



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 05:44 PM BST

PDB ID : 1KP8
Title : Structural Basis for GroEL-assisted Protein Folding from the Crystal Structure of (GroEL-KMgATP)₁₄ at 2.0 Å Resolution
Authors : Wang, J.
Deposited on : 2001-12-30
Resolution : 2.00 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

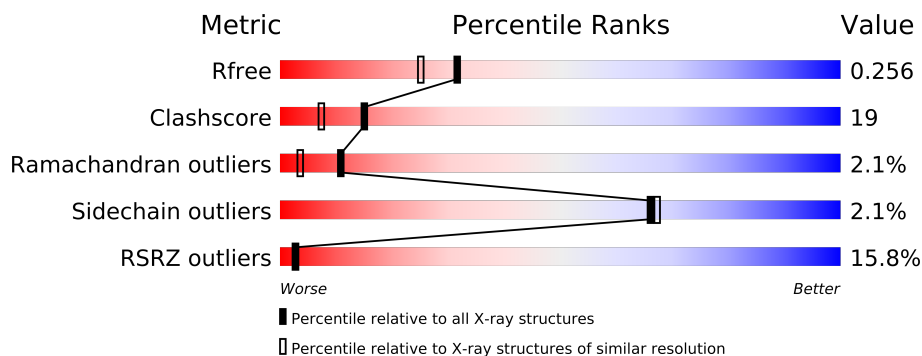
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23004
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	547	
1	B	547	
1	C	547	
1	D	547	
1	E	547	
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	4001	-	X
2	SO4	A	4007	-	X
2	SO4	A	4008	-	X
2	SO4	B	4009	-	X
2	SO4	B	4010	-	X
2	SO4	C	4011	-	X
2	SO4	C	4012	-	X
2	SO4	E	4005	-	X
2	SO4	E	4006	-	X
2	SO4	F	4004	-	X
2	SO4	G	4002	-	X
2	SO4	H	4017	-	X
2	SO4	H	4018	-	X
2	SO4	J	4019	-	X
2	SO4	J	4020	-	X
2	SO4	K	4021	-	X
2	SO4	K	4022	-	X
2	SO4	L	4003	-	X
2	SO4	M	4013	-	X
2	SO4	M	4014	-	X
2	SO4	N	4015	-	X
2	SO4	N	4016	-	X
3	MG	A	550	-	X
3	MG	B	550	-	X
3	MG	D	550	-	X
3	MG	G	550	-	X
3	MG	H	550	-	X
3	MG	J	550	-	X
3	MG	M	550	-	X
3	MG	N	550	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 57085 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

- Molecule 1 is a protein called groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	B	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	C	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	D	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	E	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	F	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	G	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	H	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	I	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	J	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	K	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	L	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	M	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	N	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			

There are 42 discrepancies between the modelled and reference sequences:

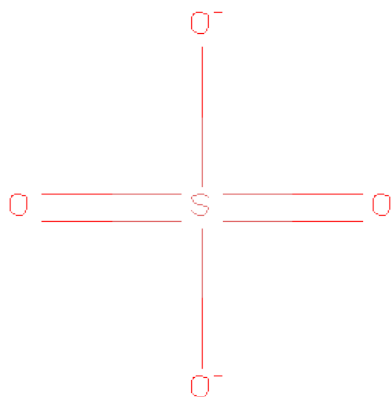
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
A	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
B	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
B	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
B	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
C	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
C	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
C	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
D	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
D	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
D	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
E	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
E	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
E	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
F	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
F	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
F	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
G	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
G	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
G	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
H	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
H	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
H	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
I	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
I	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
I	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
J	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
J	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
J	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
K	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
K	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
K	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
L	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
L	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
L	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
M	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
M	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
M	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
N	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
N	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
N	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		

Continued on next page...

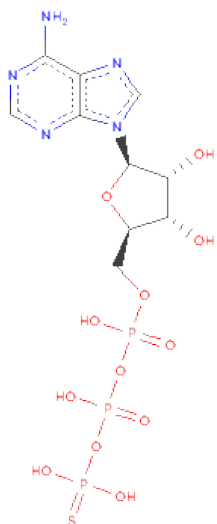
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	M	1	Total 1	Mg 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	K 1	0	0
4	J	1	Total 1	K 1	0	0
4	D	2	Total 2	K 2	0	0
4	K	1	Total 1	K 1	0	0
4	E	2	Total 2	K 2	0	0
4	H	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0
4	I	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0
4	N	1	Total 1	K 1	0	0
4	L	1	Total 1	K 1	0	0
4	F	1	Total 1	K 1	0	0
4	M	1	Total 1	K 1	0	0

- Molecule 5 is PHOSPHOTHIOPHOSPHORICACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	I	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	J	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	K	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	L	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	M	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	N	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 6 is water.

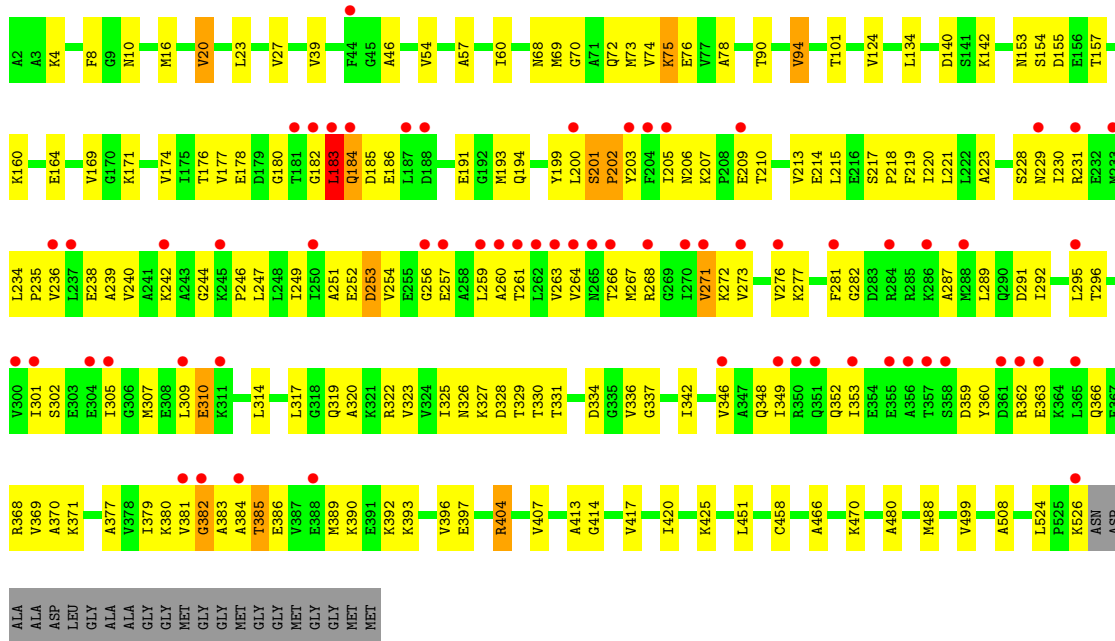
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total 156	O 156	0	0
6	B	214	Total 214	O 214	0	0
6	C	149	Total 149	O 149	0	0
6	D	261	Total 261	O 261	0	0
6	E	217	Total 217	O 217	0	0
6	F	200	Total 200	O 200	0	0
6	G	269	Total 269	O 269	0	0
6	H	204	Total 204	O 204	0	0
6	I	145	Total 145	O 145	0	0
6	J	139	Total 139	O 139	0	0
6	K	133	Total 133	O 133	0	0
6	L	163	Total 163	O 163	0	0
6	M	138	Total 138	O 138	0	0
6	N	153	Total 153	O 153	0	0

3 Residue-property plots

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

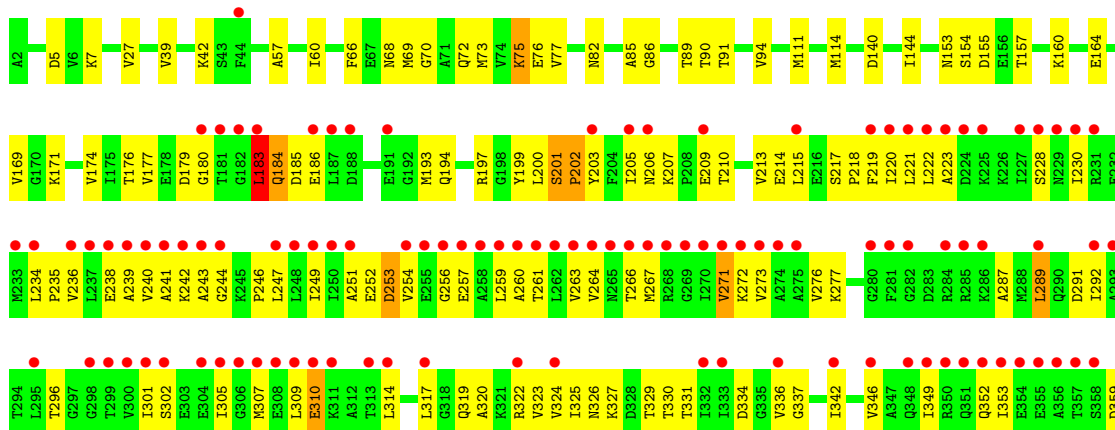
• Molecule 1: groEL protein

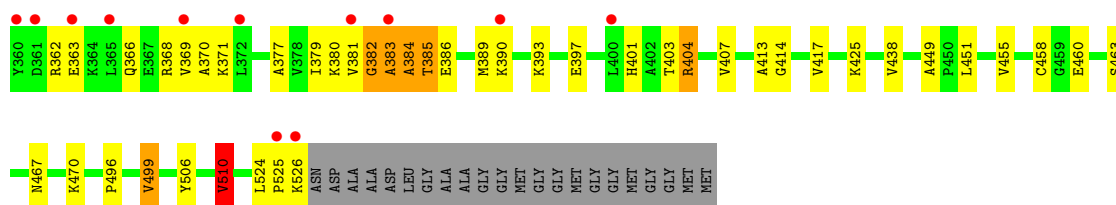
Chain A: 



