1:J:4376:LYS:NZ	2.05	0.53
1:L:6251:LEU:CD2	1:L:6333:GLU:HG3	2.38	0.53
1:A:1289:LYS:HA	1:A:1293:GLU:OE2	2.08	0.53
1:A:1539:LEU:HG	1:A:1540:LYS:HG2	1.89	0.53
1:B:2095:GLN:O	1:B:2099:GLU:HG3	2.08	0.53
1:B:2083:TYR:CZ	1:B:2108:ILE:HD13	2.43	0.53
1:B:2318:LEU:HG	3:B:2:NLX:C17	2.36	0.53
1:D:4353:GLN:O	1:D:4467:ASP:HA	2.09	0.53
1:G:1552:ALA:O	1:G:1553:LYS:HB2	2.07	0.53
1:B:2043:PHE:HB3	4:B:7515:HOH:O	2.08	0.53
1:B:2452:ARG:HD2	1:B:2464:VAL:O	2.08	0.53
1:E:5098:SER:O	1:E:5102:THR:HB	2.09	0.53
1:F:6026:VAL:CG1	1:F:6207:SER:HB3	2.39	0.53
1:F:6097:LEU:HB2	3:F:6:NLX:C19	2.39	0.53
1:G:1349:GLY:HA3	1:G:1447:TYR:CE1	2.43	0.53
1:G:1404:LEU:HB3	1:G:1413:LYS:CG	2.39	0.53
1:H:2355:PHE:CE1	1:H:2360:PRO:HB3	2.43	0.53
1:L:6324:ASP:OD1	1:L:6326:MET:N	2.39	0.53
1:A:1086:MET:CE	1:A:1110:LEU:HB2	2.39	0.53
1:C:3364:MET:CE	3:C:3:NLX:C18	2.73	0.53
1:C:3302:LYS:HD2	1:D:4092:LYS:HD3	1.90	0.53
1:I:3357:TRP:O	1:I:3360:PRO:HD2	2.09	0.53
1:I:3348:VAL:O	1:I:3446:MET:HA	2.08	0.53
1:J:4313:ARG:HD3	1:J:4383:TRP:HH2	1.74	0.53
1:L:6417:PHE:O	1:L:6420:LEU:HB3	2.08	0.53
1:C:3382:LEU:HD11	1:C:3420:LEU:HD11	1.90	0.53
1:G:1086:MET:HE3	1:G:1110:LEU:HD12	1.90	0.53
1:G:1304:LEU:HD11	1:G:1318:LEU:HD23	1.89	0.53
1:H:2306:LEU:HD22	1:H:2366:TYR:CE1	2.44	0.53
1:I:3355:PHE:CE1	1:I:3360:PRO:HG3	2.44	0.53
1:I:3429:PRO:O	1:I:3433:VAL:HG23	2.08	0.53
1:L:6235:LEU:HD12	1:L:6327:LEU:CD1	2.32	0.53
1:B:2149:ALA:CB	1:B:2169:GLN:HG3	2.39	0.52
3:D:4:NLX:O2	4:D:7001:HOH:O	2.19	0.52
1:E:5140:HIS:CD2	1:E:5147:GLY:HA3	2.44	0.52



	at pagetti	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:5308:LEU:HD21	1:E:5367:PRO:HG2	1.90	0.52
1:F:6359:ILE:HA	3:F:6:NLX:H162	1.91	0.52
1:G:1026:VAL:HG12	1:G:1027:ASP:N	2.24	0.52
1:H:2350:ILE:HD12	1:H:2350:ILE:O	2.09	0.52
3:H:2:NLX:H203	3:H:2:NLX:O4	2.09	0.52
1:J:4132:ARG:HH12	1:J:4206:ALA:HB2	1.73	0.52
1:K:5342:HIS:HA	4:K:7948:HOH:O	2.08	0.52
1:C:3092:LYS:CD	1:D:4302:LYS:HD2	2.39	0.52
1:D:4266:GLU:O	1:D:4270:ILE:HG13	2.08	0.52
1:E:5313:ARG:HA	1:E:5386:TYR:CD2	2.45	0.52
1:H:2024:PRO:HD3	1:H:2037:PHE:CE1	2.45	0.52
1:H:2107:ASN:ND2	1:H:2108:ILE:H	2.07	0.52
1:I:3250:ALA:O	1:I:3256:VAL:HG21	2.08	0.52
1:B:2103:ASN:ND2	1:B:2481:LEU:HD12	2.24	0.52
1:G:1218:PHE:HB2	1:G:1244:ILE:HB	1.91	0.52
1:H:2097:LEU:HD11	1:H:2101:PHE:CE2	2.45	0.52
1:I:3386:TYR:O	1:I:3390:CYS:N	2.40	0.52
1:K:5465:ILE:N	1:K:5465:ILE:HD12	2.24	0.52
1:C:3024:PRO:HG3	1:C:3037:PHE:CZ	2.45	0.52
1:A:1278:THR:HG21	1:C:3115:ASP:OD2	2.10	0.52
1:C:3286:LEU:HA	1:C:3289:LYS:HG2	1.92	0.52
1:E:5348:VAL:O	1:E:5446:MET:HA	2.09	0.52
1:F:6258:LYS:CE	1:F:6258:LYS:H	2.21	0.52
1:G:1348:VAL:O	1:G:1446:MET:HA	2.10	0.52
1:H:2260:ASP:OD1	1:H:2263:PRO:HD3	2.10	0.52
1:K:5370:GLU:O	1:K:5372:GLN:HG3	2.10	0.52
1:L:6023:PRO:HB2	1:L:6034:LEU:CD2	2.38	0.52
1:D:4089:GLN:OE1	1:D:4146:VAL:HB	2.10	0.52
1:E:5140:HIS:HD2	1:E:5141:GLY:O	1.92	0.52
1:G:1452:ARG:HG2	1:G:1452:ARG:NH1	2.24	0.52
1:G:1221:SER:HB2	3:G:1:NLX:O1	2.10	0.52
1:H:2228:SER:CB	1:H:2250:ALA:H	2.23	0.52
1:H:2370:GLU:C	1:H:2372:GLN:N	2.63	0.52
1:K:5246:GLU:O	1:K:5247:SER:HB2	2.10	0.52
1:L:6526:TYR:HE1	1:L:6528:GLN:HG2	1.74	0.52
1:L:6533:THR:O	1:L:6534:GLN:HG3	2.10	0.52
1:E:5404:LEU:CD2	1:E:5416:LEU:HB2	2.40	0.52
1:E:5538:LYS:O	1:E:5541:ASP:HB2	2.08	0.52
1:I:3026:VAL:HG12	1:I:3027:ASP:N	2.24	0.52
1:I:3152:TYR:CD1	1:I:3152:TYR:N	2.77	0.52
1:I:3432:ILE:O	1:I:3435:ARG:HB2	2.09	0.52



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	overlap (Å)
1:J:4482:LYS:HE2	4:J:7544:HOH:O	2.07	0.52
1:K:5223:GLY:O	1:K:5227:VAL:HG23	2.10	0.52
1:L:6225:GLU:HG3	1:L:6255:LEU:HD13	1.91	0.52
1:L:6290:THR:OG1	1:L:6293:GLU:HG3	2.09	0.52
1:A:1133:LEU:HB3	1:A:1134:PRO:HD2	1.91	0.52
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.91	0.52
1:C:3436:ASN:N	1:C:3436:ASN:HD22	2.08	0.52
1:F:6395:LEU:HD13	1:F:6550:LEU:HD23	1.91	0.52
1:F:6097:LEU:HD13	3:F:6:NLX:C19	2.40	0.52
1:I:3215:VAL:H	1:I:3241:HIS:CD2	2.25	0.52
1:K:5428:VAL:O	1:K:5432:ILE:HG13	2.09	0.52
1:E:5297:THR:O	1:E:5301:MET:HG2	2.10	0.52
1:H:2371:GLY:HA2	1:H:2414:LYS:CD	2.37	0.52
1:J:4431:VAL:HG21	1:J:4540:LYS:HB2	1.92	0.52
1:J:4079:ASN:ND2	2:J:479:NAG:C5	2.72	0.52
1:K:5186:ARG:HB3	1:K:5324:ASP:HB2	1.91	0.52
1:K:5367:PRO:C	1:K:5368:LEU:HD12	2.30	0.52
1:K:5346:TYR:HB3	1:K:5437:HIS:CD2	2.45	0.52
1:A:1351:ASN:ND2	1:A:1449:PHE:HB3	2.25	0.52
1:A:1498:LYS:CD	1:A:1514:LEU:HD11	2.30	0.52
1:B:2340:ASN:HB3	4:B:7205:HOH:O	2.08	0.52
1:D:4235:LEU:HD12	1:D:4327:LEU:HD12	1.90	0.52
1:I:3389:VAL:HB	1:I:3424:VAL:HG11	1.92	0.52
1:I:3490:ILE:O	1:I:3494:LYS:HG3	2.10	0.52
1:J:4100:LEU:O	1:J:4101:PHE:HD1	1.93	0.52
1:J:4104:ARG:NH2	1:J:4150:SER:O	2.40	0.52
1:J:4252:THR:O	1:J:4254:VAL:N	2.43	0.52
1:B:2190:GLY:O	1:B:2194:GLN:HG3	2.09	0.52
1:D:4042:GLY:N	4:D:7218:HOH:O	2.43	0.52
1:F:6529:ILE:HA	1:F:6533:THR:HG23	1.91	0.52
1:G:1233:SER:OG	1:G:1327:LEU:HD12	2.10	0.52
1:G:1399:ALA:HB2	1:G:1550:LEU:CD2	2.40	0.52
1:I:3407:THR:HG21	1:I:3412:LYS:HD3	1.92	0.52
1:K:5392:ALA:O	1:K:5396:ILE:HG12	2.09	0.52
1:B:2452:ARG:HG2	1:B:2452:ARG:HH11	1.75	0.51
1:D:4023:PRO:HB2	1:D:4034:LEU:HD21	1.90	0.51
1:H:2079:ASN:OD1	2:H:279:NAG:C1	2.58	0.51
1:H:2409:ASP:OD2	1:H:2412:LYS:HB2	2.10	0.51
1:I:3330:LYS:HG3	1:I:3335:LEU:HD21	1.92	0.51
1:H:2459:MET:SD	1:K:5308:LEU:HD22	2.50	0.51
1:A:1402:LYS:O	1:A:1402:LYS:HG3	2.10	0.51



	A + 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:B:2359:ILE:HG23	3:B:2:NLX:C7	2.40	0.51
1:C:3186:ARG:HB3	1:C:3324:ASP:HB2	1.91	0.51
1:E:5370:GLU:C	1:E:5372:GLN:H	2.13	0.51
1:E:5079:ASN:HD21	2:E:579:NAG:C1	2.22	0.51
1:F:6107:ASN:HD22	1:F:6108:ILE:N	2.07	0.51
1:F:6359:ILE:HG12	3:F:6:NLX:H151	1.91	0.51
1:G:1371:GLY:C	1:G:1414:LYS:HD3	2.30	0.51
1:I:3151:THR:HB	1:I:3152:TYR:CD1	2.44	0.51
1:I:3364:MET:HE1	3:I:3:NLX:H171	1.92	0.51
1:K:5278:THR:OG1	1:K:5281:VAL:HG23	2.10	0.51
1:B:2359:ILE:HD13	3:B:2:NLX:H72	1.91	0.51
1:C:3371:GLY:O	1:C:3411:VAL:HG13	2.10	0.51
1:C:3104:ARG:O	1:C:3482:LYS:HE3	2.09	0.51
1:D:4420:LEU:C	1:D:4420:LEU:HD12	2.31	0.51
1:E:5491:ARG:HG2	1:E:5491:ARG:HH11	1.74	0.51
1:E:5363:LEU:HD13	3:E:5:NLX:H203	1.91	0.51
1:H:2501:ALA:O	1:H:2505:ARG:HG2	2.09	0.51
1:J:4230:LEU:O	1:J:4342:HIS:HE1	1.93	0.51
1:K:5057:LYS:HG3	1:K:5058:PRO:HD2	1.92	0.51
1:L:6304:LEU:CD2	3:L:6:NLX:H102	2.38	0.51
1:L:6188:ASN:ND2	1:L:6327:LEU:HD23	2.25	0.51
1:L:6410:THR:HA	1:L:6413:LYS:HG3	1.91	0.51
1:B:2527:LEU:HD11	1:B:2533:THR:HG22	1.93	0.51
1:E:5220:GLU:HG3	4:E:7086:HOH:O	2.11	0.51
1:G:1145:MET:HE1	1:G:1303:PHE:HD1	1.76	0.51
1:I:3386:TYR:N	1:I:3387:PRO:HD2	2.25	0.51
1:J:4221:SER:OG	3:J:4:NLX:O1	2.28	0.51
1:K:5110:LEU:HD11	1:K:5150:SER:HB2	1.92	0.51
1:A:1215:VAL:N	1:A:1241:HIS:HD2	1.96	0.51
1:C:3100:LEU:HD13	1:C:3358:LEU:CD1	2.41	0.51
1:E:5203:ASP:OD1	1:E:5203:ASP:N	2.42	0.51
1:A:1462:LYS:HE3	1:F:6374:ASP:OD2	2.10	0.51
1:F:6426:PHE:O	1:F:6429:PRO:HD2	2.10	0.51
1:H:2343:THR:HB	1:H:2442:ALA:HB2	1.92	0.51
1:A:1124:PRO:HD3	1:A:1158:ALA:HB1	1.92	0.51
1:A:1304:LEU:CG	3:A:1:NLX:H203	2.40	0.51
1:D:4427:GLY:O	1:D:4431:VAL:HG23	2.11	0.51
1:F:6214:SER:HA	1:F:6241:HIS:CD2	2.45	0.51
1:G:1120:ASN:HB2	1:G:1167:THR:OG1	2.11	0.51
1:G:1339:ARG:NH1	1:G:1436:ASN:HD22	2.09	0.51
1:I:3139:ILE:HG12	1:I:3168:ILE:HD11	1.91	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:3431:VAL:HG21	1:I:3540:LYS:HB2	1.93	0.51
1:J:4313:ARG:HA	1:J:4386:TYR:CD2	2.45	0.51
1:J:4174:ILE:HA	1:J:4319:LEU:HD12	1.92	0.51
1:J:4235:LEU:HD12	1:J:4327:LEU:HD12	1.92	0.51
1:J:4542:LYS:HB2	4:J:7954:HOH:O	2.09	0.51
1:K:5063:LEU:O	1:K:5066:THR:HG23	2.11	0.51
1:A:1104:ARG:HG2	1:A:1104:ARG:HH11	1.74	0.51
1:B:2493:SER:O	1:B:2497:MET:HG3	2.11	0.51
1:C:3333:GLU:N	1:C:3333:GLU:OE1	2.43	0.51
1:D:4289:LYS:HA	1:D:4293:GLU:OE2	2.11	0.51
1:E:5107:ASN:HD22	1:E:5108:ILE:N	2.08	0.51
1:E:5354:GLU:OE1	1:E:5354:GLU:HA	2.11	0.51
1:E:5318:LEU:HD11	3:E:5:NLX:H11	1.92	0.51
1:K:5217:ILE:CD1	1:K:5227:VAL:HG13	2.41	0.51
1:E:5126:ASP:H	1:E:5131:ASN:HD21	1.56	0.51
1:E:5478:ALA:N	1:E:5479:PRO:CD	2.74	0.51
1:F:6025:VAL:HG22	1:F:6034:LEU:HD23	1.92	0.51
1:I:3029:VAL:HG23	1:I:3204:ASN:OD1	2.11	0.51
1:A:1435:ARG:O	1:A:1438:ARG:HB3	2.11	0.51
1:B:2179:SER:O	1:B:2265:ALA:HB2	2.11	0.51
1:B:2531:ALA:C	1:B:2532:ASN:HD22	2.13	0.51
1:G:1334:GLU:O	1:G:1338:GLU:HG2	2.11	0.51
1:H:2104:ARG:HG2	1:H:2104:ARG:NH1	2.26	0.51
1:H:2176:GLY:CA	1:H:2189:TRP:HB2	2.38	0.51
1:H:2252:THR:HG22	1:H:2252:THR:O	2.11	0.51
1:I:3236:ALA:O	1:I:3239:LEU:HB2	2.11	0.51
1:I:3364:MET:SD	3:I:3:NLX:H201	2.50	0.51
1:I:3400:THR:HG23	1:I:3404:LEU:HD12	1.92	0.51
1:L:6444:THR:HG22	1:L:6520:TYR:HB3	1.92	0.51
1:A:1364:MET:HG3	3:A:1:NLX:H82	1.92	0.51
1:A:1486:SER:O	1:A:1490:ILE:HG13	2.11	0.51
1:E:5034:LEU:HB3	1:E:5079:ASN:HA	1.92	0.51
1:E:5220:GLU:HA	1:E:5246:GLU:O	2.11	0.51
1:G:1350:ILE:C	1:G:1351:ASN:HD22	2.14	0.51
1:H:2268:ILE:HD11	1:H:2319:LEU:HD21	1.91	0.51
1:H:2492:LEU:O	1:H:2496:VAL:HG23	2.11	0.51
1:I:3338:GLU:HB2	1:I:3340:ASN:HB2	1.93	0.51
1:K:5371:GLY:CA	1:K:5414:LYS:HD3	2.37	0.51
1:A:1431:VAL:HG11	1:A:1544:VAL:HG21	1.92	0.50
1:B:2385:SER:C	1:B:2387:PRO:HD2	2.32	0.50
$1:E:52\overline{20:GLU:HG2}$	1:E:5472:LEU:HD21	1.92	0.50



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:1355:PHE:CE2	1:G:1425:MET:HE2	2.46	0.50
1:G:1526:TYR:CD2	1:G:1539:LEU:HB2	2.45	0.50
1:I:3244:ILE:HG23	1:I:3347:MET:HB3	1.92	0.50
1:J:4508:ASN:OD1	1:J:4510:ASN:HB2	2.11	0.50
1:K:5393:LYS:HA	1:K:5396:ILE:CG1	2.41	0.50
1:K:5429:PRO:O	1:K:5433:VAL:HG23	2.11	0.50
1:A:1045:GLN:HB2	1:L:6486:SER:HA	1.93	0.50
1:D:4171:ARG:O	1:D:4176:GLY:HA3	2.11	0.50
1:F:6447:TYR:CD2	1:F:6447:TYR:C	2.85	0.50
1:G:1152:TYR:N	1:G:1152:TYR:CD1	2.79	0.50
1:H:2097:LEU:HD11	3:H:2:NLX:H11	1.93	0.50
1:K:5420:LEU:HD12	1:K:5547:TRP:CZ2	2.44	0.50
1:L:6420:LEU:HD13	1:L:6547:TRP:CZ2	2.46	0.50
1:L:6452:ARG:HD2	1:L:6464:VAL:O	2.11	0.50
1:B:2359:ILE:CG1	3:B:2:NLX:C7	2.85	0.50
1:C:3143:GLY:CA	3:C:3:NLX:H152	2.34	0.50
1:D:4197:ALA:O	1:D:4201:VAL:HG23	2.11	0.50
1:G:1105:LYS:HE3	1:G:1483:GLU:OE1	2.12	0.50
1:I:3125:ALA:HB1	1:I:3131:ASN:ND2	2.25	0.50
1:I:3467:ASP:OD1	1:I:3468:HIS:N	2.41	0.50
1:J:4262:LYS:HB3	1:J:4263:PRO:HD3	1.92	0.50
1:J:4332:PRO:O	1:J:4336:GLN:HG2	2.11	0.50
1:J:4532:ASN:HB2	4:J:7463:HOH:O	2.10	0.50
1:J:4363:LEU:HD22	3:J:4:NLX:H192	1.93	0.50
1:L:6386:TYR:N	1:L:6387:PRO:HD2	2.27	0.50
1:C:3143:GLY:HA2	3:C:3:NLX:H51	1.94	0.50
1:D:4447:TYR:CD2	1:D:4447:TYR:C	2.84	0.50
1:D:4101:PHE:CE2	3:D:4:NLX:H21	2.46	0.50
1:E:5372:GLN:HB3	4:E:7425:HOH:O	2.11	0.50
1:G:1234:PRO:O	1:G:1237:LYS:HB2	2.12	0.50
1:H:2283:VAL:O	1:H:2287:ARG:HB2	2.11	0.50
1:I:3223:GLY:O	1:I:3227:VAL:HG23	2.10	0.50
1:I:3526:TYR:CD2	1:I:3539:LEU:HB2	2.46	0.50
1:L:6225:GLU:HG3	1:L:6255:LEU:CD1	2.42	0.50
1:A:1498:LYS:HD3	1:A:1502:ASN:HD21	1.76	0.50
1:D:4121:ILE:HG12	1:D:4166:VAL:HG22	1.94	0.50
1:D:4543:GLU:OE2	1:D:4543:GLU:N	2.31	0.50
1:E:5527:LEU:HD11	1:E:5533:THR:HG22	1.92	$0.\overline{50}$
1:F:6161:GLU:HG3	1:F:6501:ALA:HB2	1.93	0.50
1:G:1244:ILE:HD11	1:G:1503:PHE:HD2	1.76	0.50
1:I:3252:THR:HG23	1:I:3425:MET:O	2.12	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:3404:LEU:HD22	1:I:3413:LYS:O	2.10	0.50
1:J:4363:LEU:HD22	3:J:4:NLX:H181	1.92	0.50
1:K:5517:TRP:CE3	1:K:5527:LEU:HD23	2.47	0.50
1:K:5524:GLU:O	1:K:5537:GLN:O	2.29	0.50
1:K:5363:LEU:HB3	3:K:5:NLX:H201	1.93	0.50
1:C:3104:ARG:CZ	1:C:3153:ASP:HB2	2.41	0.50
1:E:5079:ASN:ND2	2:E:579:NAG:C1	2.75	0.50
1:E:5412:LYS:O	1:E:5416:LEU:HG	2.11	0.50
1:F:6543:GLU:CD	1:F:6543:GLU:H	2.14	0.50
1:F:6428:VAL:HG21	1:F:6547:TRP:CD1	2.47	0.50
1:I:3103:ASN:ND2	1:I:3481:LEU:HD12	2.25	0.50
1:I:3330:LYS:HG3	1:I:3335:LEU:CD2	2.41	0.50
1:L:6149:ALA:HB2	1:L:6169:GLN:HG3	1.94	0.50
1:H:2144:LEU:HD22	1:H:2177:PHE:CZ	2.46	0.50
1:I:3038:VAL:HG12	1:I:3039:SER:N	2.26	0.50
1:I:3218:PHE:HA	1:I:3244:ILE:O	2.12	0.50
1:J:4452:ARG:HD2	1:J:4464:VAL:O	2.12	0.50
1:K:5370:GLU:C	1:K:5372:GLN:H	2.15	0.50
3:K:5:NLX:O4	3:K:5:NLX:H203	2.12	0.50
1:L:6420:LEU:C	1:L:6420:LEU:HD12	2.32	0.50
1:D:4480:PHE:O	1:D:4481:LEU:HD23	2.12	0.50
1:A:1463:THR:HG21	1:F:6372:GLN:CB	2.41	0.50
1:G:1363:LEU:HD22	3:G:1:NLX:H181	1.94	0.50
1:H:2257:LYS:CE	1:H:2316:GLN:HE22	2.25	0.50
1:J:4526:TYR:CE1	1:J:4539:LEU:HD13	2.46	0.50
1:K:5264:LEU:HD21	1:K:5319:LEU:HD23	1.94	0.50
1:D:4126:ASP:OD2	1:D:4129:LYS:HG3	2.12	0.50
1:E:5158:ALA:O	1:E:5162:ASN:HA	2.11	0.50
1:F:6252:THR:HG22	1:F:6254:VAL:HG12	1.93	0.50
1:F:6242:ARG:HD3	1:F:6503:PHE:O	2.12	0.50
1:G:1260:ASP:O	1:G:1263:PRO:HD2	2.12	0.50
1:G:1383:TRP:CZ3	1:G:1393:LYS:HB2	2.47	0.50
1:I:3134:PRO:HG2	1:I:3163:VAL:HG12	1.94	0.50
1:I:3257:LYS:NZ	1:I:3316:GLN:CG	2.75	0.50
1:I:3309:GLN:HG3	1:J:4095:GLN:NE2	2.27	0.50
1:K:5271:THR:HG22	1:K:5297:THR:HG23	1.94	0.50
1:A:1233:SER:OG	1:A:1327:LEU:HD12	2.12	0.49
1:B:2053:ILE:HD12	1:B:2121:ILE:HD12	1.94	0.49
1:D:4201:VAL:HG13	1:D:4205:ILE:HB	1.94	0.49
1:E:5135:VAL:HG21	1:E:5205:ILE:HG21	1.93	0.49
1:F:6186:ARG:HB3	1:F:6324:ASP:HB2	1.94	0.49