• Molecule 1: groEL protein

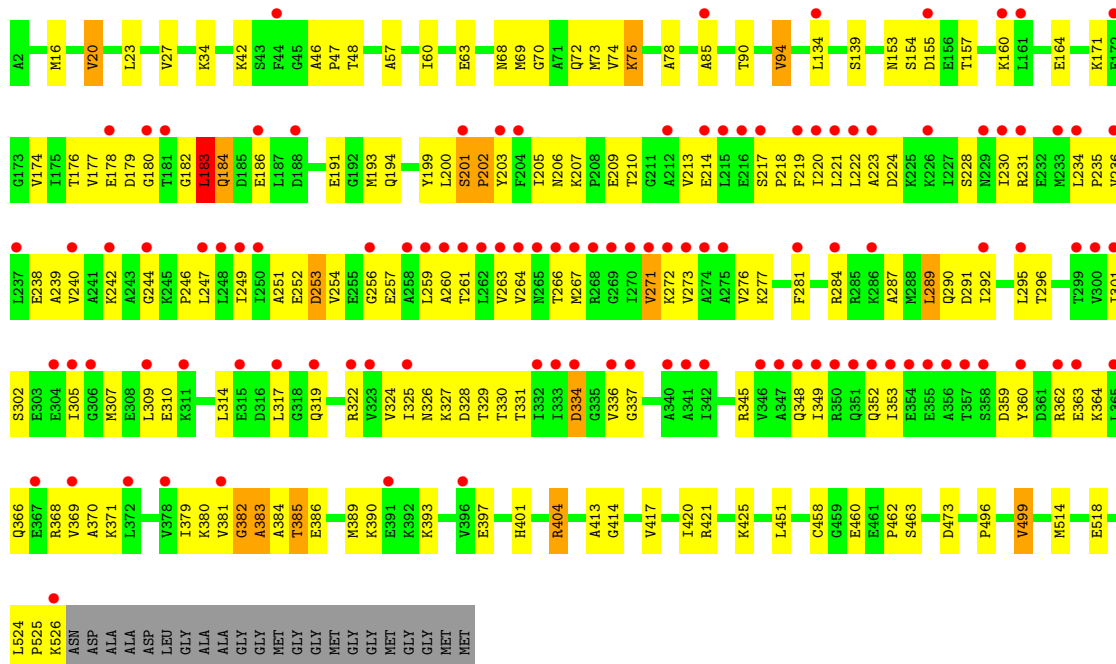
Chain B: 





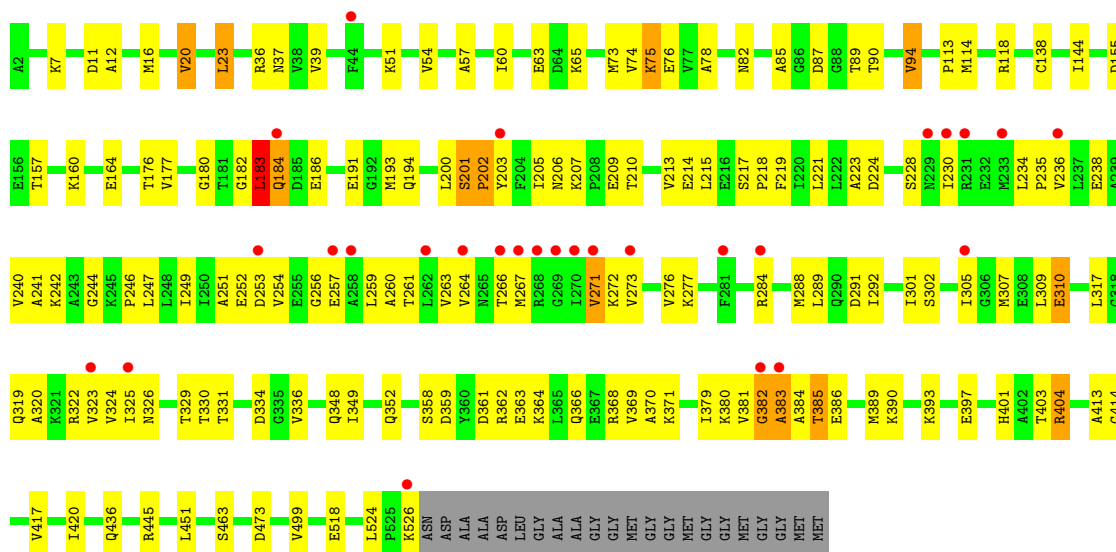
• Molecule 1: groEL protein

Chain C:



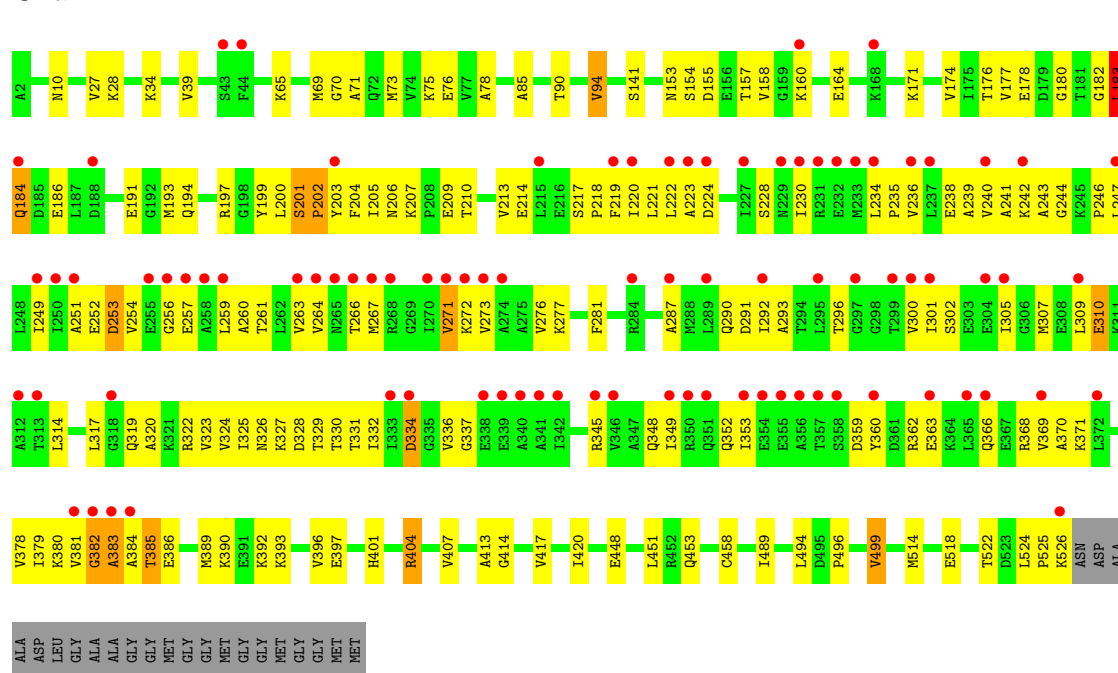
• Molecule 1: groEL protein

Chain D:



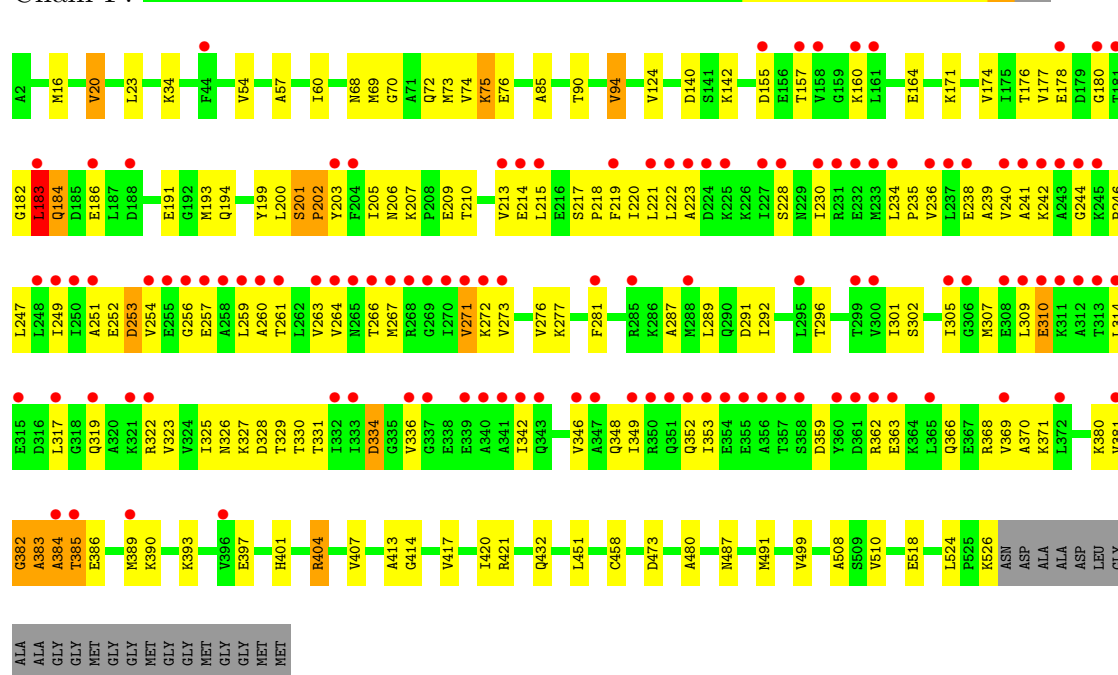
• Molecule 1: groEL protein

Chain E:



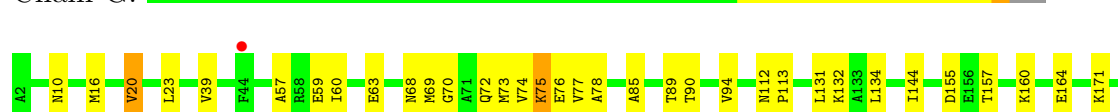
- Molecule 1: groEL protein

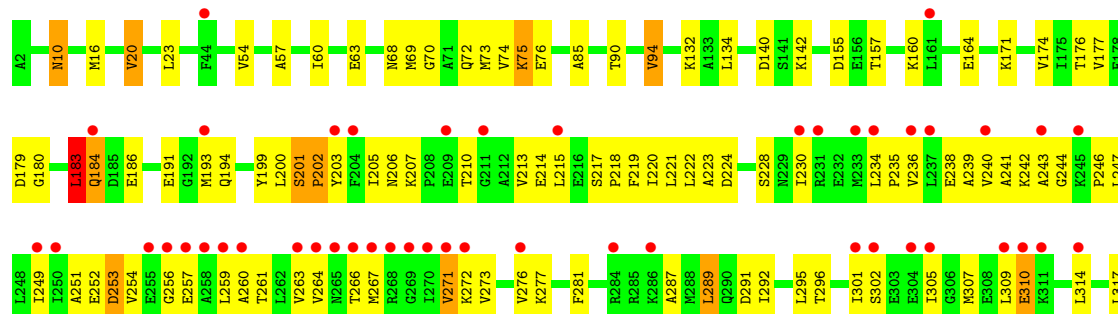
Chain F:

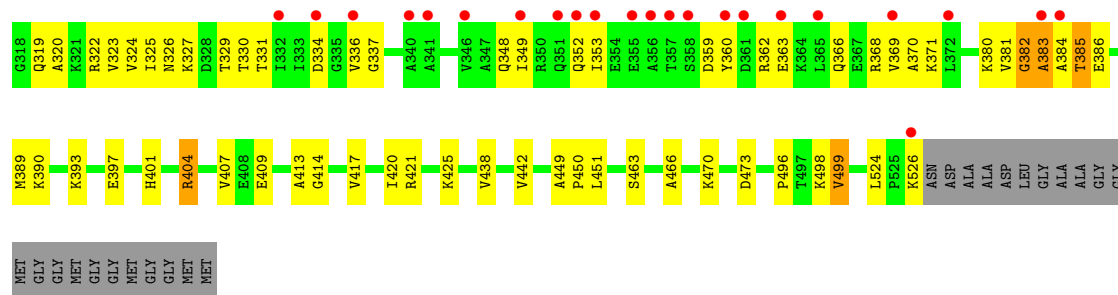


- Molecule 1: groEL protein

Chain G:

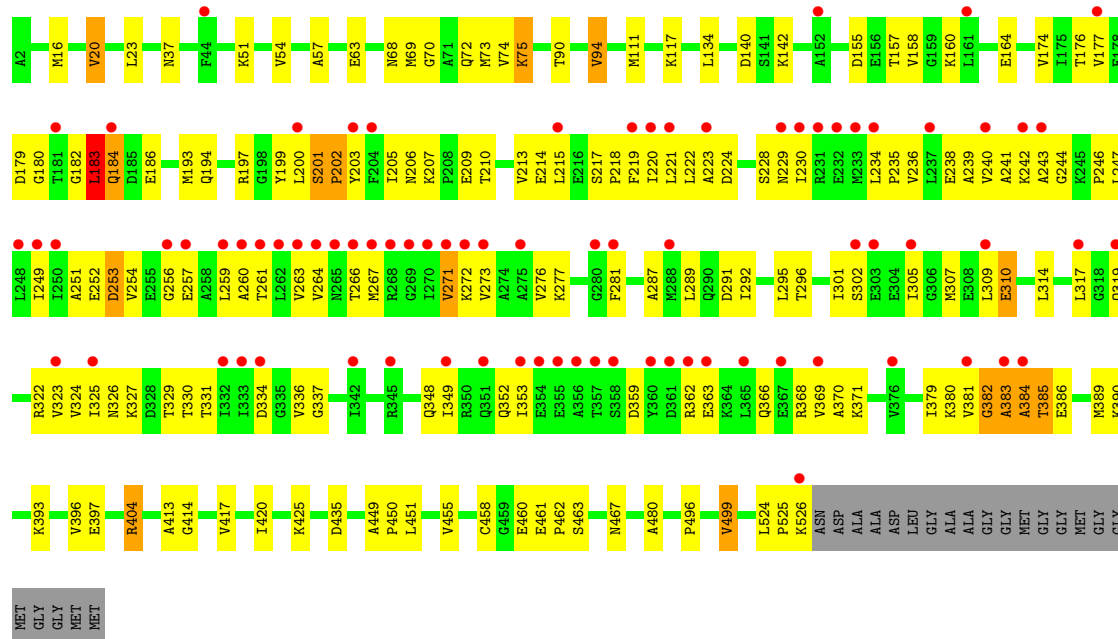






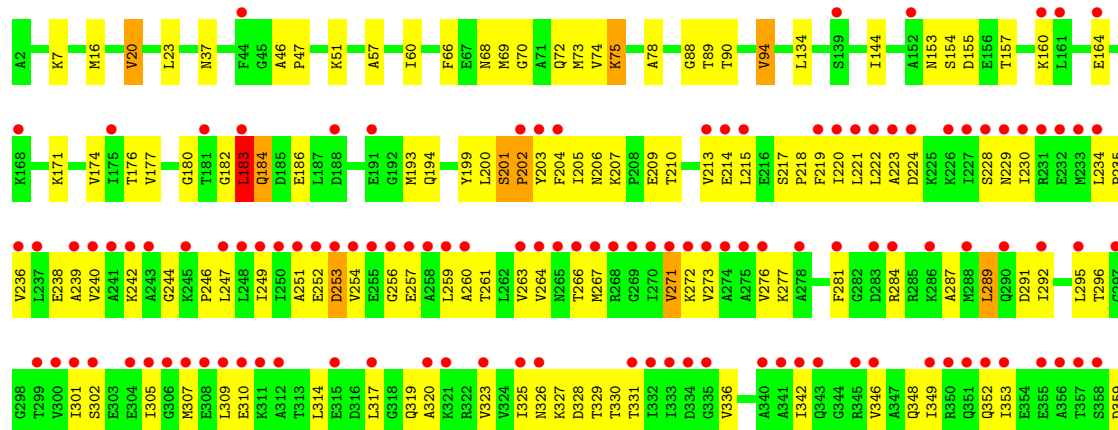
• Molecule 1: groEL protein

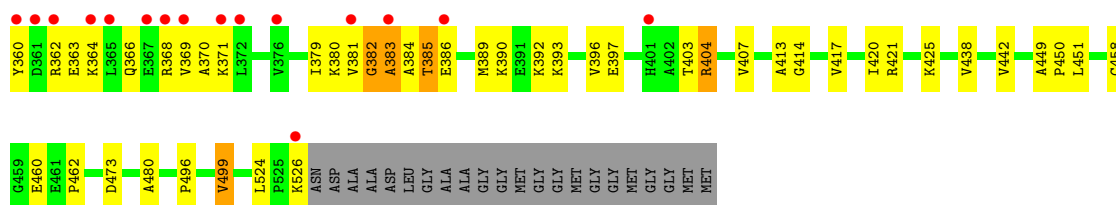
Chain J:



• Molecule 1: groEL protein

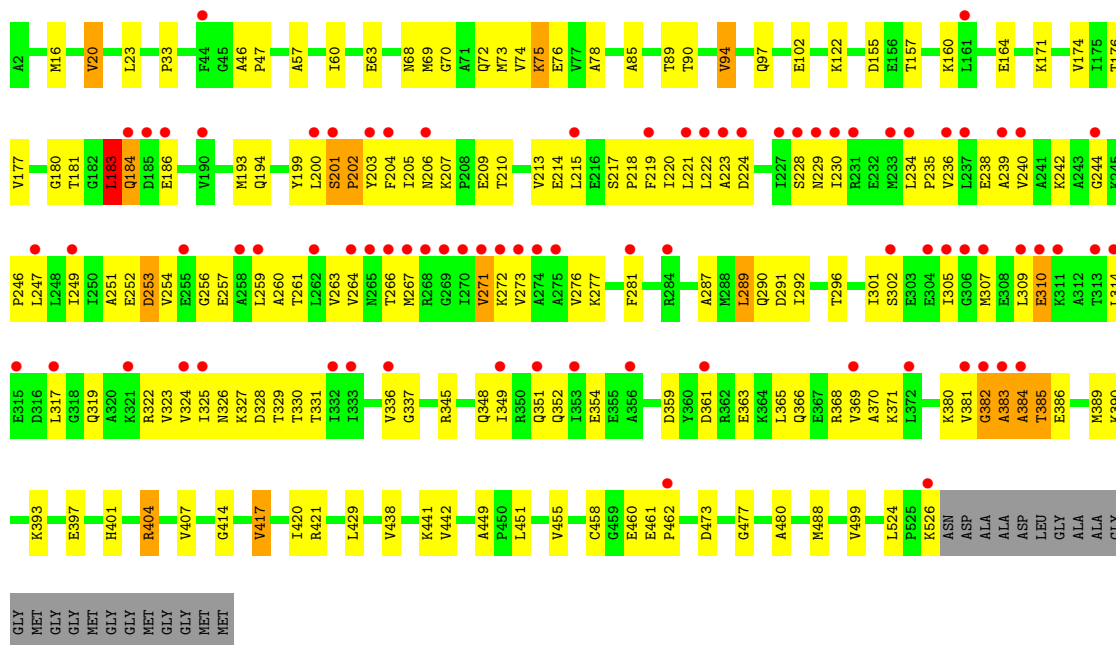
Chain K:





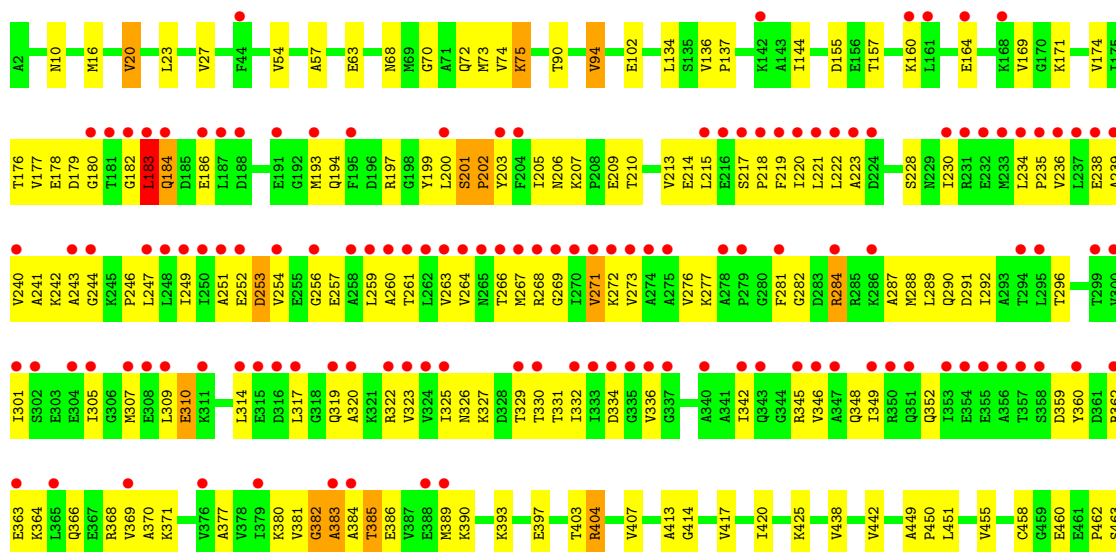
• Molecule 1: groEL protein

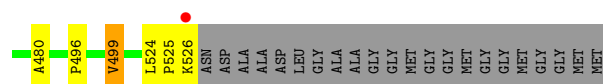
Chain L:



• Molecule 1: groEL protein

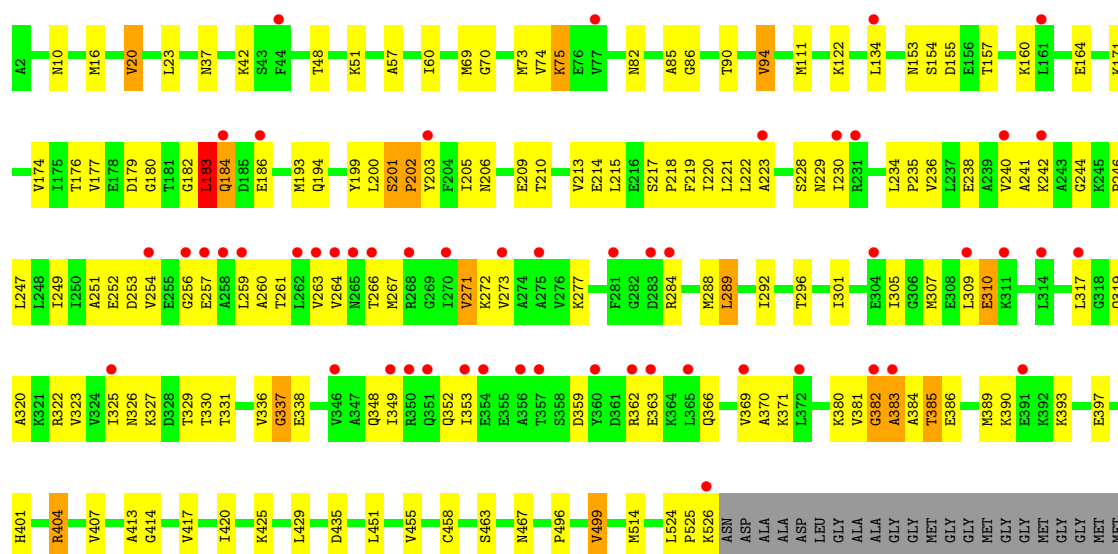
Chain M:





- Molecule 1: groEL protein

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.57Å 260.11Å 150.20Å 90.00° 101.14° 90.00°	Depositor
Resolution (Å)	39.89 – 2.00 39.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	78.9 (39.89-2.00) 79.1 (39.89-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.258 0.241 , 0.256	Depositor DCC
R_{free} test set	10647 reflections (1.97%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 645898 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	57085	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, K, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	0/3883	0.55	0/5243
1	B	0.35	0/3883	0.57	1/5243 (0.0%)
1	C	0.32	0/3883	0.55	0/5243
1	D	0.36	0/3883	0.58	0/5243
1	E	0.34	0/3883	0.57	0/5243
1	F	0.32	0/3883	0.55	0/5243
1	G	0.36	0/3883	0.58	0/5243
1	H	0.33	0/3883	0.56	0/5243
1	I	0.30	0/3883	0.55	0/5243
1	J	0.30	0/3883	0.54	0/5243
1	K	0.30	0/3883	0.54	0/5243
1	L	0.32	0/3883	0.55	0/5243
1	M	0.30	0/3883	0.54	0/5243
1	N	0.31	0/3883	0.55	0/5243
All	All	0.32	0/54362	0.55	1/73402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	VAL	CB-CA-C	-5.51	100.94	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3982	161	0
1	B	3855	0	3982	170	0
1	C	3855	0	3982	153	0
1	D	3855	0	3982	146	0
1	E	3855	0	3982	154	0
1	F	3855	0	3982	136	0
1	G	3855	0	3982	153	1
1	H	3855	0	3982	149	0
1	I	3855	0	3982	150	0
1	J	3855	0	3982	149	0
1	K	3855	0	3982	154	0
1	L	3855	0	3982	149	0
1	M	3855	0	3982	151	0
1	N	3855	0	3982	145	1
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	0	0
2	L	5	0	0	0	0
2	M	10	0	0	0	0
2	N	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	31	0	12	3	0
5	B	31	0	12	4	0
5	C	31	0	12	3	0
5	D	31	0	12	4	0
5	E	31	0	12	4	0
5	F	31	0	12	3	0
5	G	31	0	12	4	0
5	H	31	0	12	4	0
5	I	31	0	12	4	0
5	J	31	0	12	3	0
5	K	31	0	12	5	0
5	L	31	0	12	5	0
5	M	31	0	12	5	0
5	N	31	0	12	4	0
6	A	156	0	0	7	0
6	B	214	0	0	8	0
6	C	149	0	0	9	0
6	D	261	0	0	19	0
6	E	217	0	0	12	0
6	F	200	0	0	5	0
6	G	269	0	0	12	0
6	H	204	0	0	8	0
6	I	145	0	0	5	0
6	J	139	0	0	2	0
6	K	133	0	0	0	0
6	L	163	0	0	9	0
6	M	138	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	153	0	0	7	0
All	All	57085	0	55916	2099	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (2099) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:1:AGS:PG	5:B:1:AGS:S1G	1.50	1.50
5:A:1:AGS:S1G	5:A:1:AGS:PG	1.50	1.49
5:H:1:AGS:PG	5:H:1:AGS:S1G	1.49	1.49
5:M:1:AGS:S1G	5:M:1:AGS:PG	1.49	1.48
5:K:1:AGS:S1G	5:K:1:AGS:PG	1.49	1.48
5:D:551:AGS:PG	5:D:551:AGS:S1G	1.48	1.48
5:J:1:AGS:S1G	5:J:1:AGS:PG	1.49	1.48
5:F:1:AGS:PG	5:F:1:AGS:S1G	1.49	1.48
5:L:1:AGS:PG	5:L:1:AGS:S1G	1.49	1.47
5:N:1:AGS:PG	5:N:1:AGS:S1G	1.49	1.47
5:E:1:AGS:PG	5:E:1:AGS:S1G	1.48	1.47
5:C:1:AGS:PG	5:C:1:AGS:S1G	1.49	1.47
5:I:1:AGS:PG	5:I:1:AGS:S1G	1.49	1.47
5:G:1:AGS:PG	5:G:1:AGS:S1G	1.48	1.46
1:B:77:VAL:HG21	1:B:510:VAL:HG22	1.23	1.15
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.31	1.10
1:J:183:LEU:H	1:J:383:ALA:HB3	1.12	1.10
1:I:183:LEU:H	1:I:383:ALA:HB3	1.13	1.10
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.33	1.10
1:D:183:LEU:H	1:D:383:ALA:HB3	1.15	1.10
1:D:7:LYS:HB3	6:D:2704:HOH:O	1.47	1.10
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.33	1.09
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.33	1.09
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.30	1.09
1:L:183:LEU:H	1:L:383:ALA:HB3	1.08	1.09
1:B:183:LEU:H	1:B:383:ALA:HB3	1.07	1.08
1:F:183:LEU:H	1:F:383:ALA:HB3	1.19	1.08
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.31	1.07
1:K:183:LEU:H	1:K:383:ALA:HB3	1.19	1.07
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.32	1.07
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.31	1.06
1:N:183:LEU:H	1:N:383:ALA:HB3	1.17	1.06
1:H:183:LEU:H	1:H:383:ALA:HB3	1.13	1.06
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.36	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:LEU:H	1:A:383:ALA:HB3	1.20	1.06
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.37	1.06
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.32	1.05
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.36	1.04
1:G:325:ILE:HB	6:G:2628:HOH:O	1.55	1.04
1:B:77:VAL:HG13	1:B:506:TYR:HB3	1.36	1.04
1:E:183:LEU:H	1:E:383:ALA:HB3	1.19	1.03
1:C:183:LEU:H	1:C:383:ALA:HB3	1.23	1.03
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.33	1.03
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.34	1.02
1:M:183:LEU:H	1:M:383:ALA:HB3	1.27	0.99
1:G:183:LEU:H	1:G:383:ALA:HB3	1.25	0.99
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.46	0.98
1:L:218:PRO:HB3	1:L:246:PRO:HG2	1.48	0.96
1:H:383:ALA:HB1	1:I:281:PHE:HZ	1.31	0.95
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.48	0.95
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.48	0.95
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.49	0.95
1:H:218:PRO:HB3	1:H:246:PRO:HG2	1.50	0.94
1:J:383:ALA:HB1	1:K:281:PHE:HZ	1.33	0.94
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.49	0.94
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.49	0.94
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.50	0.93
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.47	0.93
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.50	0.93
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.51	0.93
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.49	0.93
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.50	0.93
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.52	0.92
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.51	0.92
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.52	0.91
1:G:218:PRO:HB3	1:G:246:PRO:HG2	1.53	0.91
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.53	0.91
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.49	0.91
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.53	0.90
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.52	0.90
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.54	0.90
1:B:383:ALA:HB1	1:C:281:PHE:HZ	1.36	0.90
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.55	0.89
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.51	0.89
1:A:281:PHE:HZ	1:G:383:ALA:HB1	1.36	0.89
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.51	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:383:ALA:HB1	1:C:281:PHE:CZ	2.07	0.89
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.54	0.89
1:B:94:VAL:HB	6:B:2545:HOH:O	1.70	0.88
1:L:383:ALA:HB1	1:M:281:PHE:HZ	1.36	0.88
1:G:57:ALA:O	1:G:75:LYS:HE2	1.73	0.88
1:C:171:LYS:HE2	6:C:2796:HOH:O	1.74	0.88
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.55	0.88
1:D:359:ASP:O	1:D:363:GLU:HG2	1.75	0.87
1:L:183:LEU:N	1:L:383:ALA:HB3	1.89	0.86
1:B:183:LEU:N	1:B:383:ALA:HB3	1.89	0.86
1:L:383:ALA:HB1	1:M:281:PHE:CZ	2.10	0.86