	• • • • •	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:G:1304:LEU:HD13	1:G:1318:LEU:HB3	1.93	0.49
1:H:2420:LEU:HD12	1:H:2547:TRP:CZ2	2.46	0.49
1:J:4074:TRP:CD2	1:J:4078:LYS:HE2	2.47	0.49
1:J:4370:GLU:HB3	1:J:4372:GLN:HG2	1.93	0.49
1:K:5268:ILE:HD11	1:K:5319:LEU:HD21	1.94	0.49
1:L:6086:MET:HE3	1:L:6110:LEU:HB2	1.93	0.49
1:L:6086:MET:HE2	1:L:6110:LEU:HB2	1.93	0.49
1:L:6260:ASP:O	1:L:6263:PRO:HD2	2.12	0.49
1:L:6545:ALA:HA	1:L:6548:THR:HG22	1.93	0.49
1:L:6143:GLY:HA3	3:L:6:NLX:H11	1.94	0.49
1:A:1348:VAL:O	1:A:1446:MET:HA	2.11	0.49
1:B:2024:PRO:O	1:B:2034:LEU:HD23	2.12	0.49
1:I:3079:ASN:OD1	2:I:379:NAG:C1	2.60	0.49
1:K:5540:LYS:O	1:K:5544:VAL:HG23	2.13	0.49
1:L:6420:LEU:HD11	1:L:6547:TRP:CZ2	2.46	0.49
1:A:1297:THR:O	1:A:1301:MET:HG2	2.12	0.49
1:A:1145:MET:HB2	1:A:1304:LEU:CD2	2.42	0.49
1:D:4161:GLU:OE2	1:D:4498:LYS:CA	2.60	0.49
1:E:5370:GLU:O	1:E:5372:GLN:N	2.45	0.49
1:G:1283:VAL:O	1:G:1287:ARG:HG3	2.12	0.49
1:I:3275:LYS:HG3	4:I:7145:HOH:O	2.11	0.49
1:J:4119:LEU:HD12	1:J:4119:LEU:O	2.12	0.49
1:L:6317:PRO:HG3	1:L:6387:PRO:HB2	1.94	0.49
1:A:1382:LEU:HD22	1:A:1420:LEU:HD21	1.93	0.49
1:A:1105:LYS:HD2	1:A:1483:GLU:OE2	2.12	0.49
1:C:3070:PRO:HG2	4:C:7964:HOH:O	2.12	0.49
1:E:5143:GLY:O	1:E:5318:LEU:HD22	2.13	0.49
1:G:1420:LEU:O	1:G:1424:VAL:HG23	2.12	0.49
1:I:3218:PHE:CB	1:I:3244:ILE:HB	2.43	0.49
1:K:5351:ASN:ND2	1:K:5449:PHE:HB3	2.27	0.49
1:L:6138:TRP:HA	1:L:6218:PHE:O	2.12	0.49
1:A:1302:LYS:HG3	4:A:7839:HOH:O	2.12	0.49
1:B:2478:ALA:HB3	1:B:2479:PRO:HD3	1.93	0.49
1:C:3092:LYS:HZ3	1:D:4302:LYS:HD2	1.76	0.49
1:C:3304:LEU:HD22	3:C:3:NLX:H201	1.95	0.49
1:F:6090:ASP:HB3	1:F:6093:ALA:HB3	1.93	0.49
1:F:6414:LYS:HD2	1:F:6414:LYS:C	2.32	0.49
1:H:2359:ILE:CD1	3:H:2:NLX:H71	2.39	0.49
1:J:4414:LYS:O	1:J:4418:LEU:HG	2.12	0.49
1:K:5258:LYS:H	1:K:5258:LYS:CD	2.06	0.49
1:K:5304:LEU:HD13	3:K:5:NLX:C18	2.37	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:K:5311:ASP:OD1	1:K:5313:ARG:HB2	2.12	0.49
1:L:6471:GLU:O	1:L:6475:VAL:HG23	2.12	0.49
1:L:6304:LEU:HD13	3:L:6:NLX:C18	2.41	0.49
1:A:1350:ILE:O	1:A:1448:GLU:HA	2.12	0.49
1:B:2355:PHE:CD2	1:B:2359:ILE:HG21	2.48	0.49
1:C:3313:ARG:HG2	1:C:3386:TYR:CZ	2.48	0.49
1:D:4447:TYR:HA	1:D:4527:LEU:O	2.13	0.49
1:E:5491:ARG:CD	4:E:7007:HOH:O	2.61	0.49
1:H:2057:LYS:HD2	4:H:7830:HOH:O	2.12	0.49
1:H:2264:LEU:HD21	1:H:2319:LEU:HD23	1.95	0.49
1:H:2103:ASN:ND2	1:H:2481:LEU:HD12	2.28	0.49
1:J:4244:ILE:HG12	1:J:4347:MET:HB3	1.94	0.49
1:J:4359:ILE:HG23	3:J:4:NLX:C8	2.43	0.49
1:L:6198:LEU:HD21	1:L:6217:ILE:CG2	2.42	0.49
1:C:3308:LEU:HG	4:C:7642:HOH:O	2.11	0.49
1:D:4335:LEU:HD11	4:D:7303:HOH:O	2.12	0.49
1:G:1468:HIS:NE2	3:G:1:NLX:O1	2.46	0.49
1:H:2374:ASP:O	1:H:2376:LYS:N	2.46	0.49
1:H:2348:VAL:O	1:H:2446:MET:HA	2.12	0.49
1:H:2304:LEU:HD22	3:H:2:NLX:C20	2.42	0.49
1:I:3025:VAL:HG22	1:I:3034:LEU:HD23	1.94	0.49
1:I:3229:VAL:HG11	1:I:3327:LEU:HD21	1.94	0.49
1:J:4473:PHE:HA	4:J:7950:HOH:O	2.11	0.49
1:J:4525:GLY:CA	1:J:4537:GLN:HG2	2.42	0.49
1:K:5060:LEU:CD2	1:K:5114:GLU:HB2	2.43	0.49
1:K:5393:LYS:HA	1:K:5396:ILE:HG12	1.93	0.49
1:K:5428:VAL:HG13	1:K:5544:VAL:HG22	1.94	0.49
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.95	0.49
1:A:1375:GLN:O	1:A:1378:ALA:HB3	2.12	0.49
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.91	0.49
1:C:3540:LYS:O	1:C:3544:VAL:HG23	2.13	0.49
1:D:4024:PRO:HD3	1:D:4037:PHE:CD1	2.48	0.49
1:F:6375:GLN:HG3	1:F:6400:THR:HG22	1.94	0.49
1:G:1149:ALA:HB2	1:G:1168:ILE:O	2.12	0.49
1:G:1374:ASP:O	1:G:1376:LYS:N	2.46	0.49
1:H:2349:GLY:HA3	1:H:2447:TYR:CE1	2.48	0.49
1:H:2404:LEU:HD13	1:H:2413:LYS:CG	2.43	0.49
1:I:3330:LYS:NZ	1:I:3330:LYS:HB3	2.27	0.49
1:I:3355:PHE:CD1	1:I:3360:PRO:HG3	2.48	0.49
1:A:1304:LEU:HG	3:A:1:NLX:H151	1.93	0.49
1:B:2452:ARG:NH1	4:B:7528:HOH:O	2.44	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:5068:PRO:HB3	1:E:5193:ASP:OD1	2.13	0.49
1:E:5404:LEU:HD22	1:E:5416:LEU:HB2	1.93	0.49
1:F:6478:ALA:N	1:F:6479:PRO:CD	2.75	0.49
1:G:1079:ASN:ND2	2:G:179:NAG:C1	2.76	0.49
1:H:2402:LYS:HG2	1:H:2546:PHE:CE1	2.47	0.49
1:J:4182:ASP:HB2	1:J:4183:GLU:OE2	2.13	0.49
1:J:4297:THR:O	1:J:4301:MET:HG2	2.13	0.49
1:K:5468:HIS:NE2	3:K:5:NLX:O3	2.46	0.49
1:B:2251:LEU:HB2	1:B:2429:PRO:HB3	1.95	0.49
1:D:4034:LEU:HD12	1:D:4079:ASN:OD1	2.13	0.49
1:G:1292:GLU:HG2	4:G:7529:HOH:O	2.11	0.49
1:G:1216:THR:OG1	1:G:1504:ALA:HA	2.12	0.49
1:G:1523:LYS:HB3	1:G:1537:GLN:OE1	2.12	0.49
1:H:2204:ASN:O	1:H:2206:ALA:N	2.45	0.49
1:I:3543:GLU:OE2	1:I:3543:GLU:N	2.41	0.49
1:J:4176:GLY:HA2	1:J:4189:TRP:HB2	1.95	0.49
1:K:5101:PHE:CE1	1:K:5469:GLY:HA3	2.48	0.49
1:L:6051:LEU:HD13	1:L:6083:TYR:CD1	2.48	0.49
1:L:6264:LEU:O	1:L:6268:ILE:HD13	2.12	0.49
1:A:1269:ALA:HB2	1:A:1282:MET:HE3	1.94	0.48
1:A:1330:LYS:HB2	1:A:1335:LEU:CD2	2.43	0.48
1:C:3024:PRO:HG3	1:C:3037:PHE:CE1	2.47	0.48
1:C:3156:ALA:O	1:C:3160:HIS:HB2	2.13	0.48
1:C:3464:VAL:HG22	1:D:4370:GLU:OE1	2.13	0.48
1:E:5024:PRO:HD3	1:E:5037:PHE:CD1	2.47	0.48
1:E:5339:ARG:NH1	1:E:5339:ARG:HG2	2.28	0.48
1:G:1104:ARG:HH12	1:G:1153:ASP:HB2	1.78	0.48
1:G:1338:GLU:O	1:G:1340:ASN:N	2.46	0.48
1:J:4278:THR:OG1	1:J:4281:VAL:HG23	2.13	0.48
1:K:5361:MET:SD	1:K:5363:LEU:HG	2.52	0.48
1:L:6304:LEU:HB3	3:L:6:NLX:H172	1.94	0.48
1:B:2370:GLU:O	1:B:2372:GLN:HG3	2.13	0.48
1:B:2079:ASN:HD21	2:B:279:NAG:C1	2.26	0.48
1:D:4309:GLN:NE2	1:D:4310:GLY:N	2.61	0.48
1:B:2308:LEU:HD22	1:E:5459:MET:SD	2.53	0.48
1:E:5452:ARG:HE	1:E:5462:LYS:HA	1.78	0.48
1:K:5359:ILE:HG12	3:K:5:NLX:H151	1.96	0.48
1:B:2254:VAL:HG21	1:B:2388:LEU:HD23	1.95	0.48
1:C:3257:LYS:HE3	1:C:3322:VAL:HG12	1.95	0.48
1:E:5176:GLY:HA2	1:E:5189:TRP:HB2	1.95	0.48
1:E:5538:LYS:HB3	1:E:5541:ASP:HB2	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:6202:GLN:NE2	1:F:6212:PRO:O	2.46	0.48
1:G:1142:GLY:CA	3:G:1:NLX:H152	2.43	0.48
1:H:2237:LYS:O	1:H:2238:ASN:HB2	2.11	0.48
1:J:4187:GLY:O	1:J:4188:ASN:HB2	2.13	0.48
1:J:4551:PHE:C	1:J:4553:LYS:H	2.16	0.48
1:K:5215:VAL:H	1:K:5241:HIS:CD2	2.19	0.48
1:K:5380:SER:O	1:K:5384:LYS:HG2	2.13	0.48
1:K:5420:LEU:CD1	1:K:5547:TRP:HZ2	2.24	0.48
1:A:1068:PRO:HA	4:A:7198:HOH:O	2.13	0.48
1:A:1304:LEU:HG	3:A:1:NLX:O4	2.12	0.48
1:L:6478:ALA:N	1:L:6479:PRO:CD	2.76	0.48
1:A:1358:LEU:O	1:A:1363:LEU:HD12	2.14	0.48
1:B:2255:LEU:HD23	1:B:2318:LEU:HD13	1.94	0.48
1:C:3112:LEU:O	1:C:3113:SER:HB2	2.13	0.48
1:E:5338:GLU:O	1:E:5338:GLU:HG3	2.13	0.48
1:G:1087:CYS:O	1:G:1088:THR:C	2.51	0.48
1:G:1318:LEU:O	1:G:1318:LEU:HD12	2.12	0.48
1:I:3251:LEU:HD21	1:I:3333:GLU:HG3	1.96	0.48
1:I:3251:LEU:HD12	1:I:3433:VAL:CG2	2.44	0.48
1:K:5353:GLN:O	1:K:5467:ASP:HA	2.13	0.48
1:K:5478:ALA:N	1:K:5479:PRO:CD	2.76	0.48
1:A:1251:LEU:HD12	1:A:1433:VAL:CG2	2.43	0.48
1:A:1311:ASP:OD1	1:A:1313:ARG:HB2	2.14	0.48
1:B:2520:TYR:CZ	1:B:2524:GLU:HG2	2.49	0.48
1:C:3268:ILE:HG12	1:C:3301:MET:CE	2.44	0.48
1:C:3290:THR:HG23	1:C:3293:GLU:OE2	2.12	0.48
1:F:6145:MET:HE1	1:F:6303:PHE:CD1	2.48	0.48
1:F:6136:MET:HB3	1:F:6218:PHE:HE1	1.79	0.48
1:F:6188:ASN:ND2	1:F:6324:ASP:OD2	2.44	0.48
1:G:1086:MET:HE1	4:G:7232:HOH:O	2.13	0.48
1:G:1308:LEU:HD22	1:L:6459:MET:SD	2.53	0.48
1:G:1304:LEU:CG	3:G:1:NLX:H203	2.36	0.48
1:H:2297:THR:O	1:H:2301:MET:HG2	2.14	0.48
1:J:4145:MET:HG3	1:J:4304:LEU:HD11	1.96	0.48
1:K:5349:GLY:HA3	1:K:5447:TYR:CE1	2.49	0.48
1:B:2292:GLU:O	1:B:2296:GLU:HG3	2.13	0.48
1:E:5286:LEU:HA	1:E:5289:LYS:HG3	1.96	0.48
1:G:1140:HIS:CD2	1:G:1147:GLY:HA3	2.48	0.48
1:H:2101:PHE:CE2	3:H:2:NLX:H21	2.49	0.48
1:J:4079:ASN:CG	2:J:479:NAG:C1	2.82	0.48
1:L:6182:ASP:HB2	1:L:6183:GLU:OE2	2.14	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1024:PRO:HD3	1:A:1037:PHE:CD1	2.48	0.48
1:A:1284:HIS:O	1:A:1288:GLN:OE1	2.32	0.48
1:B:2143:GLY:O	1:B:2144:LEU:HB2	2.14	0.48
1:C:3026:VAL:HG13	4:C:7260:HOH:O	2.13	0.48
1:D:4140:HIS:HD2	1:D:4141:GLY:O	1.97	0.48
1:I:3426:PHE:HE2	3:I:3:NLX:HO11	1.60	0.48
1:K:5099:GLU:HG3	1:K:5107:ASN:OD1	2.13	0.48
1:K:5217:ILE:O	1:K:5243:ALA:HA	2.14	0.48
1:L:6324:ASP:OD1	1:L:6327:LEU:N	2.36	0.48
1:L:6492:LEU:O	1:L:6496:VAL:HG23	2.14	0.48
1:B:2174:ILE:CG1	1:B:2298:THR:HG22	2.44	0.48
1:B:2318:LEU:CD1	3:B:2:NLX:H171	2.43	0.48
1:B:2499:PHE:HZ	1:B:2515:PRO:HG2	1.78	0.48
1:C:3475:VAL:HG22	1:C:3496:VAL:HG11	1.96	0.48
1:D:4143:GLY:O	1:D:4145:MET:HG2	2.13	0.48
1:E:5215:VAL:H	1:E:5241:HIS:CD2	2.28	0.48
1:E:5465:ILE:HD12	1:E:5465:ILE:N	2.29	0.48
1:E:5502:ASN:O	1:E:5506:ASN:HB2	2.14	0.48
1:F:6107:ASN:HD22	1:F:6108:ILE:H	1.62	0.48
1:F:6359:ILE:HG12	3:F:6:NLX:C15	2.43	0.48
1:H:2478:ALA:N	1:H:2479:PRO:CD	2.77	0.48
1:H:2143:GLY:HA3	3:H:2:NLX:C15	2.44	0.48
1:H:2363:LEU:HD22	3:H:2:NLX:H181	1.94	0.48
1:I:3324:ASP:OD2	1:I:3327:LEU:HB3	2.13	0.48
1:J:4079:ASN:ND2	2:J:479:NAG:H5	2.26	0.48
1:K:5104:ARG:HG2	1:K:5104:ARG:HH11	1.78	0.48
1:K:5404:LEU:O	1:K:5413:LYS:HE2	2.13	0.48
1:A:1040:LEU:HD22	1:A:1156:ALA:HA	1.96	0.48
1:C:3436:ASN:N	1:C:3436:ASN:ND2	2.61	0.48
1:C:3543:GLU:OE2	1:C:3543:GLU:N	2.42	0.48
1:D:4461:PRO:HG2	1:D:4464:VAL:CG2	2.44	0.48
1:E:5039:SER:OG	1:E:5046:PRO:HG3	2.14	0.48
1:E:5187:GLY:O	1:E:5188:ASN:HB2	2.14	0.48
1:E:5404:LEU:HD22	1:E:5413:LYS:O	2.14	0.48
1:G:1478:ALA:N	1:G:1479:PRO:CD	2.77	0.48
1:H:2202:GLN:HG2	4:H:7675:HOH:O	2.13	0.48
1:H:2311:ASP:HB3	1:H:2314:GLU:HG2	1.96	0.48
1:I:3257:LYS:HZ3	1:I:3316:GLN:CG	2.27	0.48
1:J:4130:LYS:HD3	1:J:4131:ASN:N	2.27	0.48
1:J:4353:GLN:NE2	1:J:4465:ILE:H	2.12	0.48
1:K:5309:GLN:NE2	4:K:7219:HOH:O	2.42	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:5550:LEU:HD23	1:K:5550:LEU:C	2.34	0.48
1:A:1024:PRO:HB3	1:A:1037:PHE:CZ	2.49	0.47
1:A:1128:THR:HG23	4:A:7990:HOH:O	2.13	0.47
1:B:2223:GLY:O	1:B:2227:VAL:HG23	2.14	0.47
1:B:2420:LEU:C	1:B:2420:LEU:HD12	2.34	0.47
1:D:4296:GLU:O	1:D:4300:LYS:HG3	2.14	0.47
1:D:4382:LEU:HD11	1:D:4391:ILE:HD12	1.95	0.47
1:D:4423:ASP:OD1	1:D:4540:LYS:CE	2.62	0.47
1:F:6140:HIS:CD2	1:F:6147:GLY:HA3	2.49	0.47
1:G:1104:ARG:CZ	1:G:1153:ASP:HB2	2.43	0.47
1:G:1161:GLU:OE2	1:G:1498:LYS:HG2	2.14	0.47
1:H:2143:GLY:O	1:H:2318:LEU:HD22	2.14	0.47
1:H:2338:GLU:HB3	1:H:2340:ASN:OD1	2.14	0.47
1:I:3492:LEU:O	1:I:3496:VAL:HG23	2.14	0.47
1:K:5100:LEU:HD22	1:K:5457:SER:HB2	1.96	0.47
1:G:1134:PRO:CG	1:G:1163:VAL:HG12	2.29	0.47
1:H:2225:GLU:O	1:H:2228:SER:N	2.47	0.47
1:H:2368:LEU:HB2	1:K:5369:SER:HA	1.95	0.47
1:H:2385:SER:O	1:H:2389:VAL:HG22	2.15	0.47
1:I:3237:LYS:O	1:I:3238:ASN:HB2	2.14	0.47
1:J:4319:LEU:N	1:J:4319:LEU:HD23	2.28	0.47
1:L:6313:ARG:HG2	1:L:6386:TYR:CE2	2.49	0.47
1:B:2359:ILE:CB	1:B:2360:PRO:CD	2.91	0.47
1:B:2143:GLY:HA3	3:B:2:NLX:H161	1.96	0.47
1:D:4257:LYS:NZ	1:D:4316:GLN:HG3	2.28	0.47
1:F:6409:ASP:OD2	1:F:6412:LYS:HB2	2.14	0.47
1:G:1034:LEU:O	1:G:1081:THR:HG23	2.15	0.47
1:H:2350:ILE:C	1:H:2350:ILE:HD12	2.35	0.47
1:I:3044:ALA:O	1:I:3046:PRO:HD3	2.13	0.47
1:J:4218:PHE:N	1:J:4218:PHE:CD1	2.82	0.47
1:J:4349:GLY:HA3	1:J:4447:TYR:CE1	2.50	0.47
1:J:4412:LYS:O	1:J:4416:LEU:HG	2.14	0.47
1:J:4417:PHE:O	1:J:4420:LEU:HB3	2.14	0.47
1:A:1249:VAL:HB	1:A:1433:VAL:HG21	1.96	0.47
1:B:2220:GLU:OE1	1:B:2221:SER:CB	2.58	0.47
1:C:3304:LEU:HD22	3:C:3:NLX:C20	2.43	0.47
1:C:3092:LYS:HD2	1:D:4302:LYS:HD2	1.97	0.47
1:E:5257:LYS:HA	4:E:7588:HOH:O	2.13	0.47
1:F:6396:ILE:HB	1:F:6397:PRO:HD3	1.96	0.47
1:G:1302:LYS:HB2	1:L:6092:LYS:NZ	2.29	0.47
1:G:1417:PHE:HD1	1:G:1420:LEU:HD23	1.79	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:4363:LEU:CD1	3:J:4:NLX:H181	2.32	0.47
1:A:1119:LEU:HD12	1:A:1119:LEU:O	2.15	0.47
1:F:6107:ASN:ND2	1:F:6108:ILE:N	2.62	0.47
1:F:6375:GLN:HG3	1:F:6400:THR:CG2	2.45	0.47
1:G:1349:GLY:HA3	1:G:1447:TYR:CZ	2.50	0.47
1:G:1547:TRP:CZ3	1:G:1550:LEU:HD23	2.50	0.47
1:H:2278:THR:OG1	1:H:2281:VAL:HG23	2.14	0.47
1:I:3024:PRO:HG3	1:I:3037:PHE:CE2	2.50	0.47
1:I:3225:GLU:CB	1:I:3255:LEU:HD13	2.44	0.47
1:I:3318:LEU:HG	3:I:3:NLX:C18	2.44	0.47
1:I:3364:MET:CG	3:I:3:NLX:H201	2.43	0.47
1:J:4183:GLU:OE2	1:J:4183:GLU:N	2.47	0.47
1:K:5104:ARG:HG2	1:K:5104:ARG:NH1	2.29	0.47
1:K:5354:GLU:HB2	1:K:5422:ALA:HB1	1.96	0.47
1:L:6414:LYS:O	1:L:6418:LEU:HG	2.14	0.47
1:A:1218:PHE:HB3	1:A:1244:ILE:HB	1.94	0.47
1:A:1375:GLN:NE2	1:A:1400:THR:HG22	2.25	0.47
1:C:3402:LYS:HG2	1:C:3546:PHE:CE1	2.49	0.47
1:E:5428:VAL:O	1:E:5429:PRO:C	2.50	0.47
1:G:1518:PRO:HG2	4:G:7779:HOH:O	2.14	0.47
1:H:2035:GLY:HA2	1:H:2081:THR:HG22	1.97	0.47
1:I:3258:LYS:H	1:I:3258:LYS:CE	2.27	0.47
1:J:4302:LYS:HB3	1:J:4302:LYS:HZ3	1.77	0.47
1:J:4449:PHE:CE2	1:J:4471:GLU:HA	2.50	0.47
1:K:5363:LEU:HD13	3:K:5:NLX:C20	2.45	0.47
1:K:5549:ASN:O	1:K:5552:ALA:HB3	2.15	0.47
1:J:4277:THR:HG21	1:L:6113:SER:HB2	1.96	0.47
1:L:6447:TYR:HB3	1:L:6517:TRP:CZ2	2.50	0.47
1:A:1296:GLU:O	1:A:1300:LYS:HG3	2.15	0.47
1:D:4145:MET:CG	1:D:4304:LEU:HD11	2.45	0.47
1:B:2092:LYS:HD2	1:E:5302:LYS:HE3	1.97	0.47
1:E:5456:SER:HB3	1:E:5460:LYS:HD2	1.97	0.47
1:G:1380:SER:O	1:G:1383:TRP:HB3	2.15	0.47
1:H:2417:PHE:O	1:H:2420:LEU:HB3	2.15	0.47
1:I:3191:HIS:CD2	1:I:3321:THR:HG23	2.50	0.47
1:I:3301:MET:HB2	1:I:3303:PHE:CE1	2.49	0.47
1:J:4258:LYS:HD3	1:J:4258:LYS:N	2.30	0.47
1:J:4264:LEU:HG	1:J:4316:GLN:HG2	1.96	0.47
1:L:6145:MET:HB3	1:L:6304:LEU:HD11	1.96	0.47
1:A:1201:VAL:O	1:A:1205:ILE:HB	2.14	0.47
1:D:4478:ALA:HB3	1:D:4479:PRO:HD3	1.96	0.47



	•	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:5339:ARG:HH11	1:E:5339:ARG:HG2	1.80	0.47
1:E:5363:LEU:HB3	3:E:5:NLX:C20	2.35	0.47
1:G:1241:HIS:O	1:G:1242:ARG:HD3	2.15	0.47
1:H:2366:TYR:OH	1:H:2385:SER:HB3	2.15	0.47
1:I:3366:TYR:HA	1:I:3367:PRO:HD3	1.76	0.47
1:J:4398:GLU:OE2	1:J:4550:LEU:HD13	2.15	0.47
1:L:6363:LEU:HD22	3:L:6:NLX:C20	2.44	0.47
1:L:6526:TYR:CZ	1:L:6536:ALA:HB3	2.50	0.47
1:A:1304:LEU:HD12	1:A:1318:LEU:HD23	1.96	0.47
1:B:2366:TYR:HD2	1:B:2368:LEU:HD13	1.79	0.47
1:G:1262:LYS:HB3	1:G:1263:PRO:HD3	1.97	0.47
1:G:1508:ASN:OD1	1:G:1510:ASN:HB2	2.15	0.47
1:I:3428:VAL:HG21	1:I:3547:TRP:CD1	2.48	0.47
1:I:3478:ALA:O	1:I:3482:LYS:HB2	2.15	0.47
1:A:1374:ASP:O	1:A:1375:GLN:C	2.54	0.47
1:B:2074:TRP:CD2	1:B:2078:LYS:HE2	2.50	0.47
1:C:3395:LEU:HB3	1:C:3550:LEU:HD11	1.97	0.47
1:G:1140:HIS:HE1	4:G:7298:HOH:O	1.97	0.47
1:G:1354:GLU:HG3	1:G:1426:PHE:HB2	1.97	0.47
1:H:2101:PHE:HE2	3:H:2:NLX:H21	1.80	0.47
1:H:2126:ASP:OD1	1:H:2128:THR:HG23	2.14	0.47
1:I:3024:PRO:HG3	1:I:3037:PHE:CZ	2.49	0.47
1:I:3125:ALA:HB2	1:I:3133:LEU:CD1	2.45	0.47
1:I:3221:SER:OG	1:I:3222:ALA:N	2.47	0.47
1:J:4218:PHE:N	1:J:4218:PHE:HD1	2.12	0.47
1:I:3381:LEU:CD2	1:J:4459:MET:HG2	2.44	0.47
1:K:5254:VAL:O	1:K:5254:VAL:HG22	2.15	0.47
1:K:5264:LEU:HD22	1:K:5316:GLN:NE2	2.29	0.47
1:G:1302:LYS:CG	1:L:6092:LYS:HZ3	2.20	0.47
1:L:6339:ARG:HH21	1:L:6439:ASP:HB2	1.80	0.47
1:A:1304:LEU:CD2	3:A:1:NLX:H151	2.45	0.47
1:E:5083:TYR:CE2	1:E:5108:ILE:HD13	2.49	0.47
1:E:5114:GLU:HG3	1:E:5291:GLU:OE2	2.16	0.47
1:G:1087:CYS:HB3	4:G:7585:HOH:O	2.15	0.47
1:G:1201:VAL:O	1:G:1205:ILE:HB	2.14	0.47
1:H:2179:SER:O	1:H:2265:ALA:HB2	2.15	0.47
1:H:2363:LEU:CB	3:H:2:NLX:H181	2.25	0.47
1:L:6029:VAL:HG13	4:L:7981:HOH:O	2.15	0.47
1:D:4304:LEU:HB3	3:D:4:NLX:C20	2.40	0.46
1:E:5437:HIS:CD2	1:E:5444:THR:OG1	2.69	0.46
1:G:1513:GLY:O	1:G:1514:LEU:HD23	2.15	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:2375:GLN:NE2	1:H:2400:THR:HG22	2.30	0.46
1:I:3317:PRO:C	3:I:3:NLX:H192	2.36	0.46
1:J:4107:ASN:HD22	1:J:4108:ILE:N	2.12	0.46
1:J:4376:LYS:HA	1:J:4379:MET:HE2	1.96	0.46
1:K:5068:PRO:HB3	1:K:5193:ASP:OD1	2.14	0.46
1:K:5258:LYS:CD	1:K:5258:LYS:N	2.71	0.46
1:K:5407:THR:OG1	1:K:5408:ASP:N	2.48	0.46
1:L:6136:MET:HB3	1:L:6218:PHE:CE1	2.50	0.46
1:L:6435:ARG:NH1	1:L:6544:VAL:HG11	2.30	0.46
1:L:6480:PHE:CD1	1:L:6480:PHE:N	2.83	0.46
1:L:6499:PHE:HD2	1:L:6509:PRO:O	1.99	0.46
1:A:1188:ASN:O	1:A:1189:TRP:C	2.53	0.46
3:B:2:NLX:H203	3:B:2:NLX:O4	2.15	0.46
1:D:4041:GLU:HB3	4:D:7218:HOH:O	2.14	0.46
1:E:5183:GLU:OE2	1:E:5183:GLU:N	2.41	0.46
1:F:6143:GLY:O	1:F:6145:MET:HG2	2.15	0.46
1:G:1543:GLU:O	1:G:1547:TRP:CD1	2.68	0.46
1:K:5420:LEU:CD1	1:K:5547:TRP:CZ2	2.98	0.46
1:L:6107:ASN:HD22	1:L:6108:ILE:H	1.63	0.46
1:E:5540:LYS:O	1:E:5544:VAL:HG23	2.15	0.46
1:F:6142:GLY:C	3:F:6:NLX:H82	2.36	0.46
1:K:5395:LEU:HD13	1:K:5550:LEU:HD23	1.98	0.46
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.15	0.46
1:F:6330:LYS:HG3	1:F:6335:LEU:CD2	2.44	0.46
1:G:1437:HIS:O	1:G:1440:ALA:HB3	2.16	0.46
1:G:1438:ARG:NH1	1:G:1524:GLU:HG2	2.31	0.46
1:H:2359:ILE:HG12	3:H:2:NLX:C8	2.46	0.46
1:J:4274:CYS:SG	1:J:4285:CYS:SG	3.04	0.46
1:J:4318:LEU:O	1:J:4318:LEU:HD12	2.16	0.46
1:I:3368:LEU:O	1:J:4369:SER:HA	2.14	0.46
1:L:6416:LEU:O	1:L:6419:ASP:HB2	2.15	0.46
1:A:1129:LYS:HD3	4:A:7882:HOH:O	2.15	0.46
1:F:6120:ASN:HB2	1:F:6167:THR:OG1	2.16	0.46
1:G:1211:ASN:HD22	1:G:1214:SER:HB3	1.80	0.46
1:H:2386:TYR:N	1:H:2387:PRO:CD	2.78	0.46
1:I:3218:PHE:N	1:I:3218:PHE:CD1	2.84	0.46
1:K:5183:GLU:N	1:K:5183:GLU:OE2	2.44	0.46
1:K:5264:LEU:HD22	1:K:5316:GLN:HE21	1.80	0.46
1:K:5447:TYR:HB3	1:K:5517:TRP:CZ2	2.51	0.46
1:L:6107:ASN:HD22	1:L:6108:ILE:N	2.13	0.46
1:L:6363:LEU:HB3	3:L:6:NLX:C20	2.44	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1099:GLU:HG2	1:A:1107:ASN:OD1	2.16	0.46
1:A:1220:GLU:OE2	1:A:1221:SER:HB2	2.16	0.46
1:A:1394:GLU:O	1:A:1397:PRO:HD2	2.14	0.46
1:B:2452:ARG:HG2	1:B:2452:ARG:NH1	2.29	0.46
1:E:5343:THR:HB	1:E:5442:ALA:HB2	1.98	0.46
1:F:6492:LEU:HD12	1:F:6495:MET:HE2	1.97	0.46
1:G:1216:THR:HG23	1:G:1242:ARG:HB2	1.96	0.46
1:H:2241:HIS:C	1:H:2242:ARG:HD2	2.36	0.46
1:H:2353:GLN:HG3	1:H:2465:ILE:O	2.16	0.46
1:I:3057:LYS:HD3	1:I:3063:LEU:HD11	1.98	0.46
1:I:3446:MET:HE1	1:I:3539:LEU:HD23	1.97	0.46
1:K:5160:HIS:CE1	1:K:5480:PHE:CE2	3.04	0.46
1:B:2218:PHE:HB3	1:B:2244:ILE:HB	1.98	0.46
1:B:2428:VAL:HG13	1:B:2544:VAL:HG22	1.96	0.46
1:C:3375:GLN:HE21	1:C:3375:GLN:HB3	1.57	0.46
1:E:5373:LEU:H	1:E:5410:THR:HB	1.81	0.46
1:E:5491:ARG:NE	4:E:7007:HOH:O	2.42	0.46
1:F:6268:ILE:HG12	1:F:6301:MET:CE	2.46	0.46
1:G:1086:MET:CE	1:G:1148:ALA:HB2	2.45	0.46
1:G:1079:ASN:CG	2:G:179:NAG:C1	2.84	0.46
1:K:5550:LEU:C	1:K:5552:ALA:H	2.18	0.46
1:A:1152:TYR:N	1:A:1152:TYR:CD1	2.84	0.46
1:B:2258:LYS:O	1:B:2258:LYS:HD2	2.16	0.46
1:B:2304:LEU:HD23	3:B:2:NLX:H191	1.98	0.46
1:C:3140:HIS:HD2	1:C:3141:GLY:O	1.97	0.46
1:C:3329:LEU:C	1:C:3330:LYS:HG2	2.36	0.46
1:E:5358:LEU:HG	1:E:5363:LEU:HD12	1.98	0.46
1:F:6359:ILE:CD1	3:F:6:NLX:H151	2.45	0.46
1:G:1536:ALA:O	1:G:1537:GLN:HG2	2.16	0.46
1:H:2361:MET:CE	1:H:2363:LEU:HG	2.46	0.46
1:H:2363:LEU:HD22	3:H:2:NLX:C18	2.46	0.46
1:I:3096:LEU:HD13	1:J:4309:GLN:HB2	1.98	0.46
1:J:4375:GLN:HE21	1:J:4375:GLN:HB3	1.55	0.46
1:L:6060:LEU:CD2	1:L:6114:GLU:HB3	2.45	0.46
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.16	0.46
2:A:179:NAG:O4	2:A:180:NAG:C1	2.64	0.46
1:B:2458:ASP:HB2	4:E:7333:HOH:O	2.16	0.46
1:B:2353:GLN:HE22	1:B:2465:ILE:H	1.62	0.46
1:C:3445:TYR:CZ	1:C:3509:PRO:HD2	2.51	0.46
1:C:3501:ALA:O	1:C:3505:ARG:HG2	2.14	0.46
1:E:5242:ARG:NH1	1:E:5242:ARG:HG3	2.28	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:6103:ASN:ND2	1:F:6476:PHE:HB3	2.31	0.46
1:F:6296:GLU:O	1:F:6300:LYS:HG3	2.15	0.46
1:F:6349:GLY:HA3	1:F:6447:TYR:CE1	2.51	0.46
1:G:1145:MET:HG3	1:G:1304:LEU:HD21	1.98	0.46
1:G:1355:PHE:CD1	1:G:1360:PRO:HG3	2.50	0.46
1:I:3103:ASN:HD22	1:I:3481:LEU:HD12	1.80	0.46
1:L:6205:ILE:HA	1:L:6205:ILE:HD12	1.69	0.46
1:L:6452:ARG:HH11	1:L:6452:ARG:HG2	1.81	0.46
1:L:6161:GLU:HB3	1:L:6501:ALA:CB	2.46	0.46
1:A:1104:ARG:NH1	1:A:1153:ASP:HB2	2.29	0.46
1:A:1334:GLU:O	1:A:1337:ALA:HB3	2.16	0.46
1:D:4251:LEU:HD12	1:D:4433:VAL:HG23	1.96	0.46
1:D:4453:PRO:HD2	1:D:4470:ASP:OD2	2.15	0.46
1:E:5186:ARG:HB3	1:E:5324:ASP:HB2	1.98	0.46
1:H:2087:CYS:HB3	4:H:7192:HOH:O	2.15	0.46
1:J:4256:VAL:HG12	1:J:4258:LYS:HD2	1.98	0.46
1:K:5428:VAL:N	1:K:5429:PRO:CD	2.79	0.46
1:A:1386:TYR:N	1:A:1387:PRO:CD	2.79	0.45
1:A:1425:MET:O	1:A:1429:PRO:HG2	2.16	0.45
1:B:2417:PHE:O	1:B:2420:LEU:HB3	2.15	0.45
1:E:5354:GLU:O	1:E:5468:HIS:HB2	2.17	0.45
1:G:1103:ASN:ND2	1:G:1476:PHE:HB3	2.31	0.45
1:H:2143:GLY:O	1:H:2144:LEU:HB2	2.16	0.45
1:H:2346:TYR:HD2	1:H:2347:MET:N	2.14	0.45
1:I:3161:GLU:HB3	1:I:3501:ALA:CB	2.46	0.45
1:I:3462:LYS:NZ	1:J:4376:LYS:HZ2	2.14	0.45
1:J:4143:GLY:N	3:J:4:NLX:H152	2.31	0.45
1:K:5212:PRO:HG2	4:K:7443:HOH:O	2.16	0.45
1:K:5395:LEU:HD23	4:K:7575:HOH:O	2.15	0.45
1:L:6187:GLY:O	1:L:6188:ASN:HB2	2.16	0.45
1:L:6351:ASN:ND2	4:L:7041:HOH:O	2.49	0.45
1:L:6304:LEU:HD13	3:L:6:NLX:C19	2.46	0.45
1:B:2124:PRO:HD3	1:B:2158:ALA:HB1	1.98	0.45
1:B:2540:LYS:O	1:B:2544:VAL:HG23	2.16	0.45
1:C:3409:ASP:HB3	1:C:3412:LYS:HB3	1.98	0.45
1:C:3355:PHE:CE1	1:C:3421:ILE:HG21	2.50	0.45
1:E:5091:PRO:HG3	1:E:5112:LEU:CD1	2.37	0.45
1:H:2190:GLY:O	1:H:2193:ASP:HB2	2.16	0.45
1:I:3123:THR:OG1	1:I:3164:VAL:HG22	2.16	0.45
1:J:4420:LEU:HD12	1:J:4547:TRP:HZ2	1.81	0.45
1:K:5161:GLU:CD	1:K:5498:LYS:HA	2.36	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:5318:LEU:HD11	3:K:5:NLX:H21	1.98	0.45
1:K:5431:VAL:O	1:K:5435:ARG:HG3	2.16	0.45
1:L:6244:ILE:HG12	1:L:6347:MET:HB3	1.98	0.45
1:L:6349:GLY:HA3	1:L:6447:TYR:CZ	2.52	0.45
1:A:1289:LYS:HD3	4:A:8105:HOH:O	2.16	0.45
1:B:2023:PRO:HB2	1:B:2034:LEU:HD21	1.98	0.45
1:B:2040:LEU:HD13	1:B:2155:LEU:HD11	1.97	0.45
1:C:3142:GLY:HA3	1:C:3146:VAL:O	2.16	0.45
1:D:4182:ASP:HB2	1:D:4183:GLU:OE2	2.16	0.45
1:D:4215:VAL:N	1:D:4241:HIS:HD2	1.97	0.45
1:H:2027:ASP:CG	1:H:2032:LYS:HZ3	2.20	0.45
1:H:2338:GLU:O	1:H:2339:ARG:HD3	2.17	0.45
1:H:2453:PRO:C	1:H:2455:PHE:H	2.18	0.45
1:I:3217:ILE:HD12	1:I:3227:VAL:HG13	1.99	0.45
1:I:3383:TRP:CZ3	1:I:3393:LYS:HB2	2.51	0.45
1:J:4073:PRO:HB2	4:J:7805:HOH:O	2.16	0.45
1:J:4251:LEU:HD12	1:J:4433:VAL:CG2	2.46	0.45
1:J:4498:LYS:HB3	1:J:4514:LEU:HD11	1.98	0.45
1:K:5368:LEU:N	1:K:5368:LEU:HD12	2.31	0.45
1:K:5409:ASP:OD2	1:K:5412:LYS:HG3	2.16	0.45
1:B:2218:PHE:HB2	1:B:2244:ILE:HB	1.99	0.45
1:G:1179:SER:O	1:G:1265:ALA:HB2	2.16	0.45
1:I:3104:ARG:CZ	1:I:3153:ASP:HB2	2.46	0.45
1:J:4455:PHE:CD2	1:J:4482:LYS:HD3	2.50	0.45
1:A:1351:ASN:HB3	1:A:1466:GLY:O	2.16	0.45
1:A:1372:GLN:NE2	1:A:1410:THR:HG21	2.29	0.45
1:C:3092:LYS:NZ	1:D:4302:LYS:HD2	2.32	0.45
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.16	0.45
1:E:5051:LEU:O	1:E:5080:ALA:HB1	2.16	0.45
1:E:5252:THR:HG22	1:E:5254:VAL:HG12	1.98	0.45
1:F:6366:TYR:HA	1:F:6367:PRO:HD3	1.81	0.45
1:F:6426:PHE:C	1:F:6429:PRO:HD2	2.37	0.45
1:K:5100:LEU:CD2	1:K:5457:SER:HB2	2.47	0.45
1:K:5414:LYS:HB3	1:K:5414:LYS:HE2	1.80	0.45
1:K:5486:SER:O	1:K:5490:ILE:HG13	2.17	0.45
1:L:6149:ALA:CB	1:L:6169:GLN:HG3	2.47	0.45
1:C:3420:LEU:HD12	1:C:3420:LEU:C	2.37	0.45
1:D:4038:VAL:CG2	1:D:4049:ILE:HD12	2.45	0.45
1:D:4234:PRO:O	1:D:4237:LYS:HB2	2.17	0.45
1:E:5174:ILE:HA	1:E:5319:LEU:HD13	1.99	0.45
1:B:2372:GLN:NE2	1:E:5463:THR:HG21	2.32	0.45