1:H:281:PHE:HZ	1:N:383:ALA:HB1	1.38	0.86
1:D:383:ALA:HB1	1:E:281:PHE:HZ	1.42	0.85
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.40	0.85
1:G:359:ASP:O	1:G:363:GLU:HG2	1.75	0.85
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.58	0.85
1:A:281:PHE:CZ	1:G:383:ALA:HB1	2.12	0.84
1:D:57:ALA:O	1:D:75:LYS:HE2	1.77	0.84
1:E:293:ALA:HB2	6:E:2717:HOH:O	1.77	0.84
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.60	0.83
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.60	0.83
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.60	0.83
1:H:183:LEU:N	1:H:383:ALA:HB3	1.93	0.82
1:E:222:LEU:HD13	6:E:2717:HOH:O	1.79	0.82
1:M:420:ILE:HD12	1:M:451:LEU:HD13	1.60	0.82
1:H:289:LEU:HG	6:H:2938:HOH:O	1.77	0.82
1:J:57:ALA:O	1:J:75:LYS:HE2	1.80	0.82
1:I:183:LEU:N	1:I:383:ALA:HB3	1.93	0.82
1:B:86:GLY:HA3	1:B:401:HIS:CE1	2.15	0.82
1:D:183:LEU:N	1:D:383:ALA:HB3	1.94	0.81
1:I:57:ALA:O	1:I:75:LYS:HE2	1.80	0.81
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.62	0.81
1:B:77:VAL:CG2	1:B:510:VAL:HG22	2.07	0.81
1:J:183:LEU:N	1:J:383:ALA:HB3	1.92	0.81
1:H:383:ALA:HB1	1:I:281:PHE:CZ	2.16	0.80
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.63	0.80
1:N:420:ILE:HD12	1:N:451:LEU:HD13	1.62	0.80
1:J:383:ALA:HB1	1:K:281:PHE:CZ	2.17	0.80
1:M:359:ASP:O	1:M:363:GLU:HG2	1.82	0.80
1:N:57:ALA:O	1:N:75:LYS:HE2	1.80	0.80
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.64	0.80
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:57:ALA:O	1:F:75:LYS:HE2	1.81	0.79
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.64	0.79
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.64	0.79
1:J:359:ASP:O	1:J:363:GLU:HG2	1.81	0.79
1:C:463:SER:HB2	6:C:2549:HOH:O	1.82	0.79
1:C:359:ASP:O	1:C:363:GLU:HG2	1.83	0.79
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.65	0.79
1:C:57:ALA:O	1:C:75:LYS:HE2	1.83	0.78
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.64	0.78
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.65	0.78
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.66	0.78
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.65	0.78
1:K:183:LEU:N	1:K:383:ALA:HB3	1.98	0.78
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.65	0.78
1:H:57:ALA:O	1:H:75:LYS:HE2	1.83	0.78
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.66	0.78
1:N:183:LEU:N	1:N:383:ALA:HB3	1.97	0.77
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.65	0.77
1:B:359:ASP:O	1:B:363:GLU:HG2	1.85	0.77
1:M:57:ALA:O	1:M:75:LYS:HE2	1.85	0.77
1:K:359:ASP:O	1:K:363:GLU:HG2	1.85	0.77
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.66	0.77
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.66	0.77
1:F:359:ASP:O	1:F:363:GLU:HG2	1.85	0.77
1:I:420:ILE:HD12	1:I:451:LEU:HD13	1.67	0.77
1:M:463:SER:HB2	6:M:3029:HOH:O	1.85	0.77
1:N:359:ASP:O	1:N:363:GLU:HG2	1.84	0.76
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.68	0.76
1:I:359:ASP:O	1:I:363:GLU:HG2	1.86	0.76
1:G:213:VAL:HB	1:G:325:ILE:CG1	2.15	0.76
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.68	0.76
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.68	0.76
1:F:414:GLY:O	1:F:417:VAL:HG13	1.86	0.76
1:M:381:VAL:HG21	1:M:393:LYS:HA	1.65	0.76
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.66	0.75
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.66	0.75
1:L:359:ASP:O	1:L:363:GLU:HG2	1.85	0.75
1:N:381:VAL:HG21	1:N:393:LYS:HA	1.68	0.75
1:F:183:LEU:N	1:F:383:ALA:HB3	1.97	0.75
1:J:381:VAL:HG21	1:J:393:LYS:HA	1.68	0.75
1:E:194:GLN:O	1:E:371:LYS:HE3	1.87	0.75
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.67	0.75
1:K:381:VAL:HG21	1:K:393:LYS:HA	1.67	0.75
1:H:359:ASP:O	1:H:363:GLU:HG2	1.86	0.75
1:E:359:ASP:O	1:E:363:GLU:HG2	1.87	0.74
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.69	0.74
1:D:183:LEU:H	1:D:383:ALA:CB	1.99	0.74
1:E:183:LEU:N	1:E:383:ALA:HB3	2.00	0.74
5:J:1:AGS:O3B	5:J:1:AGS:S1G	2.45	0.74
1:H:381:VAL:HG21	1:H:393:LYS:HA	1.70	0.74
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.70	0.74
1:C:514:MET:HE3	6:C:2670:HOH:O	1.88	0.73
1:I:194:GLN:O	1:I:371:LYS:HE3	1.87	0.73
1:A:359:ASP:O	1:A:363:GLU:HG2	1.88	0.73
5:G:1:AGS:S1G	5:G:1:AGS:O3B	2.45	0.73
1:C:183:LEU:N	1:C:383:ALA:HB3	2.02	0.73
1:A:183:LEU:N	1:A:383:ALA:HB3	1.99	0.73
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.69	0.73
1:G:473:ASP:HB2	6:G:2130:HOH:O	1.89	0.73
1:L:414:GLY:O	1:L:417:VAL:HG13	1.88	0.73
1:I:381:VAL:HG21	1:I:393:LYS:HA	1.71	0.73
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.71	0.73
5:H:1:AGS:S1G	5:H:1:AGS:O3B	2.46	0.72
1:J:194:GLN:O	1:J:371:LYS:HE3	1.88	0.72
5:N:1:AGS:O3G	5:N:1:AGS:S1G	2.46	0.72
1:A:57:ALA:O	1:A:75:LYS:HE2	1.89	0.72
5:G:1:AGS:S1G	5:G:1:AGS:O3G	2.46	0.72
1:F:263:VAL:O	1:F:267:MET:HB2	1.89	0.72
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.72	0.72
1:L:420:ILE:HD12	1:L:451:LEU:HD13	1.72	0.72
1:L:381:VAL:HG21	1:L:393:LYS:HA	1.72	0.72
5:D:551:AGS:O3B	5:D:551:AGS:S1G	2.46	0.72
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.71	0.72
1:B:194:GLN:O	1:B:371:LYS:HE3	1.89	0.72
1:K:57:ALA:O	1:K:75:LYS:HE2	1.89	0.72
1:I:383:ALA:HB1	1:J:281:PHE:HZ	1.55	0.72
1:C:514:MET:HB3	6:C:2670:HOH:O	1.89	0.72
5:K:1:AGS:S1G	5:K:1:AGS:O3G	2.46	0.72
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.70	0.72
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.72	0.72
1:F:432:GLN:HG2	6:F:2120:HOH:O	1.88	0.72
1:L:305:ILE:HD12	1:L:307:MET:HE2	1.72	0.72
5:I:1:AGS:O3B	5:I:1:AGS:S1G	2.47	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:GLY:O	1:A:417:VAL:HG13	1.90	0.71
5:C:1:AGS:O3B	5:C:1:AGS:S1G	2.48	0.71
1:H:404:ARG:NH1	6:H:2827:HOH:O	2.24	0.71
1:D:186:GLU:HB2	1:D:380:LYS:HB2	1.72	0.71
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.71	0.71
1:L:57:ALA:O	1:L:75:LYS:HE2	1.89	0.71
1:M:183:LEU:N	1:M:383:ALA:HB3	2.05	0.71
1:G:177:VAL:HG21	1:G:397:GLU:CG	2.21	0.71
1:M:305:ILE:HD12	1:M:307:MET:HE2	1.73	0.71
5:F:1:AGS:S1G	5:F:1:AGS:O3B	2.48	0.71
1:B:305:ILE:HD12	1:B:307:MET:HE2	1.72	0.71
1:G:263:VAL:O	1:G:267:MET:HB2	1.91	0.71
5:E:1:AGS:O3B	5:E:1:AGS:S1G	2.48	0.70
1:B:183:LEU:H	1:B:383:ALA:CB	1.95	0.70
1:D:263:VAL:O	1:D:267:MET:HB2	1.91	0.70
1:D:305:ILE:HD12	1:D:307:MET:HE2	1.72	0.70
1:K:414:GLY:O	1:K:417:VAL:HG13	1.91	0.70
1:D:420:ILE:HD12	1:D:451:LEU:HD13	1.72	0.70
1:I:183:LEU:H	1:I:383:ALA:CB	1.98	0.70
1:M:194:GLN:O	1:M:371:LYS:HE3	1.91	0.70
1:L:194:GLN:O	1:L:371:LYS:HE3	1.91	0.70
1:F:305:ILE:HD12	1:F:307:MET:HE2	1.72	0.70
1:A:183:LEU:H	1:A:383:ALA:CB	2.03	0.70
5:M:1:AGS:S1G	5:M:1:AGS:O3B	2.50	0.70
5:F:1:AGS:S1G	5:F:1:AGS:O3G	2.46	0.70
5:C:1:AGS:S1G	5:C:1:AGS:O3G	2.45	0.70
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.72	0.70
1:E:525:PRO:HD3	6:E:1182:HOH:O	1.91	0.70
1:D:291:ASP:OD2	1:D:368:ARG:HD2	1.92	0.69
1:L:183:LEU:H	1:L:383:ALA:CB	1.95	0.69