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:I:3266:GLU:O	1:I:3270:ILE:HG13	2.17	0.45
1:J:4023:PRO:CB	1:J:4034:LEU:HD21	2.46	0.45
1:J:4089:GLN:OE1	1:J:4146:VAL:HB	2.17	0.45
1:J:4093:ALA:HB1	3:J:4:NLX:H191	1.98	0.45
1:K:5237:LYS:HA	1:K:5237:LYS:CE	2.31	0.45
1:K:5386:TYR:N	1:K:5387:PRO:HD2	2.32	0.45
1:L:6348:VAL:O	1:L:6446:MET:HA	2.17	0.45
1:A:1370:GLU:HA	1:A:1370:GLU:OE2	2.16	0.45
1:B:2260:ASP:OD1	1:B:2263:PRO:HD3	2.16	0.45
1:B:2389:VAL:HB	1:B:2424:VAL:HG11	1.98	0.45
1:C:3107:ASN:ND2	1:C:3108:ILE:H	2.14	0.45
1:C:3361:MET:CE	1:C:3363:LEU:HG	2.47	0.45
1:D:4049:ILE:HD11	1:D:4155:LEU:HD13	1.98	0.45
1:D:4186:ARG:HH11	1:D:4186:ARG:HG3	1.82	0.45
1:D:4221:SER:CB	3:D:4:NLX:O1	2.65	0.45
1:F:6218:PHE:HB3	1:F:6244:ILE:HB	1.99	0.45
1:G:1180:THR:HB	1:G:1279:SER:OG	2.17	0.45
1:G:1180:THR:HG22	1:G:1282:MET:HE2	1.98	0.45
1:G:1304:LEU:HD12	1:G:1318:LEU:HD23	1.96	0.45
1:G:1395:LEU:HD22	1:G:1550:LEU:CD1	2.47	0.45
1:H:2187:GLY:O	1:H:2188:ASN:HB2	2.17	0.45
1:H:2423:ASP:O	1:H:2428:VAL:HG23	2.15	0.45
1:H:2528:GLN:HB2	1:H:2534:GLN:HE21	1.82	0.45
1:I:3201:VAL:HB	4:I:7603:HOH:O	2.16	0.45
1:I:3143:GLY:HA2	1:I:3222:ALA:HB2	1.99	0.45
1:J:4304:LEU:CB	3:J:4:NLX:H203	2.46	0.45
1:K:5091:PRO:HG3	1:K:5112:LEU:CD2	2.46	0.45
1:L:6156:ALA:HB3	4:L:8057:HOH:O	2.17	0.45
1:L:6500:TRP:HE3	1:L:6500:TRP:N	2.15	0.45
1:D:4105:LYS:HG3	1:D:4481:LEU:O	2.16	0.45
1:G:1265:ALA:HB1	1:G:1282:MET:HE1	1.99	0.45
1:G:1524:GLU:O	1:G:1538:LYS:N	2.50	0.45
1:H:2143:GLY:CA	3:H:2:NLX:H152	2.46	0.45
1:H:2311:ASP:HA	1:H:2312:PRO:HD3	1.80	0.45
1:K:5026:VAL:CG1	1:K:5027:ASP:N	2.80	0.45
1:K:5526:TYR:CE2	1:K:5536:ALA:HB3	2.52	0.45
1:L:6121:ILE:HG22	1:L:6122:TYR:N	2.32	0.45
1:L:6414:LYS:HD2	1:L:6414:LYS:C	2.37	0.45
1:L:6501:ALA:O	1:L:6504:ALA:HB3	2.17	0.45
1:C:3214:SER:HA	1:C:3241:HIS:CD2	2.52	0.45
1:E:5371:GLY:C	1:E:5414:LYS:HD3	2.37	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:5336:GLN:HE22	1:E:5433:VAL:HA	1.82	0.45
1:F:6049:ILE:HG12	1:F:6122:TYR:CD2	2.52	0.45
1:F:6268:ILE:HD11	1:F:6319:LEU:HD21	1.97	0.45
1:F:6528:GLN:O	1:F:6533:THR:HG23	2.16	0.45
1:G:1373:LEU:HG	1:G:1378:ALA:HB2	1.98	0.45
1:G:1540:LYS:O	1:G:1544:VAL:HG23	2.17	0.45
1:H:2404:LEU:HD13	1:H:2413:LYS:HG2	1.98	0.45
1:I:3268:ILE:HG12	1:I:3301:MET:HE2	1.98	0.45
1:K:5057:LYS:HG3	1:K:5058:PRO:CD	2.47	0.45
1:K:5125:ALA:HB1	1:K:5131:ASN:ND2	2.32	0.45
1:K:5240:PHE:N	1:K:5240:PHE:CD1	2.85	0.45
1:L:6235:LEU:CD1	1:L:6327:LEU:HA	2.47	0.45
1:A:1043:PHE:CD2	1:L:6484:GLY:HA2	2.52	0.45
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.98	0.45
1:E:5407:THR:HG21	1:E:5412:LYS:CB	2.41	0.45
1:E:5403:TYR:O	1:E:5416:LEU:HD13	2.17	0.45
1:F:6283:VAL:O	1:F:6287:ARG:HG3	2.16	0.45
1:G:1467:ASP:HB3	1:G:1470:ASP:OD1	2.17	0.45
1:G:1079:ASN:CB	2:G:179:NAG:H82	2.34	0.45
1:I:3057:LYS:HD3	1:I:3063:LEU:CD1	2.46	0.45
1:I:3359:ILE:HB	1:I:3360:PRO:HD3	1.98	0.45
1:K:5125:ALA:HB2	1:K:5133:LEU:HD12	1.98	0.45
1:K:5487:GLU:HG2	4:K:8070:HOH:O	2.17	0.45
1:K:5318:LEU:HD21	3:K:5:NLX:H11	1.97	0.45
1:L:6286:LEU:O	1:L:6289:LYS:HB2	2.16	0.45
1:L:6251:LEU:HD21	1:L:6333:GLU:HG3	1.98	0.45
1:L:6526:TYR:CE2	1:L:6539:LEU:HA	2.51	0.45
1:A:1034:LEU:C	1:A:1034:LEU:HD13	2.38	0.44
1:A:1375:GLN:HE21	1:A:1375:GLN:CA	2.29	0.44
1:D:4260:ASP:OD1	1:D:4262:LYS:CB	2.65	0.44
1:E:5142:GLY:HA2	3:E:5:NLX:C8	2.42	0.44
1:E:5143:GLY:O	1:E:5144:LEU:HB2	2.16	0.44
1:E:5257:LYS:HB2	1:E:5322:VAL:HG12	1.99	0.44
1:F:6214:SER:HA	1:F:6241:HIS:HD2	1.82	0.44
1:G:1090:ASP:HB3	1:G:1093:ALA:HB3	1.97	0.44
1:I:3364:MET:CE	3:I:3:NLX:H201	2.47	0.44
1:J:4174:ILE:HG12	1:J:4319:LEU:HD11	1.99	0.44
1:J:4493:SER:O	1:J:4497:MET:HG3	2.16	0.44
1:K:5249:VAL:CB	1:K:5433:VAL:HG21	2.46	0.44
1:A:1199:ARG:HG3	4:A:7447:HOH:O	2.17	0.44
1:B:2216:THR:HG23	1:B:2242:ARG:HB3	1.97	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:4225:GLU:O	1:D:4229:VAL:HG23	2.17	0.44
1:D:4437:HIS:NE2	1:D:4442:ALA:HB3	2.32	0.44
1:E:5254:VAL:HG22	1:E:5318:LEU:HD12	1.99	0.44
1:F:6227:VAL:O	1:F:6231:VAL:HG23	2.17	0.44
1:F:6236:ALA:HA	1:F:6239:LEU:HD12	1.99	0.44
1:F:6452:ARG:CB	1:F:6465:ILE:HG12	2.44	0.44
1:G:1313:ARG:HG3	1:G:1313:ARG:NH1	2.32	0.44
1:G:1399:ALA:HB2	1:G:1550:LEU:HD21	1.98	0.44
1:I:3136:MET:HB3	1:I:3218:PHE:CE1	2.52	0.44
1:J:4045:GLN:NE2	1:J:4046:PRO:HD2	2.32	0.44
1:J:4116:CYS:O	1:J:4118:TYR:N	2.51	0.44
1:J:4303:PHE:CB	1:J:4304:LEU:HD22	2.47	0.44
1:K:5461:PRO:HG2	1:K:5464:VAL:HG23	1.99	0.44
1:L:6161:GLU:HG3	1:L:6497:MET:O	2.18	0.44
1:A:1375:GLN:HG2	1:A:1413:LYS:NZ	2.32	0.44
1:C:3353:GLN:NE2	1:C:3465:ILE:H	2.15	0.44
1:C:3361:MET:HE3	1:C:3363:LEU:HG	2.00	0.44
1:G:1049:ILE:HG12	1:G:1122:TYR:CD2	2.52	0.44
1:H:2191:HIS:O	1:H:2195:VAL:HG23	2.18	0.44
1:I:3462:LYS:HZ1	1:J:4376:LYS:HZ2	1.64	0.44
1:I:3491:ARG:HH11	1:I:3491:ARG:HB3	1.81	0.44
1:I:3495:MET:O	1:I:3498:LYS:HB2	2.18	0.44
3:I:3:NLX:O4	3:I:3:NLX:H203	2.17	0.44
1:L:6194:GLN:OE1	1:L:6226:SER:HB3	2.18	0.44
1:A:1304:LEU:HG	3:A:1:NLX:H203	2.00	0.44
1:A:1241:HIS:O	1:A:1344:VAL:HB	2.17	0.44
1:A:1480:PHE:HZ	1:A:1494:LYS:HG3	1.83	0.44
1:B:2023:PRO:HA	1:B:2024:PRO:HD3	1.87	0.44
1:B:2355:PHE:CE2	1:B:2359:ILE:CG2	2.99	0.44
1:C:3361:MET:SD	1:C:3361:MET:C	2.96	0.44
1:F:6317:PRO:HD3	1:F:6387:PRO:HB2	1.98	0.44
1:F:6501:ALA:O	1:F:6504:ALA:HB3	2.17	0.44
1:G:1101:PHE:CD1	1:G:1472:LEU:HD12	2.52	0.44
1:I:3160:HIS:HE1	1:I:3480:PHE:CE2	2.36	0.44
1:J:4045:GLN:HE21	1:J:4046:PRO:HD2	1.81	0.44
1:J:4220:GLU:O	1:J:4221:SER:HB3	2.18	0.44
1:K:5246:GLU:HG2	1:K:5447:TYR:OH	2.17	0.44
1:L:6125:ALA:HB2	1:L:6133:LEU:HD12	1.97	0.44
1:A:1136:MET:HB3	1:A:1218:PHE:CE1	2.53	0.44
1:A:1319:LEU:H	1:A:1319:LEU:CD1	2.28	0.44
1:B:2437:HIS:HD2	1:B:2444:THR:OG1	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:3262:LYS:HB3	1:C:3263:PRO:HD3	1.98	0.44
1:E:5241:HIS:HB3	4:E:7347:HOH:O	2.17	0.44
1:F:6147:GLY:HA2	4:F:7265:HOH:O	2.17	0.44
1:G:1221:SER:O	1:G:1224:GLY:N	2.49	0.44
1:G:1267:GLN:HA	4:G:7984:HOH:O	2.18	0.44
1:G:1265:ALA:HB1	1:G:1282:MET:CE	2.48	0.44
1:H:2404:LEU:N	1:H:2404:LEU:HD23	2.32	0.44
1:I:3026:VAL:HG23	1:I:3050:PHE:CZ	2.53	0.44
1:I:3257:LYS:HZ3	1:I:3316:GLN:HG2	1.83	0.44
1:I:3143:GLY:O	1:I:3318:LEU:HD22	2.17	0.44
1:J:4251:LEU:HD12	1:J:4433:VAL:HG22	1.99	0.44
1:K:5354:GLU:O	1:K:5468:HIS:HB2	2.18	0.44
1:L:6126:ASP:O	1:L:6128:THR:N	2.51	0.44
1:L:6530:GLY:O	1:L:6531:ALA:C	2.56	0.44
1:A:1064:ARG:O	1:A:1066:THR:HG23	2.18	0.44
1:B:2355:PHE:CD2	1:B:2359:ILE:HD12	2.53	0.44
1:B:2455:PHE:CD2	1:B:2482:LYS:HD3	2.53	0.44
1:G:1205:ILE:HD12	1:G:1205:ILE:HA	1.78	0.44
1:G:1191:HIS:HB2	1:G:1327:LEU:HD22	1.99	0.44
1:H:2064:ARG:NH1	1:H:2294:LEU:HD11	2.33	0.44
1:J:4072:GLU:HG2	4:K:7791:HOH:O	2.17	0.44
1:J:4218:PHE:HB3	1:J:4244:ILE:HB	2.00	0.44
1:J:4256:VAL:HG12	1:J:4258:LYS:CD	2.48	0.44
1:J:4364:MET:HG3	3:J:4:NLX:H82	1.98	0.44
1:L:6032:LYS:HB2	1:L:6077:VAL:HG22	2.00	0.44
1:L:6220:GLU:HG2	1:L:6472:LEU:HD21	1.99	0.44
1:L:6185:SER:HB2	1:L:6283:VAL:CG2	2.48	0.44
1:B:2285:CYS:HB2	4:B:7947:HOH:O	2.17	0.44
1:D:4132:ARG:HD2	4:D:7062:HOH:O	2.17	0.44
1:D:4258:LYS:HB2	4:D:7713:HOH:O	2.17	0.44
1:E:5179:SER:HB3	1:E:5187:GLY:HA3	1.98	0.44
1:G:1302:LYS:HB2	1:L:6092:LYS:HZ1	1.83	0.44
1:G:1543:GLU:O	1:G:1547:TRP:HD1	2.00	0.44
1:H:2351:ASN:N	1:H:2351:ASN:HD22	2.16	0.44
1:K:5098:SER:O	1:K:5102:THR:HB	2.17	0.44
1:B:2428:VAL:O	1:B:2432:ILE:HG13	2.18	0.44
1:B:2549:ASN:O	1:B:2550:LEU:C	2.56	0.44
1:E:5099:GLU:O	1:E:5102:THR:HG22	2.17	0.44
1:E:5211:ASN:HD22	1:E:5214:SER:HB3	1.82	0.44
1:F:6097:LEU:CB	3:F:6:NLX:H192	2.47	0.44
1:H:2132:ARG:NH1	4:H:7324:HOH:O	2.50	0.44



	A + 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:H:2524:GLU:O	1:H:2537:GLN:HA	2.18	0.44
1:I:3140:HIS:CD2	1:I:3147:GLY:HA3	2.53	0.44
1:I:3228:SER:CB	1:I:3250:ALA:H	2.31	0.44
1:I:3257:LYS:HB2	1:I:3322:VAL:HG12	2.00	0.44
1:K:5039:SER:HB3	1:K:5046:PRO:CB	2.48	0.44
1:K:5339:ARG:HB2	1:K:5440:ALA:HA	1.99	0.44
1:K:5527:LEU:HD12	1:K:5528:GLN:H	1.83	0.44
1:A:1405:GLY:O	1:A:1406:GLY:C	2.56	0.44
1:A:1463:THR:HG21	1:F:6372:GLN:HB3	2.00	0.44
1:B:2161:GLU:HG3	1:B:2501:ALA:HB2	1.98	0.44
1:B:2453:PRO:C	1:B:2455:PHE:H	2.22	0.44
1:D:4309:GLN:HE21	1:D:4309:GLN:C	2.20	0.44
1:G:1386:TYR:N	1:G:1387:PRO:HD2	2.33	0.44
1:I:3344:VAL:HG22	4:I:7956:HOH:O	2.16	0.44
1:J:4236:ALA:O	1:J:4239:LEU:HB2	2.18	0.44
1:K:5235:LEU:HD12	1:K:5327:LEU:CD1	2.40	0.44
1:A:1032:LYS:HD2	1:A:1077:VAL:HG22	2.00	0.43
1:B:2183:GLU:OE2	1:B:2183:GLU:N	2.45	0.43
1:B:2294:LEU:O	1:B:2298:THR:HG23	2.18	0.43
1:C:3160:HIS:NE2	1:C:3480:PHE:CD2	2.86	0.43
1:C:3260:ASP:OD1	1:C:3263:PRO:HD3	2.19	0.43
1:C:3351:ASN:ND2	4:C:7038:HOH:O	2.51	0.43
1:C:3389:VAL:HB	1:C:3424:VAL:HG11	2.00	0.43
1:D:4064:ARG:HD3	1:D:4065:PHE:CE2	2.53	0.43
1:D:4242:ARG:CG	1:D:4242:ARG:HH11	2.20	0.43
1:E:5361:MET:SD	1:E:5361:MET:C	2.97	0.43
1:F:6512:GLU:N	1:F:6512:GLU:CD	2.71	0.43
1:F:6363:LEU:CD1	3:F:6:NLX:H171	2.40	0.43
1:G:1073:PRO:O	1:H:2186:ARG:NH2	2.51	0.43
1:G:1237:LYS:O	1:G:1238:ASN:HB2	2.17	0.43
1:H:2132:ARG:HD2	4:H:7324:HOH:O	2.17	0.43
1:I:3217:ILE:HG13	1:I:3227:VAL:HG13	1.99	0.43
1:I:3271:THR:HG22	1:I:3297:THR:HG23	2.00	0.43
1:I:3461:PRO:HB2	1:I:3464:VAL:HG23	2.00	0.43
1:L:6487:GLU:HB3	4:L:7856:HOH:O	2.17	0.43
1:B:2051:LEU:HD13	1:B:2083:TYR:CE1	2.53	0.43
1:B:2258:LYS:H	1:B:2258:LYS:HD2	1.83	0.43
1:B:2447:TYR:C	1:B:2447:TYR:CD2	2.91	0.43
1:B:2491:ARG:O	1:B:2492:LEU:C	2.55	0.43
1:C:3132:ARG:HD3	1:C:3132:ARG:HA	1.78	0.43
1:D:4538:LYS:HB3	1:D:4541:ASP:HB2	1.99	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:F:6097:LEU:HD12	1:F:6097:LEU:O	2.18	0.43
1:F:6386:TYR:N	1:F:6387:PRO:HD2	2.32	0.43
1:H:2143:GLY:N	3:H:2:NLX:H152	2.32	0.43
1:H:2409:ASP:OD2	1:H:2412:LYS:HD2	2.18	0.43
1:H:2420:LEU:CD1	1:H:2547:TRP:CZ2	3.01	0.43
1:I:3199:ARG:NH2	4:I:7409:HOH:O	2.47	0.43
1:I:3391:ILE:O	1:I:3392:ALA:C	2.57	0.43
1:I:3480:PHE:HZ	1:I:3494:LYS:HG2	1.82	0.43
1:J:4104:ARG:O	1:J:4482:LYS:NZ	2.51	0.43
1:K:5225:GLU:OE1	1:K:5225:GLU:C	2.56	0.43
1:L:6093:ALA:HB1	3:L:6:NLX:C19	2.47	0.43
1:A:1363:LEU:CB	3:A:1:NLX:H91	2.48	0.43
1:B:2105:LYS:HE3	1:B:2483:GLU:OE1	2.19	0.43
1:C:3200:TRP:O	1:C:3204:ASN:ND2	2.45	0.43
1:C:3264:LEU:CD1	1:C:3316:GLN:HG2	2.47	0.43
1:C:3343:THR:CB	1:C:3442:ALA:HB2	2.40	0.43
1:D:4551:PHE:C	1:D:4553:LYS:H	2.22	0.43
1:E:5304:LEU:CD1	3:E:5:NLX:H181	2.34	0.43
1:G:1130:LYS:HB3	1:G:1130:LYS:HE2	1.78	0.43
1:G:1359:ILE:HG23	3:G:1:NLX:H81	1.98	0.43
1:H:2106:GLU:HA	4:H:7831:HOH:O	2.19	0.43
1:H:2176:GLY:O	1:H:2189:TRP:HB2	2.18	0.43
1:I:3143:GLY:O	1:I:3144:LEU:HB2	2.18	0.43
1:I:3191:HIS:O	1:I:3195:VAL:HG23	2.18	0.43
1:J:4370:GLU:O	1:J:4372:GLN:HG2	2.18	0.43
1:K:5217:ILE:HD12	1:K:5227:VAL:HG13	2.00	0.43
1:K:5370:GLU:C	1:K:5372:GLN:N	2.72	0.43
1:K:5388:LEU:HD22	1:K:5425:MET:CE	2.48	0.43
1:K:5449:PHE:CE2	1:K:5451:TYR:HB3	2.52	0.43
1:A:1064:ARG:NH2	1:A:1114:GLU:OE2	2.49	0.43
1:A:1508:ASN:OD1	1:A:1510:ASN:HB2	2.18	0.43
1:B:2408:ASP:HA	1:B:2413:LYS:HE2	2.00	0.43
1:B:2471:GLU:O	1:B:2475:VAL:HG23	2.19	0.43
1:C:3034:LEU:HB3	1:C:3079:ASN:HA	2.01	0.43
1:D:4079:ASN:HB2	2:D:479:NAG:C8	2.48	0.43
1:G:1138:TRP:O	1:G:1168:ILE:HG12	2.18	0.43
1:G:1266:GLU:O	1:G:1270:ILE:HG13	2.17	0.43
1:G:1403:TYR:CE2	1:G:1420:LEU:HA	2.52	0.43
1:H:2264:LEU:HD21	1:H:2319:LEU:CD2	2.47	0.43
1:J:4526:TYR:CZ	1:J:4539:LEU:HD13	2.52	0.43
1:L:6143:GLY:O	1:L:6145:MET:HG2	2.18	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2051:LEU:HD13	1:B:2083:TYR:CD1	2.54	0.43
1:B:2359:ILE:CD1	3:B:2:NLX:H72	2.48	0.43
1:C:3431:VAL:HG21	1:C:3539:LEU:O	2.18	0.43
1:D:4420:LEU:C	1:D:4420:LEU:CD1	2.87	0.43
1:E:5023:PRO:HB2	1:E:5034:LEU:HD21	2.00	0.43
1:E:5237:LYS:NZ	1:E:5340:ASN:ND2	2.67	0.43
1:G:1352:LYS:HD3	1:G:1450:GLN:NE2	2.33	0.43
1:H:2361:MET:HG2	1:K:5367:PRO:HB3	2.00	0.43
1:I:3262:LYS:HB3	1:I:3263:PRO:HD3	1.99	0.43
1:L:6067:PRO:HG2	4:L:7322:HOH:O	2.18	0.43
1:L:6091:PRO:HB3	1:L:6112:LEU:HD11	1.99	0.43
1:L:6349:GLY:HA3	1:L:6447:TYR:CE2	2.53	0.43
1:B:2220:GLU:OE1	1:B:2221:SER:N	2.52	0.43
1:B:2332:PRO:O	1:B:2336:GLN:HG3	2.18	0.43
1:D:4236:ALA:HA	1:D:4239:LEU:HD12	2.01	0.43
1:D:4252:THR:HG22	1:D:4252:THR:O	2.18	0.43
1:E:5047:VAL:HG21	1:E:5155:LEU:HD23	2.00	0.43
1:E:5153:ASP:OD2	1:E:5155:LEU:HB2	2.19	0.43
1:G:1140:HIS:CE1	1:G:1170:TYR:CE1	3.07	0.43
1:G:1220:GLU:O	1:G:1221:SER:HB3	2.19	0.43
1:G:1374:ASP:O	1:G:1375:GLN:C	2.56	0.43
1:G:1438:ARG:HH12	1:G:1524:GLU:HG2	1.83	0.43
1:H:2145:MET:HG3	1:H:2304:LEU:HD21	2.00	0.43
1:I:3155:LEU:O	1:I:3155:LEU:HD23	2.19	0.43
1:I:3350:ILE:C	1:I:3351:ASN:HD22	2.22	0.43
1:J:4233:SER:HA	1:J:4234:PRO:HD3	1.89	0.43
1:J:4239:LEU:HD23	1:J:4239:LEU:HA	1.73	0.43
1:K:5527:LEU:HG	1:K:5529:ILE:CG1	2.49	0.43
1:L:6336:GLN:HE22	1:L:6433:VAL:HA	1.83	0.43
1:L:6366:TYR:HA	1:L:6367:PRO:HD3	1.75	0.43
1:B:2139:ILE:O	1:B:2223:GLY:HA3	2.19	0.43
1:B:2402:LYS:HG2	1:B:2546:PHE:CZ	2.54	0.43
1:B:2414:LYS:HE2	1:B:2414:LYS:HB3	1.86	0.43
1:B:2536:ALA:O	1:B:2537:GLN:HG3	2.18	0.43
1:C:3025:VAL:HG22	1:C:3034:LEU:HD23	2.00	0.43
1:C:3435:ARG:NH2	4:C:7404:HOH:O	2.40	0.43
1:E:5468:HIS:NE2	3:E:5:NLX:O3	2.51	0.43
1:G:1252:THR:HG23	1:G:1425:MET:O	2.18	0.43
1:H:2138:TRP:CZ3	1:H:2219:GLY:HA2	2.53	0.43
1:I:3090:ASP:HB3	1:I:3093:ALA:HB3	1.98	0.43
1:I:3317:PRO:HB3	4:I:7891:HOH:O	2.17	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:3352:LYS:HE3	1:I:3450:GLN:CD	2.38	0.43
1:I:3354:GLU:O	1:I:3468:HIS:HB2	2.17	0.43
1:J:4140:HIS:HD2	1:J:4147:GLY:HA3	1.83	0.43
1:J:4185:SER:HB2	1:J:4283:VAL:HG21	2.00	0.43
1:K:5087:CYS:O	1:K:5088:THR:C	2.57	0.43
1:L:6237:LYS:HG3	1:L:6238:ASN:ND2	2.34	0.43
1:L:6064:ARG:NH1	1:L:6286:LEU:O	2.52	0.43
1:A:1361:MET:HE1	1:A:1363:LEU:HD21	2.01	0.43
1:A:1412:LYS:O	1:A:1416:LEU:HB2	2.19	0.43
1:A:1445:TYR:OH	1:A:1508:ASN:ND2	2.51	0.43
1:B:2355:PHE:HA	1:B:2359:ILE:HD12	2.01	0.43
1:C:3318:LEU:HD11	3:C:3:NLX:C16	2.48	0.43
1:C:3331:THR:OG1	1:C:3334:GLU:HG3	2.19	0.43
1:C:3414:LYS:HG3	1:C:3415:ASP:N	2.33	0.43
1:F:6324:ASP:OD2	1:F:6327:LEU:HB3	2.19	0.43
1:G:1252:THR:HG22	1:G:1254:VAL:HG12	2.01	0.43
1:G:1304:LEU:HD13	1:G:1317:PRO:O	2.19	0.43
1:G:1384:LYS:O	1:G:1387:PRO:HD2	2.19	0.43
1:G:1396:ILE:HB	1:G:1397:PRO:CD	2.38	0.43
1:G:1528:GLN:HB2	1:G:1534:GLN:NE2	2.34	0.43
1:I:3318:LEU:HD11	3:I:3:NLX:H101	2.01	0.43
1:J:4353:GLN:HE22	1:J:4465:ILE:H	1.67	0.43
1:J:4452:ARG:HH11	1:J:4452:ARG:HG2	1.83	0.43
1:L:6363:LEU:HD22	3:L:6:NLX:H201	2.01	0.43
1:A:1218:PHE:HB2	1:A:1244:ILE:HB	1.99	0.43
1:A:1257:LYS:HD2	1:A:1320:GLY:N	2.30	0.43
1:B:2463:THR:HG23	4:B:7799:HOH:O	2.18	0.43
1:E:5329:LEU:HD12	1:E:5329:LEU:N	2.33	0.43
1:F:6358:LEU:HD23	1:F:6468:HIS:HB3	2.00	0.43
1:G:1308:LEU:HD21	1:G:1367:PRO:HG3	2.01	0.43
1:H:2303:PHE:CD2	1:H:2318:LEU:HA	2.53	0.43
1:I:3206:ALA:HA	1:I:3210:GLY:O	2.19	0.43
1:L:6145:MET:CB	1:L:6304:LEU:HD11	2.49	0.43
1:A:1104:ARG:HG2	1:A:1104:ARG:NH1	2.33	0.43
1:C:3447:TYR:HA	1:C:3527:LEU:O	2.19	0.43
1:E:5064:ARG:O	1:E:5065:PHE:HB2	2.19	0.43
1:G:1523:LYS:HD3	1:G:1537:GLN:HE22	1.84	0.43
1:I:3227:VAL:O	1:I:3231:VAL:HG23	2.19	0.43
1:I:3480:PHE:HZ	1:I:3494:LYS:CG	2.32	0.43
1:J:4407:THR:HG21	1:J:4412:LYS:CD	2.47	0.43
1:L:6533:THR:C	1:L:6534:GLN:HG3	2.39	0.43



		Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	$ ext{overlap}( ext{\AA})$
1:A:1330:LYS:HB2	1:A:1335:LEU:HD21	2.01	0.42
1:B:2174:ILE:HD12	1:B:2298:THR:CG2	2.49	0.42
1:B:2290:THR:OG1	1:B:2293:GLU:HG3	2.19	0.42
1:B:2477:GLY:HA2	1:B:2493:SER:OG	2.19	0.42
1:C:3023:PRO:HA	1:C:3024:PRO:HD3	1.78	0.42
1:C:3044:ALA:O	1:C:3046:PRO:HD3	2.19	0.42
1:E:5218:PHE:HB3	1:E:5244:ILE:HB	1.99	0.42
1:F:6351:ASN:N	1:F:6351:ASN:HD22	2.16	0.42
1:G:1119:LEU:HD12	1:G:1119:LEU:O	2.19	0.42
1:G:1351:ASN:N	1:G:1351:ASN:HD22	2.16	0.42
1:G:1360:PRO:HB2	4:G:7264:HOH:O	2.19	0.42
1:H:2341:PHE:HE1	1:H:2437:HIS:ND1	2.17	0.42
1:L:6142:GLY:O	3:L:6:NLX:H101	2.18	0.42
1:A:1086:MET:HE2	1:A:1110:LEU:CD1	2.47	0.42
1:A:1309:GLN:HE21	1:A:1309:GLN:C	2.22	0.42
1:C:3242:ARG:NH1	1:C:3242:ARG:CG	2.77	0.42
1:E:5518:PRO:HD3	1:E:5535:ALA:HB2	2.01	0.42
1:F:6125:ALA:HB2	1:F:6133:LEU:CD1	2.49	0.42
1:F:6143:GLY:O	1:F:6144:LEU:HB2	2.20	0.42
1:H:2491:ARG:HH11	1:H:2491:ARG:HG2	1.84	0.42
1:I:3104:ARG:HG2	1:I:3104:ARG:HH11	1.84	0.42
1:I:3272:ALA:O	1:I:3289:LYS:HE3	2.19	0.42
1:I:3420:LEU:HD13	1:I:3547:TRP:HZ2	1.81	0.42
1:I:3364:MET:CE	3:I:3:NLX:H171	2.49	0.42
1:J:4125:ALA:HB2	1:J:4133:LEU:HD12	2.00	0.42
1:K:5057:LYS:HB3	1:K:5069:GLN:HB2	2.01	0.42
1:L:6125:ALA:HB2	1:L:6133:LEU:CD1	2.49	0.42
1:L:6185:SER:HB2	1:L:6283:VAL:HG21	2.01	0.42
1:L:6264:LEU:HD22	1:L:6268:ILE:HD13	2.01	0.42
1:A:1304:LEU:CG	3:A:1:NLX:H151	2.49	0.42
1:B:2257:LYS:HE2	1:B:2316:GLN:HE22	1.84	0.42
1:C:3034:LEU:C	1:C:3034:LEU:HD13	2.40	0.42
1:D:4188:ASN:HD22	1:D:4324:ASP:CG	2.22	0.42
1:E:5359:ILE:HB	1:E:5360:PRO:CD	2.50	0.42
1:G:1104:ARG:HD2	1:G:1108:ILE:HG12	2.00	0.42
1:G:1383:TRP:CE3	1:G:1383:TRP:HA	2.54	0.42
1:H:2389:VAL:HB	1:H:2424:VAL:HG11	2.00	0.42
1:J:4119:LEU:HD12	1:J:4119:LEU:C	2.39	0.42
1:J:4453:PRO:HD2	1:J:4470:ASP:OD2	2.19	0.42
1:K:5144:LEU:HB3	1:K:5177:PHE:CE2	2.55	0.42
1:A:1098:SER:O	1:A:1102:THR:HB	2.20	0.42