1:K:263:VAL:O	1:K:267:MET:HB2	1.92	0.69
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.73	0.69
1:D:176:THR:HG21	1:D:322:ARG:HH12	1.58	0.69
1:I:213:VAL:HB	1:I:325:ILE:CG1	2.23	0.69
1:H:219:PHE:HB3	1:H:317:LEU:HD23	1.74	0.69
1:A:263:VAL:O	1:A:267:MET:HB2	1.91	0.69
5:D:551:AGS:S1G	5:D:551:AGS:O3G	2.45	0.69
5:J:1:AGS:O3G	5:J:1:AGS:S1G	2.47	0.69
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.74	0.69
1:J:414:GLY:O	1:J:417:VAL:HG13	1.92	0.69
1:H:194:GLN:O	1:H:371:LYS:HE3	1.91	0.69
5:I:1:AGS:O3G	5:I:1:AGS:S1G	2.45	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:183:LEU:H	1:H:383:ALA:CB	1.98	0.69
1:M:414:GLY:O	1:M:417:VAL:HG13	1.92	0.69
1:C:525:PRO:HD3	6:C:1993:HOH:O	1.93	0.69
5:N:1:AGS:O3B	5:N:1:AGS:S1G	2.50	0.69
5:A:1:AGS:O3B	5:A:1:AGS:S1G	2.48	0.69
1:C:194:GLN:O	1:C:371:LYS:HE3	1.91	0.69
1:N:263:VAL:O	1:N:267:MET:HB2	1.93	0.69
1:H:525:PRO:HD3	6:H:2151:HOH:O	1.93	0.69
1:K:305:ILE:HD12	1:K:307:MET:HE2	1.75	0.69
1:D:213:VAL:HB	1:D:325:ILE:CG1	2.23	0.69
5:H:1:AGS:O3G	5:H:1:AGS:S1G	2.48	0.69
5:K:1:AGS:O3B	5:K:1:AGS:S1G	2.50	0.69
5:E:1:AGS:O3G	5:E:1:AGS:S1G	2.46	0.69
1:L:263:VAL:O	1:L:267:MET:HB2	1.93	0.69
1:J:420:ILE:HD12	1:J:451:LEU:HD13	1.75	0.69
1:E:213:VAL:HB	1:E:325:ILE:CG1	2.23	0.69
1:H:177:VAL:HG21	1:H:397:GLU:HG3	1.74	0.69
1:H:183:LEU:HD23	1:H:384:ALA:HB2	1.76	0.68
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.75	0.68
1:L:449:ALA:HB1	6:L:2642:HOH:O	1.93	0.68
1:J:183:LEU:H	1:J:383:ALA:CB	1.98	0.68
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.75	0.68
1:H:263:VAL:O	1:H:267:MET:HB2	1.92	0.68
1:A:213:VAL:HB	1:A:325:ILE:CG1	2.23	0.68
1:B:263:VAL:O	1:B:267:MET:HB2	1.93	0.68
1:H:305:ILE:HD12	1:H:307:MET:HE2	1.76	0.68
1:C:263:VAL:O	1:C:267:MET:HB2	1.93	0.68
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.75	0.68
1:J:305:ILE:HD12	1:J:307:MET:HE2	1.76	0.68
1:N:177:VAL:HG21	1:N:397:GLU:HG3	1.75	0.68
1:B:414:GLY:O	1:B:417:VAL:HG13	1.93	0.68
1:A:228:SER:O	1:A:257:GLU:HB3	1.94	0.68
1:B:213:VAL:HB	1:B:325:ILE:CG1	2.24	0.68
5:L:1:AGS:O3B	5:L:1:AGS:S1G	2.49	0.68
1:D:194:GLN:O	1:D:371:LYS:HE3	1.94	0.67
1:J:263:VAL:O	1:J:267:MET:HB2	1.93	0.67
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.74	0.67
1:M:263:VAL:O	1:M:267:MET:HB2	1.93	0.67
1:K:383:ALA:HB1	1:L:281:PHE:HZ	1.59	0.67
1:I:263:VAL:O	1:I:267:MET:HB2	1.93	0.67
5:B:1:AGS:O3B	5:B:1:AGS:S1G	2.50	0.67
1:G:183:LEU:N	1:G:383:ALA:HB3	2.04	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:177:VAL:HG21	1:M:397:GLU:HG3	1.75	0.67
1:N:219:PHE:HB3	1:N:317:LEU:HD23	1.77	0.67
1:G:285:ARG:HD2	6:G:2626:HOH:O	1.95	0.67
1:H:177:VAL:HG21	1:H:397:GLU:CG	2.25	0.67
1:C:228:SER:O	1:C:257:GLU:HB3	1.95	0.67
5:B:1:AGS:O3G	5:B:1:AGS:S1G	2.48	0.67
1:J:384:ALA:HA	1:K:360:TYR:OH	1.95	0.67
1:E:263:VAL:O	1:E:267:MET:HB2	1.94	0.67
1:N:305:ILE:HD12	1:N:307:MET:HE2	1.76	0.66
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.76	0.66
1:D:160:LYS:O	1:D:164:GLU:HG3	1.95	0.66
1:G:183:LEU:HD23	1:G:384:ALA:HB2	1.77	0.66
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.75	0.66
1:D:383:ALA:HB1	1:E:281:PHE:CZ	2.29	0.66
5:M:1:AGS:O3G	5:M:1:AGS:S1G	2.47	0.66
1:H:174:VAL:HG22	1:H:194:GLN:HE21	1.61	0.66
1:N:176:THR:HG21	1:N:322:ARG:HH12	1.60	0.66
1:D:23:LEU:HD22	1:D:74:VAL:HG13	1.78	0.66
1:D:414:GLY:O	1:D:417:VAL:HG13	1.96	0.66
1:N:183:LEU:HD23	1:N:384:ALA:HB2	1.78	0.66
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.75	0.66
1:L:177:VAL:HG21	1:L:397:GLU:CG	2.25	0.66
1:F:177:VAL:HG21	1:F:397:GLU:CG	2.26	0.66
1:E:414:GLY:O	1:E:417:VAL:HG13	1.95	0.66
1:B:183:LEU:HD23	1:B:384:ALA:HB2	1.77	0.66
1:A:194:GLN:O	1:A:371:LYS:HE3	1.94	0.66
5:A:1:AGS:S1G	5:A:1:AGS:O3G	2.47	0.66
1:C:414:GLY:O	1:C:417:VAL:HG13	1.96	0.66
1:L:183:LEU:HD23	1:L:384:ALA:HB2	1.78	0.66
1:I:160:LYS:O	1:I:164:GLU:HG3	1.96	0.66
1:I:183:LEU:HD23	1:I:384:ALA:HB2	1.78	0.66
1:K:247:LEU:HB3	1:K:273:VAL:HG22	1.76	0.66
1:E:392:LYS:HE3	6:E:2648:HOH:O	1.96	0.66
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.77	0.66
1:F:228:SER:O	1:F:257:GLU:HB3	1.95	0.66
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.78	0.65
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.78	0.65
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.79	0.65
1:I:414:GLY:O	1:I:417:VAL:HG13	1.96	0.65
1:H:228:SER:O	1:H:257:GLU:HB3	1.97	0.65
1:D:404:ARG:HG2	1:D:404:ARG:HH11	1.60	0.65
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:404:ARG:CG	1:H:404:ARG:HH11	2.08	0.65
1:I:305:ILE:HD12	1:I:307:MET:HE2	1.77	0.65
1:F:178:GLU:OE2	1:F:322:ARG:HD3	1.96	0.65
1:D:326:ASN:HD22	1:D:329:THR:HB	1.61	0.65
1:K:213:VAL:HB	1:K:325:ILE:CG1	2.27	0.65
1:L:228:SER:O	1:L:257:GLU:HB3	1.97	0.65
1:F:213:VAL:HB	1:F:325:ILE:CG1	2.26	0.65
1:G:242:LYS:C	1:G:244:GLY:H	1.98	0.65
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.79	0.65
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.78	0.65
1:K:177:VAL:HG21	1:K:397:GLU:HG3	1.78	0.65
1:B:228:SER:O	1:B:257:GLU:HB3	1.97	0.65
1:D:78:ALA:HB3	6:D:2581:HOH:O	1.95	0.65
1:H:281:PHE:CZ	1:N:383:ALA:HB1	2.28	0.65
1:C:221:LEU:HD23	1:C:249:ILE:HD12	1.79	0.65
1:B:91:THR:O	1:B:94:VAL:HG22	1.96	0.65
1:K:228:SER:O	1:K:257:GLU:HB3	1.97	0.65
1:H:42:LYS:HB2	6:H:2847:HOH:O	1.96	0.65
1:C:420:ILE:HD12	1:C:451:LEU:HD13	1.79	0.65
1:I:186:GLU:HB2	1:I:380:LYS:HB2	1.77	0.65
1:B:60:ILE:O	1:B:75:LYS:HE3	1.98	0.64
1:E:206:ASN:HD21	1:E:214:GLU:H	1.45	0.64
1:C:305:ILE:HD12	1:C:307:MET:HE2	1.78	0.64
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.79	0.64
1:H:69:MET:O	1:H:73:MET:HG3	1.96	0.64
1:G:228:SER:O	1:G:257:GLU:HB3	1.97	0.64
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.79	0.64
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.79	0.64
1:H:414:GLY:O	1:H:417:VAL:HG13	1.98	0.64
1:F:194:GLN:O	1:F:371:LYS:HE3	1.97	0.64
1:I:383:ALA:HB1	1:J:281:PHE:CZ	2.32	0.64
1:F:183:LEU:HD23	1:F:384:ALA:HB2	1.80	0.64
1:A:349:ILE:HA	1:A:352:GLN:CG	2.27	0.64
1:I:177:VAL:HG21	1:I:397:GLU:CG	2.28	0.64
1:I:206:ASN:HD21	1:I:214:GLU:H	1.43	0.64
1:B:160:LYS:O	1:B:164:GLU:HG3	1.97	0.64
1:M:221:LEU:HD23	1:M:249:ILE:HD12	1.80	0.64
1:D:183:LEU:O	1:D:184:GLN:HB2	1.98	0.64
1:K:183:LEU:HD23	1:K:384:ALA:HB2	1.80	0.64
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.63	0.64
1:D:177:VAL:HG21	1:D:397:GLU:CG	2.27	0.64
1:E:177:VAL:HG21	1:E:397:GLU:CG	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.80	0.64
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.80	0.64
1:J:177:VAL:HG21	1:J:397:GLU:HG3	1.80	0.64
1:N:213:VAL:HB	1:N:325:ILE:CG1	2.28	0.64
1:K:404:ARG:HH11	1:K:404:ARG:HG2	1.63	0.64
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.79	0.64
1:L:213:VAL:HB	1:L:325:ILE:CG1	2.28	0.64
1:A:268:ARG:O	1:B:257:GLU:HG3	1.97	0.64
1:A:46:ALA:HB2	1:B:76:GLU:CG	2.28	0.64
1:K:183:LEU:H	1:K:383:ALA:CB	2.03	0.63
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.28	0.63