	•	Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	overlap (Å)
1:A:1467:ASP:N	1:A:1470:ASP:OD2	2.52	0.42
1:B:2252:THR:HG22	1:B:2254:VAL:HG12	2.01	0.42
1:B:2277:THR:HG22	1:B:2278:THR:HG23	2.01	0.42
1:B:2308:LEU:HD11	1:B:2367:PRO:CG	2.49	0.42
1:B:2467:ASP:OD1	1:B:2468:HIS:N	2.46	0.42
1:E:5126:ASP:O	1:E:5128:THR:N	2.53	0.42
1:E:5211:ASN:HD22	1:E:5214:SER:CB	2.32	0.42
1:E:5304:LEU:HD22	3:E:5:NLX:C10	2.41	0.42
1:E:5309:GLN:NE2	4:E:7812:HOH:O	2.49	0.42
1:F:6097:LEU:HD23	1:F:6146:VAL:HG23	2.00	0.42
1:G:1220:GLU:OE2	1:G:1468:HIS:NE2	2.53	0.42
1:H:2026:VAL:HG12	1:H:2027:ASP:N	2.34	0.42
1:H:2040:LEU:HD13	1:H:2155:LEU:HD13	2.01	0.42
1:H:2404:LEU:HB3	1:H:2413:LYS:CG	2.38	0.42
1:J:4321:THR:HG22	1:J:4322:VAL:N	2.35	0.42
1:J:4374:ASP:O	1:J:4376:LYS:N	2.52	0.42
1:K:5336:GLN:HE22	1:K:5433:VAL:HA	1.84	0.42
1:L:6188:ASN:ND2	1:L:6324:ASP:OD2	2.52	0.42
1:L:6246:GLU:HG2	1:L:6447:TYR:OH	2.20	0.42
1:A:1175:TRP:CZ2	1:A:1294:LEU:HB2	2.54	0.42
1:A:1404:LEU:O	1:A:1413:LYS:HE2	2.19	0.42
1:A:1426:PHE:CD1	1:A:1426:PHE:N	2.87	0.42
1:A:1527:LEU:HD11	1:A:1533:THR:HG23	2.00	0.42
1:B:2367:PRO:C	1:B:2368:LEU:HD12	2.40	0.42
1:C:3022:SER:N	4:C:7654:HOH:O	2.51	0.42
1:C:3140:HIS:CD2	1:C:3147:GLY:HA3	2.54	0.42
1:C:3152:TYR:N	1:C:3152:TYR:CD1	2.88	0.42
1:C:3211:ASN:HA	1:C:3212:PRO:HD2	1.93	0.42
1:D:4139:ILE:HG12	1:D:4168:ILE:HD11	2.01	0.42
1:D:4164:VAL:HG11	1:D:4205:ILE:HD11	2.01	0.42
1:D:4079:ASN:CB	2:D:479:NAG:H82	2.49	0.42
1:E:5382:LEU:O	1:E:5385:SER:HB2	2.19	0.42
1:F:6023:PRO:HA	1:F:6024:PRO:HD3	1.74	0.42
1:F:6108:ILE:HA	1:F:6109:PRO:HD3	1.81	0.42
1:H:2152:TYR:N	1:H:2152:TYR:CD1	2.88	0.42
1:H:2330:LYS:HB3	1:H:2334:GLU:OE2	2.19	0.42
1:J:4132:ARG:HA	1:J:4132:ARG:HD3	1.79	0.42
1:J:4231:VAL:HG12	1:J:4231:VAL:O	2.19	0.42
1:J:4312:PRO:C	1:J:4314:GLU:H	2.23	0.42
1:J:4363:LEU:HD22	3:J:4:NLX:C19	2.49	0.42
1:J:4480:PHE:HZ	1:J:4494:LYS:HG3	1.83	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:5025:VAL:CG2	1:K:5034:LEU:HD23	2.50	0.42
1:K:5495:MET:HE3	1:K:5529:ILE:HG23	2.01	0.42
1:L:6096:LEU:O	1:L:6096:LEU:HD12	2.19	0.42
1:L:6085:PRO:HG2	1:L:6115:ASP:O	2.19	0.42
1:L:6290:THR:O	1:L:6291:GLU:C	2.58	0.42
1:A:1025:VAL:CG2	1:A:1034:LEU:HD23	2.33	0.42
1:A:1176:GLY:HA2	1:A:1189:TRP:HB2	2.02	0.42
1:A:1420:LEU:HD12	1:A:1547:TRP:HZ2	1.84	0.42
1:A:1421:ILE:H	1:A:1421:ILE:HD12	1.85	0.42
1:B:2104:ARG:CZ	1:B:2108:ILE:HD12	2.50	0.42
1:D:4086:MET:SD	1:D:4089:GLN:NE2	2.92	0.42
1:D:4145:MET:HB3	1:D:4304:LEU:HD21	2.00	0.42
1:E:5447:TYR:HB3	1:E:5517:TRP:CZ2	2.54	0.42
1:F:6492:LEU:O	1:F:6496:VAL:HG23	2.20	0.42
1:G:1372:GLN:HE22	1:L:6463:THR:HB	1.85	0.42
1:H:2119:LEU:HD12	1:H:2119:LEU:O	2.19	0.42
1:J:4102:THR:OG1	1:J:4103:ASN:N	2.52	0.42
1:J:4190:GLY:O	1:J:4194:GLN:HG3	2.19	0.42
1:K:5197:ALA:O	1:K:5200:TRP:HB3	2.19	0.42
1:L:6040:LEU:HD13	1:L:6155:LEU:HD13	2.01	0.42
1:L:6358:LEU:CD1	1:L:6363:LEU:HD11	2.50	0.42
1:L:6097:LEU:HD13	3:L:6:NLX:O4	2.19	0.42
1:B:2257:LYS:N	1:B:2257:LYS:HD2	2.34	0.42
1:D:4366:TYR:HA	1:D:4367:PRO:HD3	1.88	0.42
1:F:6086:MET:HB3	1:F:6110:LEU:HD13	2.00	0.42
1:G:1411:VAL:HG21	1:L:6411:VAL:HG21	2.01	0.42
1:G:1425:MET:HB2	1:G:1426:PHE:CD1	2.54	0.42
1:H:2404:LEU:O	1:H:2413:LYS:HE2	2.20	0.42
1:I:3138:TRP:CZ3	1:I:3219:GLY:HA2	2.55	0.42
1:I:3332:PRO:O	1:I:3336:GLN:HG3	2.19	0.42
1:I:3366:TYR:OH	1:I:3385:SER:OG	2.33	0.42
1:I:3420:LEU:C	1:I:3420:LEU:HD12	2.40	0.42
1:J:4517:TRP:HA	1:J:4518:PRO:HD2	1.91	0.42
1:L:6452:ARG:HB2	1:L:6465:ILE:HA	2.02	0.42
1:B:2402:LYS:HE2	1:B:2546:PHE:CD1	2.54	0.42
1:E:5414:LYS:NZ	1:E:5414:LYS:HB3	2.34	0.42
1:E:5142:GLY:CA	3:E:5:NLX:H82	2.42	0.42
1:F:6420:LEU:CD1	1:F:6547:TRP:CZ2	3.02	0.42
1:H:2255:LEU:HD23	1:H:2318:LEU:HD21	2.01	0.42
1:H:2316:GLN:HA	1:H:2317:PRO:HD2	1.91	0.42
1:H:2382:LEU:HA	1:H:2385:SER:OG	2.19	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:I:3126:ASP:OD1	1:I:3129:LYS:HG3	2.20	0.42
1:I:3268:ILE:HD11	1:I:3319:LEU:HD21	2.01	0.42
1:J:4089:GLN:OE1	1:J:4094:GLY:HA3	2.20	0.42
1:J:4107:ASN:ND2	1:J:4108:ILE:N	2.68	0.42
1:K:5061:GLY:HA3	1:K:5062:PRO:HD3	1.79	0.42
1:K:5089:GLN:O	1:K:5090:ASP:C	2.57	0.42
1:K:5395:LEU:HD13	1:K:5550:LEU:CD2	2.50	0.42
1:L:6105:LYS:HB2	1:L:6481:LEU:O	2.19	0.42
1:C:3343:THR:HB	1:C:3442:ALA:CB	2.42	0.42
1:E:5526:TYR:CE2	1:E:5539:LEU:HB2	2.55	0.42
1:F:6190:GLY:O	1:F:6193:ASP:HB2	2.20	0.42
1:G:1223:GLY:O	1:G:1227:VAL:HG23	2.19	0.42
1:H:2190:GLY:O	1:H:2194:GLN:HG3	2.19	0.42
1:I:3298:THR:HG22	1:I:3298:THR:O	2.20	0.42
1:I:3338:GLU:C	1:I:3340:ASN:N	2.71	0.42
1:I:3410:THR:HA	1:I:3413:LYS:HB2	2.01	0.42
1:I:3499:PHE:HD2	1:I:3509:PRO:O	2.03	0.42
1:J:4130:LYS:HE2	1:J:4132:ARG:HE	1.83	0.42
1:K:5420:LEU:O	1:K:5424:VAL:HG23	2.20	0.42
1:L:6171:ARG:HD2	1:L:6175:TRP:O	2.20	0.42
1:L:6375:GLN:HG3	1:L:6400:THR:CG2	2.50	0.42
1:A:1324:ASP:OD2	1:A:1325:GLY:N	2.52	0.42
1:A:1375:GLN:NE2	1:A:1375:GLN:HA	2.35	0.42
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.19	0.42
1:B:2403:TYR:OH	1:B:2423:ASP:OD2	2.30	0.42
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.49	0.42
1:C:3444:THR:HG22	1:C:3445:TYR:N	2.35	0.42
1:D:4143:GLY:C	1:D:4145:MET:H	2.23	0.42
1:D:4198:LEU:HA	1:D:4198:LEU:HD23	1.84	0.42
1:E:5537:GLN:NE2	4:E:7903:HOH:O	2.51	0.42
1:F:6243:ALA:O	1:F:6346:TYR:HA	2.19	0.42
1:F:6398:GLU:HB2	4:F:7899:HOH:O	2.18	0.42
1:H:2311:ASP:HB3	1:H:2314:GLU:CG	2.50	0.42
1:H:2304:LEU:CG	3:H:2:NLX:H201	2.49	0.42
1:K:5069:GLN:HE21	1:K:5069:GLN:HA	1.83	0.42
1:L:6545:ALA:HA	1:L:6548:THR:CG2	2.49	0.42
1:A:1049:ILE:HD13	1:A:1122:TYR:CE2	2.55	0.41
1:A:1218:PHE:HA	1:A:1244:ILE:O	2.20	0.41
1:A:1251:LEU:HD12	1:A:1433:VAL:HG23	2.02	0.41
1:A:1375:GLN:HE21	1:A:1375:GLN:HA	1.85	0.41
1:C:3512:GLU:HB3	4:C:7492:HOH:O	2.19	0.41



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:5087:CYS:O	1:E:5088:THR:C	2.58	0.41
1:E:5202:GLN:HG2	4:E:7074:HOH:O	2.19	0.41
1:F:6064:ARG:HH11	1:F:6287:ARG:HA	1.84	0.41
1:F:6453:PRO:HA	1:F:6489:GLU:OE1	2.20	0.41
1:G:1251:LEU:HB2	1:G:1429:PRO:HB3	2.00	0.41
1:G:1264:LEU:HD11	1:G:1316:GLN:HG2	2.02	0.41
1:I:3414:LYS:HD2	1:I:3414:LYS:O	2.20	0.41
1:J:4527:LEU:HD11	1:J:4533:THR:HG22	2.02	0.41
1:K:5241:HIS:O	1:K:5345:PRO:HD2	2.20	0.41
1:L:6111:LYS:NZ	4:L:7632:HOH:O	2.49	0.41
1:A:1303:PHE:CZ	1:A:1319:LEU:HD11	2.55	0.41
1:A:1363:LEU:HD22	3:A:1:NLX:C18	2.43	0.41
1:C:3427:GLY:O	1:C:3428:VAL:C	2.59	0.41
1:E:5225:GLU:O	1:E:5228:SER:HB3	2.19	0.41
1:F:6218:PHE:CB	1:F:6244:ILE:HB	2.50	0.41
1:F:6262:LYS:HA	1:F:6262:LYS:HD2	1.90	0.41
1:F:6420:LEU:CD1	1:F:6547:TRP:HZ2	2.33	0.41
1:F:6445:TYR:CE1	1:F:6509:PRO:HD2	2.55	0.41
1:G:1398:GLU:OE1	1:G:1550:LEU:HD13	2.20	0.41
1:H:2304:LEU:HD22	3:H:2:NLX:H162	2.00	0.41
1:I:3023:PRO:HA	1:I:3024:PRO:HD3	1.68	0.41
1:I:3091:PRO:HB3	1:I:3112:LEU:HD11	2.02	0.41
1:I:3251:LEU:HD12	1:I:3433:VAL:HG22	2.02	0.41
1:K:5333:GLU:OE1	1:K:5333:GLU:N	2.31	0.41
1:K:5438:ARG:HD2	1:K:5522:GLN:NE2	2.35	0.41
1:K:5493:SER:O	1:K:5497:MET:HG3	2.20	0.41
1:K:5550:LEU:C	1:K:5552:ALA:N	2.74	0.41
1:L:6254:VAL:HG12	4:L:7486:HOH:O	2.19	0.41
1:G:1381:LEU:HD21	1:L:6459:MET:HB3	2.01	0.41
1:L:6420:LEU:HD11	1:L:6547:TRP:CH2	2.55	0.41
1:A:1246:GLU:HB3	1:A:1471:GLU:OE1	2.20	0.41
1:A:1526:TYR:CZ	1:A:1536:ALA:HB3	2.55	0.41
1:D:4079:ASN:CG	2:D:479:NAG:C1	2.88	0.41
1:D:4317:PRO:O	1:D:4318:LEU:HB3	2.20	0.41
1:E:5372:GLN:HB3	1:E:5410:THR:OG1	2.20	0.41
1:E:5221:SER:HB2	3:E:5:NLX:O3	2.19	0.41
1:G:1145:MET:CG	1:G:1304:LEU:HD21	2.50	0.41
1:G:1244:ILE:HD11	1:G:1503:PHE:CD2	2.55	0.41
1:G:1367:PRO:O	1:G:1368:LEU:HD23	2.20	0.41
1:G:1435:ARG:NH2	1:G:1541:ASP:OD2	2.53	0.41
1:H:2368:LEU:O	1:K:5368:LEU:O	2.38	0.41


		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:I:3220:GLU:HA	1:I:3246:GLU:O	2.20	0.41	
1:K:5051:LEU:HD22	1:K:5083:TYR:CE1	2.55	0.41	
1:K:5401:GLU:O	1:K:5402:LYS:C	2.58	0.41	
1:K:5404:LEU:HD22	1:K:5413:LYS:O	2.20	0.41	
1:K:5480:PHE:CD1	1:K:5480:PHE:N	2.88	0.41	
1:K:5540:LYS:HA	1:K:5543:GLU:OE2	2.21	0.41	
1:L:6383:TRP:HA	1:L:6383:TRP:CE3	2.55	0.41	
1:B:2237:LYS:HA	1:B:2237:LYS:HD3	1.89	0.41	
1:C:3366:TYR:HA	1:C:3367:PRO:HD3	1.79	0.41	
1:C:3348:VAL:O	1:C:3446:MET:HA	2.20	0.41	
1:C:3304:LEU:HA	3:C:3:NLX:H201	2.02	0.41	
1:D:4040:LEU:O	1:D:4041:GLU:C	2.57	0.41	
1:D:4351:ASN:ND2	1:D:4449:PHE:HB3	2.35	0.41	
1:D:4486:SER:HB2	1:D:4489:GLU:H	1.84	0.41	
1:E:5487:GLU:HG3	1:E:5491:ARG:CZ	2.50	0.41	
1:G:1170:TYR:N	1:G:1170:TYR:CD1	2.89	0.41	
1:G:1448:GLU:OE2	1:G:1539:LEU:CD1	2.69	0.41	
1:H:2176:GLY:O	1:H:2189:TRP:N	2.53	0.41	
1:J:4296:GLU:O	1:J:4300:LYS:HG3	2.20	0.41	
1:J:4524:GLU:HG3	1:J:4538:LYS:CE	2.50	0.41	
1:K:5255:LEU:O	1:K:5320:GLY:HA3	2.21	0.41	
1:K:5290:THR:HG23	1:K:5293:GLU:OE2	2.20	0.41	
1:L:6375:GLN:HA	1:L:6378:ALA:HB3	2.01	0.41	
1:L:6412:LYS:O	1:L:6416:LEU:HD12	2.20	0.41	
1:A:1153:ASP:OD2	1:A:1153:ASP:C	2.59	0.41	
1:A:1373:LEU:N	1:A:1373:LEU:HD12	2.36	0.41	
1:B:2161:GLU:HG3	1:B:2501:ALA:CB	2.51	0.41	
1:B:2423:ASP:HA	4:B:7059:HOH:O	2.19	0.41	
1:C:3104:ARG:NH1	1:C:3153:ASP:HB2	2.36	0.41	
1:D:4442:ALA:HA	1:D:4443:PRO:HD3	1.87	0.41	
1:E:5290:THR:HG23	1:E:5293:GLU:OE2	2.21	0.41	
1:G:1045:GLN:NE2	1:G:1046:PRO:HD2	2.35	0.41	
1:G:1345:PRO:HA	1:G:1443:PRO:O	2.21	0.41	
1:G:1452:ARG:HA	1:G:1453:PRO:HD2	1.85	0.41	
1:H:2345:PRO:HA	1:H:2443:PRO:O	2.20	0.41	
1:I:3389:VAL:HG23	1:I:3391:ILE:HG13	2.03	0.41	
1:L:6363:LEU:CB	3:L:6:NLX:H162	2.48	0.41	
1:L:6093:ALA:CB	3:L:6:NLX:H192	2.50	0.41	
1:A:1186:ARG:HB3	1:A:1324:ASP:HB2	2.03	0.41	
1:A:1398:GLU:OE2	1:A:1550:LEU:HD13	2.20	0.41	
1:D:4279:SER:O	1:D:4283:VAL:HG23	2.21	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:5321:THR:HG22	1:E:5322:VAL:N	2.35	0.41
1:E:5105:LYS:HZ2	1:E:5482:LYS:HA	1.86	0.41
1:E:5395:LEU:HD13	1:E:5550:LEU:CD1	2.50	0.41
1:F:6047:VAL:HG21	1:F:6155:LEU:CD2	2.48	0.41
1:F:6096:LEU:HD23	1:F:6363:LEU:HD21	2.03	0.41
1:G:1119:LEU:C	1:G:1119:LEU:HD12	2.41	0.41
1:H:2074:TRP:CE2	1:H:2078:LYS:HD2	2.55	0.41
1:H:2097:LEU:CD1	3:H:2:NLX:H11	2.51	0.41
1:H:2354:GLU:O	1:H:2468:HIS:HB2	2.20	0.41
1:I:3289:LYS:HA	1:I:3293:GLU:OE2	2.20	0.41
1:I:3364:MET:SD	3:I:3:NLX:H171	2.61	0.41
1:I:3304:LEU:HA	3:I:3:NLX:H202	2.01	0.41
1:J:4232:LEU:HA	1:J:4341:PHE:HB3	2.02	0.41
1:K:5252:THR:HG23	1:K:5425:MET:O	2.21	0.41
1:L:6311:ASP:OD1	1:L:6313:ARG:N	2.49	0.41
1:A:1447:TYR:HB3	1:A:1517:TRP:CZ2	2.55	0.41
1:C:3355:PHE:CD1	1:C:3421:ILE:HG21	2.56	0.41
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.35	0.41
1:C:3449:PHE:CE2	1:C:3451:TYR:HB3	2.55	0.41
1:C:3526:TYR:CD2	1:C:3539:LEU:HB2	2.55	0.41
1:D:4145:MET:CB	1:D:4304:LEU:HD21	2.51	0.41
1:D:4275:LYS:HD3	1:D:4275:LYS:HA	1.73	0.41
1:D:4325:GLY:O	1:D:4329:LEU:CD2	2.69	0.41
1:H:2103:ASN:O	1:H:2481:LEU:HB2	2.21	0.41
1:H:2107:ASN:ND2	1:H:2108:ILE:N	2.68	0.41
1:I:3043:PHE:N	1:I:3043:PHE:CD1	2.88	0.41
1:I:3112:LEU:O	1:I:3113:SER:HB2	2.20	0.41
1:J:4211:ASN:HA	1:J:4212:PRO:HD2	1.94	0.41
1:L:6546:PHE:O	1:L:6549:ASN:HB3	2.20	0.41
1:A:1140:HIS:HD2	1:A:1141:GLY:O	2.03	0.41
1:A:1367:PRO:HB3	1:F:6361:MET:HG2	2.02	0.41
1:A:1420:LEU:HD12	1:A:1547:TRP:CZ2	2.55	0.41
1:B:2381:LEU:O	1:B:2384:LYS:N	2.53	0.41
1:C:3205:ILE:HA	1:C:3205:ILE:HD12	1.95	0.41
1:D:4375:GLN:HE21	1:D:4375:GLN:HB3	1.50	0.41
1:F:6336:GLN:O	1:F:6339:ARG:HD2	2.21	0.41
1:F:6451:TYR:HE2	1:F:6489:GLU:HG3	1.86	0.41
1:G:1311:ASP:HA	1:G:1312:PRO:HD3	1.90	0.41
1:G:1352:LYS:HD3	1:G:1450:GLN:CD	2.41	0.41
1:G:1354:GLU:OE1	1:G:1354:GLU:HA	2.20	0.41
1:H:2358:LEU:HG	1:H:2363:LEU:HD12	2.03	0.41



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:2464:VAL:HG12	1:H:2467:ASP:HB2	2.03	0.41
1:I:3498:LYS:HB3	1:I:3514:LEU:CD1	2.47	0.41
1:L:6090:ASP:HB3	1:L:6093:ALA:HB3	2.03	0.41
1:L:6393:LYS:O	1:L:6396:ILE:HG12	2.21	0.41
1:A:1104:ARG:NH1	1:A:1153:ASP:OD1	2.54	0.41
1:A:1126:ASP:OD2	1:A:1129:LYS:HG2	2.21	0.41
1:C:3534:GLN:N	1:C:3534:GLN:CD	2.73	0.41
1:E:5375:GLN:HE22	1:E:5401:GLU:HA	1.85	0.41
1:F:6262:LYS:NZ	1:F:6282:MET:CE	2.84	0.41
1:G:1132:ARG:HD3	1:G:1132:ARG:HA	1.80	0.41
1:G:1402:LYS:HG3	1:G:1402:LYS:O	2.20	0.41
1:I:3177:PHE:N	1:I:3177:PHE:CD2	2.89	0.41
1:I:3473:PHE:HB3	1:I:3478:ALA:HB3	2.02	0.41
1:J:4363:LEU:HD22	3:J:4:NLX:C18	2.51	0.41
1:K:5034:LEU:HD13	1:K:5034:LEU:O	2.21	0.41
1:K:5217:ILE:HG13	1:K:5227:VAL:HG13	2.03	0.41
1:K:5527:LEU:HG	1:K:5529:ILE:HG13	2.03	0.41
1:L:6218:PHE:HB2	1:L:6244:ILE:HB	2.03	0.41
1:L:6304:LEU:HB3	3:L:6:NLX:C17	2.51	0.41
1:L:6375:GLN:O	1:L:6378:ALA:HB3	2.21	0.41
1:L:6444:THR:HG22	1:L:6445:TYR:N	2.35	0.41
1:A:1220:GLU:O	1:A:1221:SER:HB3	2.21	0.41
1:A:1417:PHE:O	1:A:1420:LEU:HB3	2.21	0.41
1:C:3067:PRO:HB3	1:C:3192:LEU:HD13	2.03	0.41
1:C:3055:PHE:CE1	1:C:3197:ALA:HB2	2.56	0.41
1:C:3175:TRP:CZ2	1:C:3294:LEU:HB2	2.56	0.41
1:C:3475:VAL:HG22	1:C:3496:VAL:CG1	2.50	0.41
1:C:3143:GLY:CA	3:C:3:NLX:C15	2.94	0.41
1:D:4488:GLU:HG2	1:D:4489:GLU:N	2.35	0.41
1:E:5455:PHE:CE1	1:E:5478:ALA:HB3	2.56	0.41
1:E:5491:ARG:HG2	1:E:5491:ARG:NH1	2.36	0.41
1:G:1428:VAL:CB	1:G:1429:PRO:HD3	2.46	0.41
1:G:1395:LEU:HD22	1:G:1550:LEU:HD12	2.03	0.41
1:H:2409:ASP:C	1:H:2411:VAL:H	2.25	0.41
1:I:3277:THR:HG22	1:I:3278:THR:HG23	2.03	0.41
1:J:4351:ASN:HB3	1:J:4466:GLY:O	2.21	0.41
1:J:4447:TYR:C	1:J:4447:TYR:CD2	2.94	0.41
1:K:5404:LEU:C	1:K:5406:GLY:H	2.23	0.41
1:L:6140:HIS:CD2	1:L:6141:GLY:N	2.89	0.41
1:A:1205:ILE:HA	1:A:1205:ILE:HD12	1.92	0.41
1:A:1494:LYS:O	1:A:1498:LYS:HB2	2.21	0.41



	A L	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:3104:ARG:HH11	1:C:3104:ARG:HG2	1.86	0.41
1:C:3371:GLY:HA2	1:D:4371:GLY:HA3	2.02	0.41
1:E:5237:LYS:HZ2	1:E:5340:ASN:ND2	2.19	0.41
1:E:5257:LYS:HE3	1:E:5316:GLN:OE1	2.20	0.41
1:E:5145:MET:CG	1:E:5318:LEU:HD23	2.51	0.41
1:E:5493:SER:O	1:E:5497:MET:HG3	2.21	0.41
1:J:4455:PHE:CE2	1:J:4482:LYS:HB2	2.56	0.41
1:L:6452:ARG:HA	1:L:6453:PRO:HD2	1.95	0.41
3:L:6:NLX:H203	3:L:6:NLX:O4	2.21	0.41
1:A:1257:LYS:NZ	1:A:1318:LEU:O	2.49	0.40
1:B:2549:ASN:O	1:B:2552:ALA:N	2.52	0.40
1:D:4030:HIS:CD2	1:D:4071:ALA:HB3	2.56	0.40
1:D:4057:LYS:HG3	1:D:4058:PRO:HD2	2.03	0.40
1:D:4079:ASN:ND2	4:D:7835:HOH:O	2.48	0.40
1:E:5346:TYR:HB3	1:E:5437:HIS:CD2	2.56	0.40
1:F:6330:LYS:HB2	1:F:6334:GLU:OE1	2.20	0.40
1:F:6338:GLU:C	1:F:6340:ASN:N	2.72	0.40
1:F:6359:ILE:HG23	3:F:6:NLX:H161	2.03	0.40
1:G:1149:ALA:CB	1:G:1169:GLN:HG3	2.51	0.40
1:H:2435:ARG:O	1:H:2438:ARG:HB3	2.22	0.40
1:I:3107:ASN:HD22	1:I:3108:ILE:H	1.69	0.40
1:I:3354:GLU:HB2	1:I:3422:ALA:HB1	2.04	0.40
1:J:4313:ARG:HG2	1:J:4386:TYR:CE2	2.57	0.40
1:K:5313:ARG:HA	1:K:5386:TYR:CD2	2.57	0.40
1:L:6048:ALA:HB3	1:L:6123:THR:CG2	2.50	0.40
1:L:6382:LEU:HD21	1:L:6420:LEU:HD21	2.02	0.40
1:L:6452:ARG:HG2	1:L:6452:ARG:NH1	2.36	0.40
1:A:1254:VAL:O	1:A:1254:VAL:HG22	2.22	0.40
1:A:1349:GLY:HA3	1:A:1447:TYR:CD1	2.56	0.40
1:A:1449:PHE:CE2	1:A:1471:GLU:HA	2.56	0.40
1:B:2241:HIS:O	1:B:2242:ARG:HD2	2.21	0.40
1:C:3495:MET:HG3	1:C:3514:LEU:CD2	2.49	0.40
1:D:4338:GLU:H	1:D:4338:GLU:HG3	1.54	0.40
1:D:4370:GLU:HA	1:D:4370:GLU:OE2	2.22	0.40
1:D:4455:PHE:CD2	1:D:4482:LYS:HD3	2.56	0.40
1:F:6303:PHE:HB3	1:F:6317:PRO:O	2.21	0.40
1:G:1517:TRP:CE3	1:G:1527:LEU:HD22	2.56	0.40
1:H:2428:VAL:HB	1:H:2429:PRO:HD3	2.03	0.40
1:I:3087:CYS:O	1:I:3088:THR:C	2.59	0.40
1:J:4138:TRP:CH2	1:J:4220:GLU:HB2	2.57	0.40
1:J:4303:PHE:C	1:J:4304:LEU:HD22	2.41	0.40



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:K:5205:ILE:HD12	1:K:5205:ILE:HA	1.88	0.40	
1:L:6104:ARG:HD2	4:L:7255:HOH:O	2.22	0.40	
1:A:1123:THR:HG23	1:A:1123:THR:O	2.21	0.40	
1:A:1229:VAL:O	1:A:1232:LEU:N	2.51	0.40	
1:A:1316:GLN:HA	1:A:1316:GLN:OE1	2.21	0.40	
1:B:2205:ILE:HG13	1:B:2210:GLY:HA3	2.02	0.40	
1:B:2373:LEU:CD2	1:B:2378:ALA:HB2	2.33	0.40	
1:C:3040:LEU:HD13	1:C:3155:LEU:HD13	2.03	0.40	
1:C:3223:GLY:O	1:C:3227:VAL:HG23	2.22	0.40	
1:C:3464:VAL:CG2	1:D:4370:GLU:HG3	2.51	0.40	
1:E:5221:SER:HA	1:E:5247:SER:O	2.21	0.40	
1:F:6074:TRP:NE1	1:F:6078:LYS:HB2	2.36	0.40	
1:F:6191:HIS:CD2	1:F:6321:THR:HG23	2.56	0.40	
1:F:6342:HIS:CD2	4:F:7231:HOH:O	2.74	0.40	
1:G:1221:SER:OG	1:G:1222:ALA:N	2.53	0.40	
1:H:2091:PRO:HG3	1:H:2112:LEU:HD11	2.04	0.40	
1:H:2264:LEU:HD22	1:H:2316:GLN:HG3	2.02	0.40	
1:I:3151:THR:HB	1:I:3152:TYR:CE1	2.55	0.40	
1:I:3452:ARG:CZ	1:I:3462:LYS:HA	2.52	0.40	
1:I:3359:ILE:HG23	3:I:3:NLX:C15	2.51	0.40	
1:J:4061:GLY:HA2	4:J:8043:HOH:O	2.21	0.40	
1:K:5318:LEU:HD11	3:K:5:NLX:C2	2.52	0.40	
1:K:5357:TRP:O	1:K:5361:MET:CB	2.69	0.40	
1:K:5425:MET:HG2	4:K:7147:HOH:O	2.22	0.40	
1:K:5495:MET:O	1:K:5499:PHE:HB2	2.22	0.40	
1:L:6358:LEU:HD11	1:L:6363:LEU:HD11	2.04	0.40	
1:A:1266:GLU:O	1:A:1270:ILE:HD12	2.21	0.40	
1:A:1341:PHE:N	1:A:1341:PHE:CD2	2.89	0.40	
1:A:1519:GLU:HG2	1:A:1520:TYR:N	2.36	0.40	
1:A:1539:LEU:N	4:A:7558:HOH:O	2.54	0.40	
1:B:2026:VAL:CG1	1:B:2027:ASP:N	2.84	0.40	
1:C:3431:VAL:HA	1:C:3446:MET:CE	2.51	0.40	
1:D:4211:ASN:HA	1:D:4212:PRO:HD2	1.93	0.40	
1:E:5022:SER:HB3	4:E:8085:HOH:O	2.21	0.40	
1:E:5145:MET:CB	1:E:5304:LEU:HD11	2.49	0.40	
1:F:6449:PHE:CE2	1:F:6451:TYR:HB3	2.57	0.40	
1:F:6471:GLU:O	1:F:6475:VAL:HG23	2.21	0.40	
1:F:6534:GLN:CD	1:F:6534:GLN:H	2.24	0.40	
1:G:1351:ASN:O	1:G:1352:LYS:C	2.60	0.40	
1:H:2048:ALA:HB3	1:H:2123:THR:CG2	2.47	0.40	
1:H:2244:ILE:HG12	1:H:2347:MET:HB3	2.03	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2		overlap (Å)
1:I:3191:HIS:HD2	1:I:3321:THR:HG23	1.85	0.40
1:J:4049:ILE:HG12	1:J:4122:TYR:CD2	2.56	0.40
1:J:4182:ASP:N	1:J:4182:ASP:OD2	2.54	0.40
1:J:4370:GLU:C	1:J:4372:GLN:H	2.24	0.40
1:K:5249:VAL:H	1:K:5252:THR:HG1	1.70	0.40
1:K:5450:GLN:O	1:K:5451:TYR:HB2	2.21	0.40
1:K:5498:LYS:HG2	1:K:5502:ASN:ND2	2.33	0.40
1:L:6263:PRO:HB2	4:L:7197:HOH:O	2.21	0.40
1:L:6351:ASN:HD22	1:L:6351:ASN:N	2.19	0.40
1:L:6545:ALA:C	1:L:6548:THR:HG22	2.42	0.40
1:A:1401:GLU:C	1:A:1403:TYR:H	2.25	0.40
1:A:1420:LEU:CD1	1:A:1547:TRP:CZ2	3.05	0.40
1:A:1420:LEU:CD1	1:A:1547:TRP:HZ2	2.35	0.40
1:B:2339:ARG:O	1:B:2341:PHE:CD2	2.74	0.40
1:C:3357:TRP:C	1:C:3360:PRO:HD2	2.41	0.40
1:C:3526:TYR:CE1	1:C:3539:LEU:HD13	2.57	0.40
1:E:5034:LEU:C	1:E:5034:LEU:CD2	2.90	0.40
1:F:6185:SER:HB2	1:F:6283:VAL:HG21	2.03	0.40
1:H:2420:LEU:CD1	1:H:2547:TRP:HZ2	2.33	0.40
1:J:4355:PHE:HB2	1:J:4422:ALA:HB2	2.02	0.40
1:J:4428:VAL:CB	1:J:4429:PRO:HD3	2.43	0.40
1:K:5036:LYS:HG2	1:K:5049:ILE:HB	2.03	0.40
1:K:5142:GLY:CA	3:K:5:NLX:H82	2.52	0.40
1:K:5389:VAL:HB	1:K:5391:ILE:HG13	2.03	0.40
1:L:6426:PHE:C	1:L:6429:PRO:HD2	2.42	0.40

There are no symmetry-related clashes.

# 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	Percentiles
1	А	530/548~(97%)	480 (91%)	41 (8%)	9 (2%)	9 31



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entiles
1	В	530/548~(97%)	476 (90%)	48 (9%)	6 (1%)	14	42
1	С	529/548~(96%)	489 (92%)	33~(6%)	7 (1%)	12	37
1	D	531/548~(97%)	491 (92%)	36~(7%)	4 (1%)	19	51
1	Ε	529/548~(96%)	482 (91%)	40 (8%)	7 (1%)	12	37
1	F	529/548~(96%)	477 (90%)	44 (8%)	8 (2%)	10	34
1	G	530/548~(97%)	467 (88%)	55~(10%)	8 (2%)	10	34
1	Н	529/548~(96%)	470 (89%)	52~(10%)	7 (1%)	12	37
1	Ι	529/548~(96%)	466 (88%)	56 (11%)	7 (1%)	12	37
1	J	530/548~(97%)	484 (91%)	40 (8%)	6 (1%)	14	42
1	K	529/548~(96%)	475~(90%)	48 (9%)	6 (1%)	14	42
1	L	529/548~(96%)	467 (88%)	53~(10%)	9(2%)	9	31
All	All	6354/6576~(97%)	5724 (90%)	546 (9%)	84 (1%)	12	37

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1253	SER
1	В	2342	HIS
1	С	3253	SER
1	D	4185	SER
1	D	4253	SER
1	Е	5237	LYS
1	Е	5253	SER
1	G	1253	SER
1	G	1339	ARG
1	G	1375	GLN
1	Н	2205	ILE
1	Ι	3535	ALA
1	J	4105	LYS
1	J	4253	SER
1	L	6539	LEU
1	А	1185	SER
1	А	1375	GLN
1	В	2237	LYS
1	В	2253	SER
1	В	2340	ASN
1	С	3185	SER
1	С	3405	GLY



Mol	Chain	Res	Type
1	C	3427	GLY
1	D	4552	ALA
1	E	5127	LEU
1	E	5371	GLY
1	F	6185	SER
1	F	6406	GLY
1	G	1462	LYS
1	G	1520	TYR
1	H	2185	SER
1	Н	2253	SER
1	Н	2375	GLN
1	I	3341	PHE
1	J	4185	SER
- 1		4375	GLN
1	K	5237	LYS
1	K	5340	ASN
1	L	6127	LEU
1	Ā	1358	LEU
1	C	3127	LEU
1	D	4337	ALA
1	E	5044	ALA
1	F	6357	TRP
1	G	1378	ALA
1	I	3185	SER
1	J	4343	THR
1	J	4371	GLY
1	K	5185	SER
1	K	5253	SER
1	K	5338	GLU
1	L	6142	GLY
1	A	1221	SER
1	A	1406	GLY
1	С	3079	ASN
1	C	3113	SER
1	Е	5185	SER
1	F	6253	SER
1	F	6479	PRO
1	G	1185	SER
1	Н	2343	THR
1	Н	2462	LYS
1	Ι	3205	ILE
1	L	6041	GLU



Mol	Chain	Res	Type
1	L	6253	SER
1	L	6254	VAL
1	А	1155	LEU
1	А	1538	LYS
1	В	2044	ALA
1	В	2373	LEU
1	F	6129	LYS
1	G	1352	LYS
1	Ι	3142	GLY
1	L	6358	LEU
1	L	6538	LYS
1	А	1356	GLY
1	F	6259	GLY
1	F	6358	LEU
1	L	6303	PHE
1	E	5427	GLY
1	Ι	3367	PRO
1	Ι	3427	GLY
1	K	5061	GLY
1	Н	2173	GLY

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	$\mathbf{ntiles}$
1	А	448/463~(97%)	435~(97%)	13 (3%)	42	76
1	В	448/463~(97%)	431~(96%)	17~(4%)	33	67
1	С	447/463~(96%)	420 (94%)	27~(6%)	19	49
1	D	448/463~(97%)	423~(94%)	25~(6%)	21	52
1	Е	447/463~(96%)	422 (94%)	25~(6%)	21	52
1	F	447/463~(96%)	426~(95%)	21 (5%)	26	59
1	G	448/463~(97%)	419 (94%)	29 (6%)	17	45
1	Η	447/463~(96%)	427 (96%)	20 (4%)	27	61



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	Ι	447/463~(96%)	418 (94%)	29~(6%)	17	45
1	J	448/463~(97%)	426~(95%)	22~(5%)	25	57
1	Κ	447/463~(96%)	421 (94%)	26~(6%)	20	50
1	L	447/463~(96%)	433~(97%)	14(3%)	40	74
All	All	5369/5556~(97%)	5101~(95%)	268~(5%)	24	57

Continued from previous page...

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1078	LYS
1	А	1218	PHE
1	А	1253	SER
1	А	1264	LEU
1	А	1304	LEU
1	А	1309	GLN
1	А	1341	PHE
1	А	1366	TYR
1	А	1394	GLU
1	А	1408	ASP
1	А	1410	THR
1	А	1488	GLU
1	А	1491	ARG
1	В	2034	LEU
1	В	2111	LYS
1	В	2160	HIS
1	В	2218	PHE
1	В	2220	GLU
1	В	2225	GLU
1	В	2258	LYS
1	В	2299	LEU
1	В	2309	GLN
1	В	2319	LEU
1	В	2341	PHE
1	В	2346	TYR
1	В	2366	TYR
1	В	2404	LEU
1	В	2420	LEU
1	В	2499	PHE
1	В	2512	GLU
1	С	3027	ASP
1	С	3088	THR



Mol	Chain	Res	Type
1	С	3106	GLU
1	С	3107	ASN
1	С	3155	LEU
1	C	3218	PHE
1	С	3220	GLU
1	С	3221	SER
1	С	3225	GLU
1	С	3242	ARG
1	С	3264	LEU
1	С	3296	GLU
1	С	3299	LEU
1	С	3309	GLN
1	С	3319	LEU
1	С	3330	LYS
1	С	3333	GLU
1	С	3339	ARG
1	С	3355	PHE
1	С	3374	ASP
1	С	3394	GLU
1	С	3414	LYS
1	С	3420	LEU
1	С	3483	GLU
1	С	3499	PHE
1	С	3500	TRP
1	С	3534	GLN
1	D	4027	ASP
1	D	4078	LYS
1	D	4106	GLU
1	D	4107	ASN
1	D	4218	PHE
1	D	4242	ARG
1	D	4253	SER
1	D	4264	LEU
1	D	4279	SER
1	D	4304	LEU
1	D	4309	GLN
1	D	4316	GLN
1	D	4327	LEU
1	D	4338	GLU
1	D	4341	PHE
1	D	4346	TYR
1	D	4363	LEU
		-	·]



Mol	Chain	Res	Type
1	D	4366	TYR
1	D	4372	GLN
1	D	4375	GLN
1	D	4420	LEU
1	D	4458	ASP
1	D	4471	GLU
1	D	4488	GLU
1	D	4491	ARG
1	Е	5033	VAL
1	Е	5034	LEU
1	Е	5079	ASN
1	Е	5105	LYS
1	Е	5107	ASN
1	Е	5111	LYS
1	Е	5155	LEU
1	Е	5203	ASP
1	Е	5218	PHE
1	Е	5220	GLU
1	Е	5225	GLU
1	Е	5258	LYS
1	Е	5266	GLU
1	Е	5289	LYS
1	Е	5305	SER
1	Е	5319	LEU
1	Е	5340	ASN
1	Е	5346	TYR
1	Е	5366	TYR
1	Е	5370	GLU
1	Е	5394	GLU
1	Е	5408	ASP
1	Е	5463	THR
1	Е	5499	PHE
1	Е	5500	TRP
1	F	6072	GLU
1	F	6155	LEU
1	F	6203	ASP
1	F	6214	SER
1	F	6220	GLU
1	F	6221	SER
1	F	6249	VAL
1	F	6257	LYS
1	F	6258	LYS
	1		



NonChainResType1F6264LEU1F6277THR1F6323ILE1F6346TYR1F6372GLN1F6374ASP1F6414LYS1F6471GLU1F6471GLU1F6489GLU1F6500TRP1F6541ASP1F6541ASP1G1034LEU1G1041GLU1G1104ARG1G1128THR1G1218PHE1G1225GLU1G1264LEU1G1267THR1G1264LEU1G1276THR1G1276THR1G1309GLN1G1318LEU1G1318LEU1G1340ASN1G1366TYR1G1360SER1G1363SER1G1363LYS1G1363SER1G1363SER1G1363SER1G1363SER1G1363 </th <th>Mal</th> <th>Chair</th> <th>Por</th> <th>Tuno</th>	Mal	Chair	Por	Tuno
I     F $6264$ LEU       1     F $6277$ THR       1     F $6323$ ILE       1     F $6372$ GLN       1     F $6374$ ASP       1     F $6414$ LYS       1     F $6471$ GLU       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1128$ THR       1     G $1225$ GLU       1     G $1267$ GLN       1     G $1267$ GLN	10101		nes	LTT
I     F     6277     THR       1     F     6323     ILE       1     F     6346     TYR       1     F     6372     GLN       1     F     6374     ASP       1     F     6414     LYS       1     F     6414     LYS       1     F     6471     GLU       1     F     6489     GLU       1     F     6534     GLN       1     F     6541     ASP       1     G     1041     GLU       1     G     1041     GLU       1     G     1041     GLU       1     G     1126     ASP       1     G     1128     THR       1     G     1218     PHE       1     G     1225     GLU       1     G     1267     GLN       1     G     1276     THR       1     G <td></td> <td>F F</td> <td>6264</td> <td>LEU</td>		F F	6264	LEU
I     F $6323$ ILE       1     F $6372$ GLN       1     F $6374$ ASP       1     F $6414$ LYS       1     F $6414$ LYS       1     F $6471$ GLU       1     F $6471$ GLU       1     F $6471$ GLU       1     F $6500$ TRP       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1128$ THR       1     G $1225$ GLU       1     G $1267$ GLN       1     G $1267$ GLN       1     G $1309$ GLN	1		6277	THR
1     F $6346$ TYR       1     F $6372$ GLN       1     F $6374$ ASP       1     F $6414$ LYS       1     F $6414$ LYS       1     F $6471$ GLU       1     F $6471$ GLU       1     F $6500$ TRP       1     F $6534$ GLN       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1128$ THR       1     G $1225$ GLU       1     G $1267$ GLN       1     G $1267$ GLN       1     G $1309$ GLN	1	F'	6323	ILE
1     F $6372$ GLN       1     F $6374$ ASP       1     F $6414$ LYS       1     F $6471$ GLU       1     F $6471$ GLU       1     F $6471$ GLU       1     F $6500$ TRP       1     F $6534$ GLN       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1126$ ASP       1     G $1126$ ASP       1     G $1128$ THR       1     G $1225$ GLU       1     G $1226$ SER       1     G $1277$ THR       1     G $1277$ THR       1     G $1319$ LEU	1	F	6346	TYR
1     F $6374$ ASP       1     F $6414$ LYS       1     F $6471$ GLU       1     F $6489$ GLU       1     F $6500$ TRP       1     F $6534$ GLN       1     F $6534$ GLN       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1128$ THR       1     G $1225$ GLU       1     G $1226$ SER       1     G $1267$ GLN       1     G $1277$ THR       1     G $1309$ GLN       1     G $1319$ LEU	1	F'	6372	GLN
1     F $6414$ LYS       1     F $6471$ GLU       1     F $6489$ GLU       1     F $6500$ TRP       1     F $6534$ GLN       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1034$ LEU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1128$ THR       1     G $1225$ GLU       1     G $1267$ GLN       1     G $1267$ GLN       1     G $1277$ THR       1     G $1309$ GLN       1     G $1319$ LEU	1	F	6374	ASP
1     F $6471$ GLU       1     F $6489$ GLU       1     F $6500$ TRP       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1034$ LEU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1128$ THR       1     G $1218$ PHE       1     G $1225$ GLU       1     G $1267$ GLN       1     G $1267$ GLN       1     G $1276$ THR       1     G $1309$ GLN       1     G $1319$ LEU       1     G $1340$ ASN	1	F	6414	LYS
1     F $6489$ GLU       1     F $6500$ TRP       1     F $6534$ GLN       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1034$ LEU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1128$ THR       1     G $1225$ GLU       1     G $1226$ SER       1     G $1267$ GLN       1     G $1277$ THR       1     G $1309$ GLN       1     G $1318$ LEU       1     G $1340$ ASN	1	F	6471	GLU
1     F $6500$ TRP       1     F $6534$ GLN       1     F $6541$ ASP       1     G $1034$ LEU       1     G $1041$ GLU       1     G $1041$ GLU       1     G $1104$ ARG       1     G $1126$ ASP       1     G $1126$ ASP       1     G $1128$ THR       1     G $1218$ PHE       1     G $1225$ GLU       1     G $1264$ LEU       1     G $1267$ GLN       1     G $1277$ THR       1     G $1309$ GLN       1     G $1318$ LEU       1     G $1340$ ASN       1     G $1340$ ASN       1     G $1346$ TYR	1	F	6489	GLU
1   F $6534$ GLN     1   G $1034$ LEU     1   G $1041$ GLU     1   G $1041$ GLU     1   G $1104$ ARG     1   G $1126$ ASP     1   G $1128$ THR     1   G $1128$ THR     1   G $1218$ PHE     1   G $1225$ GLU     1   G $1264$ LEU     1   G $1267$ GLN     1   G $1276$ THR     1   G $1277$ THR     1   G $1279$ SER     1   G $1309$ GLN     1   G $1340$ ASN     1   G $1340$ ASN     1   G $1346$ TYR     1   G $1366$ TYR     1   G $1393$ LYS     1   G $1463$	1	F	6500	TRP
1   F   6541   ASP     1   G   1034   LEU     1   G   1041   GLU     1   G   1104   ARG     1   G   1126   ASP     1   G   1126   ASP     1   G   1128   THR     1   G   1218   PHE     1   G   1225   GLU     1   G   1264   LEU     1   G   1267   GLN     1   G   1276   THR     1   G   1277   THR     1   G   1279   SER     1   G   1309   GLN     1   G   1318   LEU     1   G   1340   ASN     1   G   1340   ASN     1   G   1346   TYR     1   G   1366   TYR     1   G   1375   GLN     1   G   1393   LYS	1	F	6534	GLN
1   G $1034$ LEU     1   G $1041$ GLU     1   G $1104$ ARG     1   G $1126$ ASP     1   G $1126$ ASP     1   G $1128$ THR     1   G $1128$ THR     1   G $1218$ PHE     1   G $1225$ GLU     1   G $1226$ SER     1   G $1267$ GLN     1   G $1277$ THR     1   G $1277$ THR     1   G $1277$ THR     1   G $1309$ GLN     1   G $1318$ LEU     1   G $1340$ ASN     1   G $1340$ ASN     1   G $1346$ TYR     1   G $1375$ GLN     1   G $1393$ LYS     1   G $1463$	1	F	6541	ASP
1   G $1041$ GLU     1   G $1104$ ARG     1   G $1126$ ASP     1   G $1128$ THR     1   G $1128$ THR     1   G $1218$ PHE     1   G $1225$ GLU     1   G $1226$ SER     1   G $1264$ LEU     1   G $1267$ GLN     1   G $1276$ THR     1   G $1277$ THR     1   G $1279$ SER     1   G $1309$ GLN     1   G $1318$ LEU     1   G $1346$ TYR     1   G $1346$ TYR     1   G $1375$ GLN     1   G $1393$ LYS     1   G $1393$ LYS     1   G $1463$ THR     1   G $1463$	1	G	1034	LEU
1   G   1104   ARG     1   G   1126   ASP     1   G   1128   THR     1   G   1146   VAL     1   G   1218   PHE     1   G   1225   GLU     1   G   1226   SER     1   G   1264   LEU     1   G   1267   GLN     1   G   1276   THR     1   G   1277   THR     1   G   1279   SER     1   G   1309   GLN     1   G   1318   LEU     1   G   1319   LEU     1   G   1340   ASN     1   G   1346   TYR     1   G   1366   TYR     1   G   1375   GLN     1   G   1393   LYS     1   G   1393   LYS     1   G   1463   THR  1	1	G	1041	GLU
1   G   1126   ASP     1   G   1128   THR     1   G   1146   VAL     1   G   1218   PHE     1   G   1225   GLU     1   G   1226   SER     1   G   1264   LEU     1   G   1267   GLN     1   G   1276   THR     1   G   1277   THR     1   G   1279   SER     1   G   1309   GLN     1   G   1318   LEU     1   G   1319   LEU     1   G   1340   ASN     1   G   1346   TYR     1   G   1366   TYR     1   G   1375   GLN     1   G   1393   LYS     1   G   1393   LYS     1   G   1458   ASP     1   G   1463   THR	1	G	1104	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1126	ASP
1   G   1146   VAL     1   G   1218   PHE     1   G   1225   GLU     1   G   1226   SER     1   G   1267   GLN     1   G   1267   GLN     1   G   1267   GLN     1   G   1276   THR     1   G   1279   SER     1   G   1309   GLN     1   G   1318   LEU     1   G   1319   LEU     1   G   1340   ASN     1   G   1340   ASN     1   G   1340   ASN     1   G   1366   TYR     1   G   1366   TYR     1   G   1375   GLN     1   G   1393   LYS     1   G   1407   THR     1   G   1458   ASP     1   G   1463   THR	1	G	1128	THR
1   G   1218   PHE     1   G   1225   GLU     1   G   1226   SER     1   G   1264   LEU     1   G   1267   GLN     1   G   1276   THR     1   G   1277   THR     1   G   1279   SER     1   G   1309   GLN     1   G   1319   LEU     1   G   1319   LEU     1   G   1346   TYR     1   G   1366   TYR     1   G   1375   GLN     1   G   1375   GLN     1   G   1375   GLN     1   G   1393   LYS     1   G   1407   THR     1   G   1458   ASP     1   G   1453   THR     1   G   1463   THR     1   G   1500   TRP	1	G	1146	VAL
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1218	PHE
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1225	GLU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1226	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1264	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1267	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1276	THR
1   G   1279   SER     1   G   1309   GLN     1   G   1318   LEU     1   G   1319   LEU     1   G   1340   ASN     1   G   1346   TYR     1   G   1366   TYR     1   G   1366   TYR     1   G   1375   GLN     1   G   1380   SER     1   G   1393   LYS     1   G   1407   THR     1   G   1458   ASP     1   G   1453   THR     1   G   1500   TRP     1   G   1522   GLN	1	G	1277	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1279	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1309	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1318	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1319	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	1340	ASN
1     G     1366     TYR       1     G     1375     GLN       1     G     1375     GLN       1     G     1380     SER       1     G     1393     LYS       1     G     1407     THR       1     G     1458     ASP       1     G     1463     THR       1     G     1500     TRP       1     G     1522     GLN	1	G	1346	TYR
1     G     1375     GLN       1     G     1380     SER       1     G     1393     LYS       1     G     1407     THR       1     G     1458     ASP       1     G     1463     THR       1     G     1500     TRP       1     G     1522     GLN	1	G	1366	TYR
1     G     1380     SER       1     G     1393     LYS       1     G     1407     THR       1     G     1458     ASP       1     G     1463     THR       1     G     1500     TRP       1     G     1522     GLN	1	G	1375	GLN
1     G     1393     LYS       1     G     1407     THR       1     G     1458     ASP       1     G     1458     THR       1     G     1463     THR       1     G     1500     TRP       1     G     1522     GLN	1	G	1380	SER
1     G     1407     THR       1     G     1458     ASP       1     G     1463     THR       1     G     1500     TRP       1     G     1522     GLN	1	G	1393	LYS
1     G     1458     ASP       1     G     1463     THR       1     G     1500     TRP       1     G     1522     GLN	1	G	1407	THR
1     G     1463     THR       1     G     1500     TRP       1     G     1522     GLN	1	G	1458	ASP
1     G     1500     TRP       1     G     1522     GLN	1	G	1463	THR
1 G 1522 GLN	1	G	1500	TRP
	1	G	1522	GLN
$1 \mid G \mid 1541 \mid ASP \mid$	1	G	1541	ASP
1 H 2034 LEU	1	Н	2034	LEU



Mol	Chain	Res	Type
1	Н	2111	LYS
1	H	2129	LYS
 1	H	$\frac{2120}{2132}$	ARG
1	H	2152	LEU
1	H	2100	PHE
1	H	2210	GLU
1	H H	2220	
1	H H	2200	GLU
 	 Ц	2292	CIN
	 Ц	2309	CLU
1	11 U	2000	
1	П	2342	
1		2040	
1		2404	
1		2409	ASP
1	H TT	2411	VAL
	H	2483	GLU
1	H	2499	PHE
1	H	2500	TRP
1	H	2532	ASN
1	l	3034	LEU
1	I	3064	ARG
1	I	3072	GLU
1	I	3105	LYS
1	I	3107	ASN
1	Ι	3155	LEU
1	Ι	3218	PHE
1	Ι	3220	GLU
1	Ι	3225	GLU
1	I	3240	PHE
1	Ι	3258	LYS
1	Ι	3264	LEU
1	Ι	3296	GLU
1	Ι	3299	LEU
1	Ι	3330	LYS
1	Ι	3340	ASN
1	Ι	3341	PHE
1	Ι	3346	TYR
1	Ι	3372	GLN
1	Ι	3374	ASP
1	Ι	3385	SER
1	Ι	3414	LYS
1	I	3420	LEU
-	· ·		



Mol	Chain	Res	
1	I	3447	TVR
 1	I T	3/70	
1	I	3500	TRP
1	I	2512	CLU
1	I	$\frac{3312}{2524}$	CLN
1	I	2540	ASN
	I T	3049	ASN
1	J	4027	ASP
	J	4034	CLU
	J	4041	GLU
1	J	4072	GLU
1	J	4102	THR
	J	4104	ARG
1	J	4107	ASN
1	J	4218	PHE
1	J	4258	LYS
1	J	4264	LEU
1	J	4282	MET
1	J	4297	THR
1	J	4304	LEU
1	J	4316	GLN
1	J	4319	LEU
1	J	4342	HIS
1	J	4366	TYR
1	J	4375	GLN
1	J	4394	GLU
1	J	4404	LEU
1	J	4471	GLU
1	J	4506	ASN
1	K	5033	VAL
1	K	5066	THR
1	K	5069	GLN
1	K	5128	THR
1	K	5155	LEU
1	K	5220	GLU
1	K	5225	GLU
1	K	5240	PHE
1	K	5242	ARG
1	K	5258	LYS
1	K	5299	LEU
1	K	5305	SER
1	K	5309	GLN
1	K	5330	LYS
-		0000	<b>11</b>



Mol	Chain	Res	Type
1	K	5341	PHE
1	K	5366	TYR
1	K	5374	ASP
1	K	5375	GLN
1	K	5390	CYS
1	K	5426	PHE
1	K	5439	ASP
1	K	5463	THR
1	K	5499	PHE
1	K	5500	TRP
1	Κ	5512	GLU
1	K	5541	ASP
1	L	6107	ASN
1	L	6130	LYS
1	L	6155	LEU
1	L	6218	PHE
1	L	6220	GLU
1	L	6258	LYS
1	L	6264	LEU
1	L	6278	THR
1	L	6414	LYS
1	L	6419	ASP
1	L	6420	LEU
1	L	6447	TYR
1	L	6463	THR
1	L	6500	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	1030	HIS
1	А	1079	ASN
1	А	1095	GLN
1	А	1131	ASN
1	А	1140	HIS
1	А	1160	HIS
1	А	1162	ASN
1	А	1184	HIS
1	А	1238	ASN
1	А	1241	HIS
1	А	1288	GLN
1	А	1309	GLN



Mol	Chain	Res	Type
1	A	1336	GLN
1	A	1340	ASN
1	A	1342	HIS
1	A	1351	ASN
1	A	1353	GLN
1	A	1372	GLN
1	A	1375	GLN
1	А	1436	ASN
1	А	1502	ASN
1	В	2030	HIS
1	В	2045	GLN
1	В	2069	GLN
1	В	2140	HIS
1	В	2162	ASN
1	В	2241	HIS
1	В	2309	GLN
1	В	2316	GLN
1	В	2336	GLN
1	В	2351	ASN
1	В	2353	GLN
1	В	2372	GLN
1	В	2436	ASN
1	В	2450	GLN
1	В	2532	ASN
1	В	2537	GLN
1	С	3045	GLN
1	С	3095	GLN
1	С	3140	HIS
1	С	3162	ASN
1	С	3202	GLN
1	С	3238	ASN
1	С	3241	HIS
1	С	3351	ASN
1	С	3353	GLN
1	С	3375	GLN
1	C	3436	ASN
1	C	3437	HIS
1	C	3450	GLN
1	С	3532	ASN
1	C	3534	GLN
1	C	3537	GLN
1	D	4069	GLN



Mol	Chain	Res	Type
1	D	4107	ASN
1	D	4131	ASN
1	D	4140	HIS
1	D	4241	HIS
1	D	4309	GLN
1	D	4336	GLN
1	D	4342	HIS
1	D	4351	ASN
1	D	4372	GLN
1	D	4375	GLN
1	D	4450	GLN
1	D	4508	ASN
1	D	4510	ASN
1	D	4537	GLN
1	E	5131	ASN
1	Е	5140	HIS
1	Е	5162	ASN
1	Е	5211	ASN
1	Е	5241	HIS
1	Е	5309	GLN
1	Е	5336	GLN
1	Е	5340	ASN
1	Е	5353	GLN
1	Е	5375	GLN
1	Е	5436	ASN
1	Е	5437	HIS
1	Е	5506	ASN
1	Е	5532	ASN
1	Е	5537	GLN
1	F	6030	HIS
1	F	6079	ASN
1	F	6095	GLN
1	F	6140	HIS
1	F	6160	HIS
1	F	6211	ASN
1	F	6241	HIS
1	F	6336	GLN
1	F	6351	ASN
1	F	6353	GLN
1	F	6436	ASN
1	F	6532	ASN
1	F	6534	GLN
	1		



Mol	Chain	Res	Type
1	G	1045	GLN
1	G	1107	ASN
1	G	1131	ASN
1	G	1140	HIS
1	G	1211	ASN
1	G	1241	HIS
1	G	1267	GLN
1	G	1309	GLN
1	G	1340	ASN
1	G	1351	ASN
1	G	1372	GLN
1	G	1375	GLN
1	G	1436	ASN
1	G	1522	GLN
1	G	1549	ASN
1	Н	2045	GLN
1	Н	2107	ASN
1	Н	2140	HIS
1	Н	2241	HIS
1	Н	2267	GLN
1	Н	2288	GLN
1	Н	2316	GLN
1	Н	2351	ASN
1	Н	2372	GLN
1	Н	2375	GLN
1	Н	2528	GLN
1	Н	2532	ASN
1	Н	2534	GLN
1	Н	2537	GLN
1	Ι	3140	HIS
1	Ι	3160	HIS
1	Ι	3184	HIS
1	Ι	3241	HIS
1	Ι	3316	GLN
1	Ι	3336	GLN
1	Ι	3351	ASN
1	Ι	3353	GLN
1	Ι	3375	GLN
1	Ι	3534	GLN
1	Ι	3537	GLN
1	Ι	3549	ASN
1	J	4045	GLN



Mol	Chain	Res	Type
1	J	4079	ASN
1	J	4095	GLN
1	J	4107	ASN
1	J	4131	ASN
1	J	4140	HIS
1	J	4238	ASN
1	J	4241	HIS
1	J	4316	GLN
1	J	4336	GLN
1	J	4342	HIS
1	J	4351	ASN
1	J	4353	GLN
1	J	4375	GLN
1	J	4450	GLN
1	J	4537	GLN
1	K	5069	GLN
1	K	5131	ASN
1	K	5140	HIS
1	K	5160	HIS
1	K	5162	ASN
1	K	5241	HIS
1	K	5267	GLN
1	K	5288	GLN
1	K	5309	GLN
1	K	5336	GLN
1	K	5351	ASN
1	K	5353	GLN
1	K	5436	ASN
1	K	5437	HIS
1	K	5502	ASN
1	K	5522	GLN
1	K	5537	GLN
1	L	6107	ASN
1	L	6140	HIS
1	L	6238	ASN
1	L	6241	HIS
1	L	6351	ASN
1	L	6375	GLN
1	L L	6450	GLN



#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

25 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	Type	Chain	Bos	Link	B	ond leng	gths	E	Bond ang	gles
WIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	NAG	F	679	-	14, 14, 15	0.51	0	17,19,21	0.76	1(5%)
2	NAG	K	579	-	14,14,15	0.52	0	17,19,21	0.75	1 (5%)
3	NLX	С	3	-	26, 29, 29	4.40	18 (69%)	45,49,49	5.14	19 (42%)
3	NLX	Κ	5	-	26, 29, 29	<mark>3.15</mark>	15 (57%)	45,49,49	2.09	15 (33%)
3	NLX	L	6	-	26, 29, 29	<mark>3.35</mark>	15 (57%)	45,49,49	2.19	15 (33%)
3	NLX	J	4	-	26, 29, 29	<mark>3.41</mark>	14 (53%)	45,49,49	2.06	12 (26%)
2	NAG	D	479	-	14, 14, 15	0.45	0	17,19,21	0.61	0
2	NAG	С	379	-	14, 14, 15	0.48	0	17,19,21	0.73	0
2	NAG	Н	279	-	14, 14, 15	0.48	0	17,19,21	0.66	0
3	NLX	F	6	-	26, 29, 29	3.41	17 (65%)	45,49,49	5.27	22 (48%)
3	NLX	Н	2	-	26, 29, 29	<mark>3.28</mark>	15 (57%)	45,49,49	2.46	15 (33%)
3	NLX	Е	5	-	26, 29, 29	<mark>3.07</mark>	17 (65%)	45,49,49	2.05	14 (31%)
2	NAG	G	179	-	14, 14, 15	0.55	0	17,19,21	0.58	0
2	NAG	А	179	-	14, 14, 15	0.63	0	17,19,21	0.65	0
3	NLX	D	4	-	26, 29, 29	<mark>3.29</mark>	17 (65%)	45,49,49	2.30	15 (33%)



Mal	Tune	Chain	Dog	Tink	B	ond leng	gths	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NLX	В	2	-	26,29,29	2.96	15 (57%)	45,49,49	2.04	14 (31%)
3	NLX	G	1	-	26,29,29	<mark>3.39</mark>	15 (57%)	45,49,49	2.22	14 (31%)
2	NAG	J	479	-	14,14,15	0.55	0	17,19,21	0.65	0
3	NLX	А	1	-	26,29,29	<mark>3.68</mark>	16 (61%)	45,49,49	2.20	16 (35%)
2	NAG	Ι	379	-	14,14,15	0.47	0	17,19,21	0.78	1(5%)
2	NAG	L	679	-	14,14,15	0.60	0	17,19,21	0.65	0
3	NLX	Ι	3	-	26,29,29	<b>3.16</b>	17 (65%)	45,49,49	2.36	15 (33%)
2	NAG	В	279	-	14,14,15	0.49	0	17,19,21	0.59	0
2	NAG	Е	579	-	14,14,15	0.51	0	17,19,21	0.76	1 (5%)
2	NAG	А	180	-	14,14,15	0.60	0	17,19,21	0.66	0

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
3	NLX	G	1	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	K	579	-	-	4/6/23/26	0/1/1/1
3	NLX	С	3	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	В	279	-	-	2/6/23/26	0/1/1/1
3	NLX	L	6	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	J	4	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	Ι	3	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	C	379	-	-	2/6/23/26	0/1/1/1
2	NAG	Н	279	-	-	4/6/23/26	0/1/1/1
3	NLX	F	6	-	1/1/6/7	2/4/62/62	0/6/5/5
3	NLX	Н	2	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	Е	5	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	G	179	-	-	5/6/23/26	0/1/1/1
2	NAG	А	179	-	-	4/6/23/26	0/1/1/1
3	NLX	D	4	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	В	2	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	F	679	-	-	3/6/23/26	0/1/1/1
2	NAG	J	479	-	-	3/6/23/26	0/1/1/1
3	NLX	А	1	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	Ι	379	-	-	4/6/23/26	0/1/1/1
2	NAG	L	679	-	-	2/6/23/26	0/1/1/1
2	NAG	D	479	-	-	2/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NLX	K	5	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	Е	579	-	-	0/6/23/26	0/1/1/1
2	NAG	А	180	-	-	3/6/23/26	0/1/1/1

Continued from previous page...

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	С	3	NLX	C14-C9	14.77	1.78	1.55
3	D	4	NLX	C14-C9	10.24	1.71	1.55
3	Н	2	NLX	C14-C9	9.99	1.71	1.55
3	J	4	NLX	C14-C9	9.64	1.70	1.55
3	А	1	NLX	C14-C9	9.52	1.70	1.55
3	Ι	3	NLX	C14-C9	8.67	1.69	1.55
3	L	6	NLX	C14-C9	8.45	1.68	1.55
3	G	1	NLX	C14-C9	8.31	1.68	1.55
3	К	5	NLX	C14-C9	8.07	1.68	1.55
3	Е	5	NLX	C14-C9	7.96	1.67	1.55
3	А	1	NLX	C14-C13	7.26	1.63	1.53
3	F	6	NLX	C11-C12	7.02	1.50	1.39
3	F	6	NLX	C14-C13	6.89	1.63	1.53
3	L	6	NLX	C14-C13	6.84	1.63	1.53
3	G	1	NLX	C14-C13	6.68	1.62	1.53
3	Ι	3	NLX	C14-C13	6.46	1.62	1.53
3	K	5	NLX	C14-C13	6.46	1.62	1.53
3	В	2	NLX	C14-C13	6.36	1.62	1.53
3	В	2	NLX	C14-C9	6.34	1.65	1.55
3	С	3	NLX	C14-C13	6.31	1.62	1.53
3	Н	2	NLX	C14-C13	6.31	1.62	1.53
3	J	4	NLX	C14-C13	6.25	1.62	1.53
3	Е	5	NLX	C14-C13	5.97	1.61	1.53
3	А	1	NLX	C15-C13	5.69	1.62	1.54
3	D	4	NLX	C14-C13	5.64	1.61	1.53
3	С	3	NLX	C10-C11	5.60	1.62	1.51
3	С	3	NLX	C11-C12	5.38	1.48	1.39
3	L	6	NLX	C15-C13	5.34	1.61	1.54
3	С	3	NLX	C13-C5	5.33	1.61	1.54
3	G	1	NLX	C8-C14	5.31	1.60	1.53
3	F	6	NLX	C14-C9	5.26	1.63	1.55
3	G	1	NLX	C15-C13	5.18	1.61	1.54
3	С	3	NLX	O2-C5	5.14	1.54	1.47
3	А	1	NLX	C8-C14	5.14	1.60	1.53
3	С	3	NLX	C8-C14	5.04	1.60	1.53



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	NLX	C13-C5	4.82	1.60	1.54
3	J	4	NLX	C8-C14	4.80	1.60	1.53
3	А	1	NLX	C13-C5	4.80	1.60	1.54
3	Ι	3	NLX	C15-C13	4.74	1.60	1.54
3	В	2	NLX	C15-C13	4.72	1.60	1.54
3	А	1	NLX	C16-C15	4.66	1.60	1.52
3	K	5	NLX	C15-C13	4.59	1.60	1.54
3	Н	2	NLX	C15-C13	4.54	1.60	1.54
3	J	4	NLX	C15-C13	4.46	1.60	1.54
3	Е	5	NLX	C15-C13	4.46	1.60	1.54
3	L	6	NLX	C8-C14	4.43	1.59	1.53
3	D	4	NLX	C11-C12	4.41	1.46	1.39
3	D	4	NLX	C15-C13	4.41	1.60	1.54
3	F	6	NLX	O2-C5	4.38	1.53	1.47
3	F	6	NLX	C8-C7	4.34	1.62	1.53
3	F	6	NLX	C16-C15	4.33	1.60	1.52
3	В	2	NLX	C11-C12	4.16	1.46	1.39
3	K	5	NLX	C10-C11	4.08	1.59	1.51
3	L	6	NLX	C10-C11	4.07	1.59	1.51
3	Ε	5	NLX	C10-C11	4.07	1.59	1.51
3	G	1	NLX	C13-C5	4.06	1.59	1.54
3	D	4	NLX	C8-C14	3.98	1.58	1.53
3	J	4	NLX	C11-C12	3.97	1.45	1.39
3	А	1	NLX	C7-C6	3.96	1.57	1.50
3	G	1	NLX	C16-C15	3.95	1.59	1.52
3	Н	2	NLX	C8-C14	3.92	1.58	1.53
3	G	1	NLX	C10-C11	3.91	1.58	1.51
3	H	2	NLX	C11-C12	3.87	1.45	1.39
3	K	5	NLX	C8-C14	3.86	1.58	1.53
3	J	4	NLX	C16-C15	3.86	1.59	1.52
3	H	2	NLX	C13-C5	3.83	1.59	1.54
3	L	6	NLX	C16-C15	3.79	1.59	1.52
3	I	3	NLX	C11-C12	3.78	1.45	1.39
3	F	6	NLX	C2-C3	3.78	1.46	1.39
3	G	1	NLX	C11-C12	3.78	1.45	1.39
3	F	6	NLX	C20-N1	3.76	1.61	1.50
3	K	5	NLX	C7-C6	3.75	1.57	1.50
3	A	1	NLX	C11-C12	3.73	1.45	1.39
3	J	4	NLX	C7-C6	3.71	1.57	1.50
3	С	3	NLX	C4-C12	3.71	1.43	1.38
3	G	1	NLX	C7-C6	3.71	1.57	1.50
3	F	6	NLX	C17-C18	3.70	1.63	1.50



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	6	NLX	C7-C6	3.65	1.56	1.50
3	С	3	NLX	C13-C12	3.62	1.56	1.50
3	K	5	NLX	C11-C12	3.61	1.45	1.39
3	D	4	NLX	C10-C11	3.57	1.58	1.51
3	А	1	NLX	C10-C11	3.56	1.58	1.51
3	F	6	NLX	C7-C6	3.55	1.56	1.50
3	Ι	3	NLX	C13-C5	3.54	1.59	1.54
3	В	2	NLX	C16-C15	3.53	1.58	1.52
3	В	2	NLX	C8-C14	3.51	1.58	1.53
3	F	6	NLX	C13-C5	3.50	1.59	1.54
3	K	5	NLX	C16-C15	3.47	1.58	1.52
3	L	6	NLX	C13-C5	3.47	1.59	1.54
3	Е	5	NLX	C16-C15	3.43	1.58	1.52
3	F	6	NLX	C13-C12	3.39	1.56	1.50
3	D	4	NLX	C13-C5	3.39	1.58	1.54
3	С	3	NLX	C8-C7	3.37	1.60	1.53
3	В	2	NLX	C10-C11	3.30	1.57	1.51
3	А	1	NLX	C4-C12	3.27	1.43	1.38
3	Η	2	NLX	C7-C6	3.26	1.56	1.50
3	Е	5	NLX	O2-C5	3.24	1.51	1.47
3	Ι	3	NLX	C16-C15	3.23	1.58	1.52
3	В	2	NLX	O2-C5	3.22	1.51	1.47
3	D	4	NLX	C7-C6	3.22	1.56	1.50
3	Ι	3	NLX	C13-C12	3.19	1.56	1.50
3	Е	5	NLX	C8-C14	3.17	1.57	1.53
3	С	3	NLX	C7-C6	3.15	1.56	1.50
3	Н	2	NLX	O2-C5	3.14	1.51	1.47
3	L	6	NLX	C4-C12	3.13	1.42	1.38
3	K	5	NLX	C2-C1	3.11	1.44	1.38
3	J	4	NLX	C4-C12	3.11	1.42	1.38
3	L	6	NLX	O2-C5	3.10	1.51	1.47
3	С	3	NLX	C3-C4	3.09	1.46	1.40
3	G	1	NLX	C5-C6	3.09	1.60	1.52
3	F	6	NLX	C8-C14	3.08	1.57	1.53
3	В	2	NLX	C13-C5	3.06	1.58	1.54
3	E	5	NLX	C11-C12	3.05	1.44	1.39
3	E	5	NLX	C13-C5	3.04	1.58	1.54
3	I	3	NLX	C8-C14	3.03	1.57	1.53
3	L	6	NLX	C11-C12	2.98	1.44	1.39
3	H	2	NLX	C8-C7	2.98	1.59	1.53
3	E	5	NLX	C7-C6	2.96	1.55	1.50
3	J	4	NLX	C8-C7	2.94	1.59	1.53



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	5	NLX	C4-C12	2.93	1.42	1.38
3	L	6	NLX	C5-C6	2.90	1.59	1.52
3	Ι	3	NLX	C7-C6	2.88	1.55	1.50
3	В	2	NLX	C13-C12	2.86	1.55	1.50
3	Е	5	NLX	C5-C6	2.86	1.59	1.52
3	Е	5	NLX	C4-C12	2.86	1.42	1.38
3	J	4	NLX	C10-C11	2.84	1.56	1.51
3	K	5	NLX	C13-C5	2.82	1.58	1.54
3	G	1	NLX	C4-C12	2.79	1.42	1.38
3	Н	2	NLX	C16-C15	2.78	1.57	1.52
3	В	2	NLX	C5-C6	2.75	1.59	1.52
3	Ι	3	NLX	C5-C6	2.74	1.59	1.52
3	Е	5	NLX	C2-C1	2.74	1.43	1.38
3	В	2	NLX	C2-C1	2.73	1.43	1.38
3	Ι	3	NLX	C3-C4	2.72	1.45	1.40
3	G	1	NLX	O2-C5	2.72	1.50	1.47
3	D	4	NLX	C8-C7	2.70	1.58	1.53
3	D	4	NLX	C16-C15	2.70	1.57	1.52
3	G	1	NLX	C2-C1	2.69	1.43	1.38
3	С	3	NLX	C2-C1	2.69	1.43	1.38
3	Н	2	NLX	C10-C11	2.64	1.56	1.51
3	В	2	NLX	C4-C12	2.64	1.42	1.38
3	С	3	NLX	C15-C13	2.64	1.57	1.54
3	L	6	NLX	C2-C1	2.63	1.43	1.38
3	А	1	NLX	C2-C1	2.63	1.43	1.38
3	D	4	NLX	C4-C12	2.59	1.42	1.38
3	А	1	NLX	O2-C5	2.58	1.50	1.47
3	A	1	NLX	C5-C6	2.56	1.59	1.52
3	С	3	NLX	O2-C4	2.55	1.42	1.38
3	Ι	3	NLX	O2-C5	2.55	1.50	1.47
3	A	1	NLX	C8-C7	2.55	1.58	1.53
3	J	4	NLX	O2-C5	2.51	1.50	1.47
3	K	5	NLX	C5-C6	2.47	1.58	1.52
3	Ι	3	NLX	C10-C11	2.43	1.56	1.51
3	В	2	NLX	C2-C3	2.43	1.43	1.39
3	E	5	NLX	C3-C4	2.42	1.45	1.40
3	D	4	NLX	O2-C5	2.42	1.50	1.47
3	В	2	NLX	C7-C6	2.39	1.54	1.50
3	D	4	NLX	C2-C1	2.39	1.43	1.38
3	H	2	NLX	C13-C12	2.38	1.54	1.50
3	С	3	NLX	C16-C15	2.38	1.56	1.52
3	L	6	NLX	C13-C12	2.36	1.54	1.50



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(Å)	Ideal(Å)
3	Ι	3	NLX	C4-C12	2.36	1.41	1.38
3	L	6	NLX	C3-C4	2.35	1.45	1.40
3	Н	2	NLX	C3-C4	2.32	1.45	1.40
3	J	4	NLX	C2-C1	2.30	1.42	1.38
3	С	3	NLX	C2-C3	2.29	1.43	1.39
3	F	6	NLX	C16-N1	2.28	1.57	1.52
3	G	1	NLX	C8-C7	2.28	1.57	1.53
3	F	6	NLX	C10-C11	2.24	1.55	1.51
3	F	6	NLX	C19-C18	2.22	1.43	1.28
3	Н	2	NLX	C4-C12	2.19	1.41	1.38
3	Ι	3	NLX	C2-C1	2.18	1.42	1.38
3	Ι	3	NLX	C2-C3	2.16	1.43	1.39
3	Κ	5	NLX	O2-C5	2.16	1.50	1.47
3	G	1	NLX	C2-C3	2.13	1.43	1.39
3	D	4	NLX	C5-C6	2.13	1.58	1.52
3	Κ	5	NLX	C2-C3	2.13	1.43	1.39
3	А	1	NLX	C13-C12	2.12	1.54	1.50
3	Κ	5	NLX	C1-C11	2.11	1.43	1.39
3	А	1	NLX	C3-C4	2.09	1.44	1.40
3	F	6	NLX	C5-C6	2.09	1.57	1.52
3	С	3	NLX	C20-N1	2.07	1.56	1.50
3	D	4	NLX	C3-C4	2.06	1.44	1.40
3	Ι	3	NLX	C8-C7	2.06	1.57	1.53
3	D	4	NLX	C2-C3	2.05	1.43	1.39
3	Ε	5	NLX	C8-C7	2.04	1.57	1.53
3	Н	2	NLX	C5-C6	2.02	1.57	1.52
3	J	4	NLX	C5-C6	2.01	1.57	1.52
3	D	4	NLX	C13-C12	2.01	1.54	1.50
3	Е	5	NLX	C13-C12	2.00	1.54	1.50
3	E	5	NLX	C1-C11	2.00	1.43	1.39

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	3	NLX	C20-N1-C17	-23.54	63.74	108.50
3	F	6	NLX	C20-N1-C17	-22.28	66.14	108.50
3	С	3	NLX	C20-N1-C16	-17.31	68.71	108.64
3	F	6	NLX	C20-N1-C16	-15.98	71.79	108.64
3	С	3	NLX	C16-N1-C17	10.17	131.74	109.05
3	F	6	NLX	O2-C5-C6	10.12	116.90	108.51
3	F	6	NLX	C16-N1-C17	9.28	129.74	109.05
3	F	6	NLX	C15-C13-C14	8.82	116.41	109.35



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	G	1	NLX	O2-C5-C6	7.76	114.94	108.51
3	Ι	3	NLX	O2-C5-C6	7.46	114.70	108.51
3	Н	2	NLX	C18-C17-N1	7.18	124.99	114.48
3	В	2	NLX	O2-C5-C6	6.73	114.09	108.51
3	Ι	3	NLX	C18-C17-N1	6.73	124.33	114.48
3	Κ	5	NLX	O2-C5-C6	6.51	113.91	108.51
3	L	6	NLX	O2-C5-C6	6.50	113.90	108.51
3	D	4	NLX	C18-C17-N1	6.06	123.35	114.48
3	F	6	NLX	C14-C13-C5	6.06	122.62	118.10
3	Н	2	NLX	O2-C5-C6	5.88	113.38	108.51
3	Е	5	NLX	O2-C5-C6	5.88	113.38	108.51
3	F	6	NLX	C13-C14-C9	5.85	110.30	106.37
3	В	2	NLX	C18-C17-N1	5.32	122.26	114.48
3	J	4	NLX	C18-C17-N1	5.28	122.22	114.48
3	С	3	NLX	O2-C5-C6	5.17	112.80	108.51
3	А	1	NLX	O2-C5-C6 5.11 112.74		112.74	108.51
3	А	1	NLX	C18-C17-N1 5.06		121.89	114.48
3	D	4	NLX	O2-C5-C6	4.96	112.62	108.51
3	С	3	NLX	C10-C9-C14	-4.94	104.30	114.46
3	Н	2	NLX	C8-C14-C13	-4.90	107.38	111.47
3	L	6	NLX	C18-C17-N1	4.90	121.66	114.48
3	С	3	NLX	C8-C14-C13	-4.85	107.42	111.47
3	G	1	NLX	C18-C17-N1	4.80	121.51	114.48
3	D	4	NLX	C17-N1-C9	4.77	117.77	110.29
3	Н	2	NLX	C17-N1-C9	4.63	117.56	110.29
3	D	4	NLX	C8-C14-C9	4.62	118.06	111.66
3	Н	2	NLX	C8-C14-C9	4.55	117.95	111.66
3	Κ	5	NLX	C18-C17-N1	4.41	120.94	114.48
3	L	6	NLX	C7-C6-C5	4.37	123.33	116.44
3	J	4	NLX	C16-C15-C13	4.30	118.74	111.52
3	G	1	NLX	C7-C6-C5	4.29	123.21	116.44
3	А	1	NLX	C8-C14-C9	4.23	117.51	111.66
3	С	3	NLX	C8-C14-C9	4.22	117.50	111.66
3	D	4	NLX	C8-C14-C13	-4.22	107.95	111.47
3	K	5	NLX	C7-C6-C5	4.18	123.03	116.44
3	J	4	NLX	C8-C14-C9	4.15	117.40	111.66
3	Е	5	NLX	C7-C6-C5	4.14	122.97	116.44
3	A	1	NLX	C7-C6-C5	$4.0\overline{6}$	122.85	116.44
3	Ι	3	NLX	C16-C15-C13	4.05	118.32	111.52
3	В	2	NLX	C7-C6-C5	4.04	122.82	116.44
3	H	2	NLX	C16-C15-C13	4.03	118.30	111.52
3	А	1	NLX	C16-C15-C13	4.03	118.29	111.52



1	MXQ	
1	TAT V V	

Mol	Chain	$\mathbf{Res}$	Type	page		Observed(°)	Ideal(°)
3	D	4	NLX	C16-C15-C13	4.02	118.27	111.52
3	F	6	NLX	C8-C14-C9	4.00	117.20	111.66
3	J	4	NLX	C8-C14-C13	-3.97	108.15	111.47
3	J	4	NLX	C7-C6-C5	3.86	122.53	116.44
3	F	6	NLX	C15-C13-C12	-3.84	103.26	111.45
3	A	1	NLX	C8-C14-C13	-3.81	108.29	111.47
3	Ι	3	NLX	C8-C14-C13	-3.80	108.30	111.47
3	С	3	NLX	C16-N1-C9	-3.78	98.54	108.93
3	G	1	NLX	C16-C15-C13	3.78	117.87	111.52
3	Ι	3	NLX	C7-C6-C5	3.76	122.37	116.44
3	Е	5	NLX	C8-C14-C9	3.75	116.85	111.66
3	D	4	NLX	C7-C6-C5	3.74	122.34	116.44
3	G	1	NLX	C8-C14-C9	3.70	116.78	111.66
3	L	6	NLX	C8-C14-C9	3.63	116.68	111.66
3	L	6	NLX	C16-C15-C13	3.63	117.61	111.52
3	K	5	NLX	C16-C15-C13	3.61	117.59	111.52
3	Н	2	NLX	C7-C6-C5 3.61 122		122.14	116.44
3	G	1	NLX	C10-C9-C14	-3.60	107.06	114.46
3	С	3	NLX	C13-C12-C4	3.59	112.57	109.23
3	F	6	NLX	C17-N1-C9	-3.58	104.68	110.29
3	K	5	NLX	C8-C14-C9	3.56	116.59	111.66
3	J	4	NLX	O2-C5-C6	3.53	111.43	108.51
3	F	6	NLX	C14-C13-C12	-3.52	104.02	108.56
3	А	1	NLX	C20-N1-C17	-3.50	101.85	108.50
3	С	3	NLX	O2-C4-C3	3.49	132.36	126.29
3	Е	5	NLX	C16-C15-C13	3.48	117.37	111.52
3	Ε	5	NLX	C18-C17-N1	3.45	119.53	114.48
3	А	1	NLX	C10-C9-C14	-3.42	107.44	114.46
3	Ι	3	NLX	C8-C14-C9	3.36	116.32	111.66
3	Ε	5	NLX	C8-C14-C13	-3.32	108.70	111.47
3	Ε	5	NLX	C10-C9-C14	-3.31	107.66	114.46
3	K	5	NLX	C10-C9-C14	-3.28	107.72	114.46
3	L	6	NLX	C20-N1-C17	-3.22	102.39	108.50
3	А	1	NLX	C13-C12-C4	3.20	112.21	109.23
3	F	6	NLX	O2-C4-C3	3.20	131.85	126.29
3	K	5	NLX	C15-C13-C14	3.19	111.90	109.35
3	В	2	NLX	C16-C15-C13	3.18	116.87	111.52
3	L	6	NLX	C10-C9-C14	-3.17	107.95	114.46
3	F	6	NLX	C13-C12-C4	3.16	112.17	109.23
3	L	6	NLX	C13-C12-C4	3.14	112.16	109.23
3	C	3	NLX	C17-N1-C9	-3.09	$105.4\overline{5}$	110.29
3	Н	2	NLX	O2-C4-C3	3.09	131.66	126.29



	Chain	Res	Tvne	Type Atoms		Observed $(^{o})$	Ideal(°)
3	B	2005	NLX	03-C6-C7	-3.09	116.38	122 11
3	F F	6	NLX	C12-C13-C5	-3.08	95.56	98.43
3	J	4	NLX	C20-N1-C17	-3.07	102.67	108.50
3	Ċ	3	NLX	C7-C6-C5	3.06	121.27	116.44
3	H	2	NLX	C13-C12-C4	3.00	112.02	109.23
3	J	4	NLX	C10-C9-C14	-2.97	108.35	114.46
3	L	6	NLX	O2-C4-C12	-2.94	109.30	112.79
3	В	2	NLX	C10-C9-C14	-2.91	108.49	114.46
3	L	6	NLX	C8-C14-C13	-2.91	109.04	111.47
3	Е	5	NLX	O2-C4-C3	2.89	131.31	126.29
3	Е	5	NLX	C13-C12-C4	2.88	111.92	109.23
3	Ι	3	NLX	O2-C4-C3	2.87	131.28	126.29
3	Ι	3	NLX	C13-C12-C4	2.84	111.88	109.23
3	С	3	NLX	C14-C13-C5	2.84	120.22	118.10
3	L	6	NLX	O2-C4-C3	2.82	131.19	126.29
3	С	3	NLX	O2-C4-C12	02-C4-C12 -2.82 109.44		112.79
3	Е	5	NLX	O2-C4-C12 -2.80 109.45		112.79	
3	F	6	NLX	C8-C14-C13 -2.80 109.13		109.13	111.47
3	А	1	NLX	O2-C4-C3 2.80 131.15		131.15	126.29
3	G	1	NLX	O2-C4-C3 2.77		131.11	126.29
3	G	1	NLX	C15-C13-C14	2.77	111.57	109.35
3	F	6	NLX	C7-C6-C5	2.77	120.81	116.44
3	D	4	NLX	O2-C4-C3	2.77	131.10	126.29
3	Е	5	NLX	C17-N1-C9 2.76		114.62	110.29
3	В	2	NLX	O2-C4-C3	2.74	131.06	126.29
3	D	4	NLX	C15-C13-C14 2.74 111.54		111.54	109.35
3	D	4	NLX	C10-C9-C14 -2.74 108.84		108.84	114.46
3	С	3	NLX	C13-C14-C9	2.73	108.20	106.37
3	Е	5	NLX	C20-N1-C17	-2.71	103.36	108.50
3	Е	5	NLX	O3-C6-C7	-2.70	117.09	122.11
3	L	6	NLX	C15-C13-C14	2.68	111.50	109.35
3	F	6	NLX	O4-C14-C8	-2.68	102.28	107.92
3	Ι	3	NLX	O2-C4-C12	-2.68	109.60	112.79
3	J	4	NLX	C13-C12-C4	2.67	111.72	109.23
3	С	3	NLX	C15-C13-C5	2.67	114.87	111.98
3	J	4	NLX	O2-C4-C3	2.66	130.91	126.29
3	С	3	NLX	C16-C15-C13	2.66	115.98	111.52
3	H	2	NLX	C10-C9-C14	-2.65	109.02	114.46
3	C	3	NLX	C15-C13-C14	-2.64	107.24	109.35
3	В	2	NLX	C8-C14-C13	-2.63	109.28	111.47
3	K	5	NLX	C8-C14-C13	-2.62	109.28	111.47
3	G	1	NLX	C13-C12-C4	2.58	$111.6\overline{3}$	109.23



Continued from previous page								
Mol	Chain	Res	Type	Type Atoms		$Observed(^{o})$	$Ideal(^{o})$	
3	G	1	NLX	O3-C6-C7	-2.56	117.35	122.11	
3	K	5	NLX	O2-C4-C12	-2.56	109.75	112.79	
3	F	6	NLX	C3-C4-C12	-2.54	117.71	120.91	
3	K	5	NLX	O2-C4-C3	2.53	130.68	126.29	
3	Н	2	NLX	C14-C13-C5	2.52	119.98	118.10	
3	Н	2	NLX	O2-C4-C12	-2.51	109.80	112.79	
3	В	2	NLX	C13-C12-C4	2.51	111.57	109.23	
3	А	1	NLX	C12-C13-C5	-2.51	96.09	98.43	
3	K	5	NLX	C13-C12-C4	2.51	111.57	109.23	
3	Ι	3	NLX	C12-C13-C5	-2.50	96.10	98.43	
3	Ι	3	NLX	O3-C6-C7	-2.50	117.47	122.11	
3	L	6	NLX	O3-C6-C7	-2.49	117.48	122.11	
3	G	1	NLX	C20-N1-C17	-2.47	103.81	108.50	
3	В	2	NLX	O2-C4-C12	-2.46	109.86	112.79	
3	А	1	NLX	O2-C4-C12	-2.46	109.86	112.79	
3	В	2	NLX	C20-N1-C17	-2.45	103.84	108.50	
3	А	1	NLX	C17-N1-C9	2.45	114.14	110.29	
3	D	4	NLX	O2-C4-C12	-2.45	109.88	112.79	
3	Ι	3	NLX	C17-N1-C9	2.43	114.10	110.29	
3	J	4	NLX	C17-N1-C9	2.42	114.08	110.29	
3	F	6	NLX	C16-C15-C13	2.41	115.58	111.52	
3	Ι	3	NLX	C10-C9-C14	-2.41	109.52	114.46	
3	Н	2	NLX	C20-N1-C17	-2.40	103.93	108.50	
3	Ι	3	NLX	C20-N1-C17	-2.39	103.95	108.50	
3	А	1	NLX	C15-C13-C14	2.39	111.26	109.35	
3	D	4	NLX	C13-C12-C4	2.37	111.44	109.23	
3	G	1	NLX	C15-C13-C12	-2.36	106.40	111.45	
3	Е	5	NLX	C15-C13-C14	2.36	111.24	109.35	
3	G	1	NLX	O2-C4-C12	-2.36	109.98	112.79	
3	Н	2	NLX	C15-C13-C14	2.36	111.24	109.35	
3	L	6	NLX	C12-C13-C5	-2.35	96.24	98.43	
3	D	4	NLX	C4-O2-C5	2.34	107.29	104.79	
3	G	1	NLX	C8-C14-C13	-2.31	109.54	111.47	
2	Ι	379	NAG	C2-N2-C7	-2.30	119.63	122.90	
3	В	2	NLX	C12-C13-C5	-2.30	96.29	98.43	
3	D	4	NLX	C20-N1-C17	-2.28	104.16	108.50	
3	K	5	NLX	O3-C6-C7	-2.27	117.89	122.11	
3	Ι	3	NLX	C15-C13-C14	2.26	111.16	109.35	
3	F	6	NLX	C16-N1-C9	2.23	115.06	108.93	
2	K	579	NAG	C2-N2-C7	-2.22	119.74	122.90	
3	K	5	NLX	C12-C13-C5	-2.22	96.36	98.43	
3	K	5	NLX	C20-N1-C17	-2.21	104.30	108.50	



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	1	NLX	O3-C6-C7	-2.20	118.02	122.11
2	F	679	NAG	C2-N2-C7	-2.19	119.78	122.90
2	Е	579	NAG	C2-N2-C7	-2.18	119.80	122.90
3	С	3	NLX	C3-C4-C12	-2.17	118.17	120.91
3	K	5	NLX	C17-N1-C9	2.17	113.69	110.29
3	В	2	NLX	C15-C13-C14	2.11	111.04	109.35
3	А	1	NLX	O2-C5-C13	2.08	106.20	104.90
3	F	6	NLX	O4-C14-C9	-2.07	104.00	108.27
3	J	4	NLX	O2-C5-C13	2.07	106.19	104.90
3	Н	2	NLX	C16-N1-C17	-2.05	104.49	109.05
3	L	6	NLX	C17-N1-C9	2.03	113.48	110.29
3	F	6	NLX	O4-C14-C13	2.02	113.77	109.83
3	D	4	NLX	C20-N1-C9	-2.02	107.71	113.04
3	В	2	NLX	C8-C14-C9	2.01	114.45	111.66

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	С	3	NLX	N1
3	Κ	5	NLX	N1
3	L	6	NLX	N1
3	J	4	NLX	N1
3	F	6	NLX	N1
3	Н	2	NLX	N1
3	Е	5	NLX	N1
3	D	4	NLX	N1
3	В	2	NLX	N1
3	G	1	NLX	N1
3	А	1	NLX	N1
3	Ι	3	NLX	N1

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	679	NAG	C8-C7-N2-C2
2	F	679	NAG	O7-C7-N2-C2
2	Κ	579	NAG	C8-C7-N2-C2
2	К	579	NAG	O7-C7-N2-C2
3	С	3	NLX	N1-C17-C18-C19
2	Н	279	NAG	C8-C7-N2-C2
2	Н	279	NAG	O7-C7-N2-C2
2	А	179	NAG	C8-C7-N2-C2



		1		
Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	А	179	NAG	O7-C7-N2-C2
3	G	1	NLX	N1-C17-C18-C19
2	J	479	NAG	C3-C2-N2-C7
2	Ι	379	NAG	O7-C7-N2-C2
2	В	279	NAG	C8-C7-N2-C2
2	В	279	NAG	O7-C7-N2-C2
2	А	180	NAG	C8-C7-N2-C2
2	А	180	NAG	O7-C7-N2-C2
2	С	379	NAG	C8-C7-N2-C2
2	С	379	NAG	O7-C7-N2-C2
2	G	179	NAG	C8-C7-N2-C2
2	G	179	NAG	O7-C7-N2-C2
2	Ι	379	NAG	C8-C7-N2-C2
2	L	679	NAG	C8-C7-N2-C2
2	L	679	NAG	O7-C7-N2-C2
2	A	179	NAG	C4-C5-C6-O6
2	G	179	NAG	C1-C2-N2-C7
2	K	579	NAG	C4-C5-C6-O6
2	Н	279	NAG	O5-C5-C6-O6
2	Н	279	NAG	C4-C5-C6-O6
2	D	479	NAG	C8-C7-N2-C2
2	А	179	NAG	O5-C5-C6-O6
2	K	579	NAG	O5-C5-C6-O6
2	Ι	379	NAG	C4-C5-C6-O6
2	Ι	379	NAG	O5-C5-C6-O6
2	D	479	NAG	O7-C7-N2-C2
2	G	179	NAG	C4-C5-C6-O6
2	G	179	NAG	O5-C5-C6-O6
3	F	6	NLX	C18-C17-N1-C20
2	J	479	NAG	C8-C7-N2-C2
3	F	6	NLX	N1-C17-C18-C19
2	J	479	NAG	O7-C7-N2-C2
2	F	679	NAG	C4-C5-C6-O6
2	A	180	NAG	C3-C2-N2-C7

Continued from previous page...

There are no ring outliers.

22 monomers are involved in 273 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	579	NAG	1	0
3	С	3	NLX	27	0
3	K	5	NLX	18	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	6	NLX	23	0
3	J	4	NLX	20	0
2	D	479	NAG	4	0
2	Н	279	NAG	1	0
3	F	6	NLX	23	0
3	Н	2	NLX	30	0
3	Е	5	NLX	18	0
2	G	179	NAG	4	0
2	А	179	NAG	3	0
3	D	4	NLX	15	0
3	В	2	NLX	21	0
3	G	1	NLX	12	0
2	J	479	NAG	7	0
3	А	1	NLX	20	0
2	Ι	379	NAG	1	0
3	Ι	3	NLX	19	0
2	В	279	NAG	4	0
2	Е	579	NAG	2	0
2	А	180	NAG	1	0

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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

#### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