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.80	0.63
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.79	0.63
1:L:177:VAL:HG21	1:L:397:GLU:HG3	1.80	0.63
1:K:194:GLN:O	1:K:371:LYS:HE3	1.98	0.63
1:I:177:VAL:HG21	1:I:397:GLU:HG3	1.80	0.63
1:M:326:ASN:HD22	1:M:329:THR:HB	1.64	0.63
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.79	0.63
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.80	0.63
1:A:183:LEU:HD23	1:A:384:ALA:HB2	1.81	0.63
1:C:213:VAL:HB	1:C:325:ILE:CG1	2.28	0.63
1:D:221:LEU:HD23	1:D:249:ILE:HD12	1.80	0.63
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.81	0.63
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.80	0.63
1:C:90:THR:O	1:C:94:VAL:HG13	1.98	0.63
1:D:193:MET:CE	1:D:292:ILE:HG12	2.28	0.63
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.81	0.63
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.79	0.63
1:F:183:LEU:H	1:F:383:ALA:CB	2.03	0.63
1:N:177:VAL:HG21	1:N:397:GLU:CG	2.29	0.63
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.80	0.63
1:E:305:ILE:HD12	1:E:307:MET:HE2	1.80	0.63
1:H:362:ARG:O	1:H:366:GLN:HG3	1.99	0.63
1:J:183:LEU:HD23	1:J:384:ALA:HB2	1.81	0.63
1:D:193:MET:HE2	1:D:292:ILE:HG12	1.80	0.63
1:J:54:VAL:HG23	6:J:2067:HOH:O	1.98	0.63
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.79	0.63
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.29	0.63
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.81	0.62
1:G:194:GLN:O	1:G:371:LYS:HE3	1.99	0.62
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.64	0.62
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:305:ILE:HD12	1:G:307:MET:HE2	1.81	0.62
1:N:228:SER:O	1:N:257:GLU:HB3	1.99	0.62
1:M:228:SER:O	1:M:257:GLU:HB3	1.99	0.62
5:L:1:AGS:S1G	5:L:1:AGS:O3G	2.49	0.62
1:C:139:SER:HB3	6:C:2796:HOH:O	2.00	0.62
1:K:200:LEU:O	1:K:201:SER:HB3	1.99	0.62
1:F:420:ILE:HD12	1:F:451:LEU:HD13	1.81	0.62
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.80	0.62
1:B:186:GLU:HB2	1:B:380:LYS:HB2	1.80	0.62
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.81	0.62
1:M:176:THR:HG21	1:M:322:ARG:HH12	1.63	0.62
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.27	0.62
1:F:160:LYS:O	1:F:164:GLU:HG3	2.00	0.62
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.82	0.62
1:E:228:SER:O	1:E:257:GLU:HB3	1.99	0.62
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.81	0.62
1:A:360:TYR:OH	1:G:384:ALA:HA	2.00	0.62
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.81	0.62
1:D:82:ASN:HA	6:D:2757:HOH:O	1.98	0.62
1:C:404:ARG:HH11	1:C:404:ARG:HG2	1.63	0.62
1:N:183:LEU:H	1:N:383:ALA:CB	2.02	0.62
1:C:200:LEU:O	1:C:201:SER:HB3	1.99	0.62
1:B:68:ASN:O	1:B:72:GLN:HG2	1.98	0.62
1:F:413:ALA:HB3	1:F:417:VAL:HG22	1.82	0.62
1:D:200:LEU:O	1:D:201:SER:HB3	2.00	0.62
1:M:178:GLU:OE2	1:M:322:ARG:HD3	2.00	0.62
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.81	0.62
1:H:420:ILE:HD12	1:H:451:LEU:HD13	1.80	0.62
1:N:272:LYS:HD2	1:N:272:LYS:N	2.15	0.62
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.80	0.62
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.80	0.62
1:H:206:ASN:HD21	1:H:214:GLU:H	1.46	0.62
1:H:384:ALA:HA	1:I:360:TYR:OH	2.00	0.62
1:L:218:PRO:CB	1:L:246:PRO:HG2	2.27	0.62
1:K:205:ILE:HA	1:K:213:VAL:HG22	1.82	0.61
1:J:221:LEU:HD23	1:J:249:ILE:HD12	1.82	0.61
1:B:77:VAL:CG1	1:B:506:TYR:HB3	2.22	0.61
1:H:349:ILE:HA	1:H:352:GLN:CG	2.28	0.61
1:L:78:ALA:HB3	6:L:2535:HOH:O	1.99	0.61
1:N:404:ARG:HH11	1:N:404:ARG:HG2	1.65	0.61
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.81	0.61
1:N:414:GLY:O	1:N:417:VAL:HG13	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:16:MET:O	1:F:20:VAL:HG13	2.00	0.61
1:M:525:PRO:HD3	6:M:2817:HOH:O	1.99	0.61
1:J:177:VAL:HG21	1:J:397:GLU:CG	2.30	0.61
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.83	0.61
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.82	0.61
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.82	0.61
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.81	0.61
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.82	0.61
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.01	0.61
1:B:200:LEU:O	1:B:201:SER:HB3	2.00	0.61
1:D:404:ARG:NH1	6:D:2552:HOH:O	2.33	0.61
1:G:78:ALA:HB3	6:G:1724:HOH:O	1.98	0.61
1:E:78:ALA:HB3	6:E:2338:HOH:O	2.00	0.61
1:D:183:LEU:HD23	1:D:384:ALA:HB2	1.83	0.61
1:N:200:LEU:O	1:N:201:SER:HB3	2.00	0.61
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.82	0.61
1:M:268:ARG:O	1:N:257:GLU:HG3	1.99	0.61
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.00	0.61
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.83	0.61
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.83	0.61
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.83	0.61
1:J:160:LYS:O	1:J:164:GLU:HG3	2.01	0.61
1:G:183:LEU:O	1:G:184:GLN:HB2	2.00	0.61
1:A:69:MET:O	1:A:73:MET:HG3	2.00	0.61
1:C:183:LEU:HD12	1:C:184:GLN:HG3	1.83	0.61
1:M:177:VAL:HG21	1:M:397:GLU:CG	2.30	0.61
1:C:272:LYS:HD2	1:C:272:LYS:N	2.16	0.61
1:M:319:GLN:O	1:M:336:VAL:HG23	2.01	0.61
1:I:228:SER:O	1:I:257:GLU:HB3	2.01	0.60
1:J:183:LEU:HD12	1:J:184:GLN:HG3	1.83	0.60
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.83	0.60
1:F:206:ASN:HD21	1:F:214:GLU:H	1.49	0.60
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.83	0.60
1:C:23:LEU:HD22	1:C:74:VAL:HG13	1.84	0.60
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.01	0.60
1:D:39:VAL:HG12	1:E:69:MET:HE2	1.83	0.60
1:C:177:VAL:HG21	1:C:397:GLU:CG	2.31	0.60
1:B:90:THR:O	1:B:94:VAL:HG13	2.02	0.60
1:I:218:PRO:CB	1:I:246:PRO:HG2	2.28	0.60
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.81	0.60
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.82	0.60
1:M:362:ARG:O	1:M:366:GLN:HG3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.83	0.60
1:B:177:VAL:HG21	1:B:397:GLU:CG	2.32	0.60
1:B:221:LEU:HD23	1:B:249:ILE:HD12	1.82	0.60
1:M:200:LEU:O	1:M:201:SER:HB3	1.99	0.60
1:A:46:ALA:CB	1:B:76:GLU:HG3	2.31	0.60
1:B:425:LYS:HB2	6:B:2916:HOH:O	2.01	0.60
1:G:414:GLY:O	1:G:417:VAL:HG13	2.01	0.60
1:G:420:ILE:HD12	1:G:451:LEU:HD13	1.82	0.60
1:J:23:LEU:CD2	1:J:74:VAL:HG13	2.31	0.60
1:D:272:LYS:HD2	1:D:272:LYS:N	2.17	0.60
1:D:228:SER:O	1:D:257:GLU:HB3	2.01	0.60
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.83	0.60
1:B:57:ALA:O	1:B:75:LYS:HE2	2.01	0.60
1:N:194:GLN:O	1:N:371:LYS:HE3	2.00	0.60
1:A:177:VAL:HG21	1:A:397:GLU:CG	2.31	0.60
1:J:228:SER:O	1:J:257:GLU:HB3	2.02	0.60
1:F:383:ALA:O	1:F:384:ALA:HB3	2.01	0.59
1:J:349:ILE:HA	1:J:352:GLN:CG	2.31	0.59
1:J:272:LYS:N	1:J:272:LYS:HD2	2.17	0.59
1:B:496:PRO:HB2	1:B:499:VAL:HG13	1.84	0.59
1:I:404:ARG:HG2	1:I:404:ARG:HH11	1.67	0.59
1:C:183:LEU:HD23	1:C:384:ALA:HB2	1.85	0.59
1:E:349:ILE:HA	1:E:352:GLN:CG	2.32	0.59
1:E:183:LEU:HD23	1:E:384:ALA:HB2	1.85	0.59
1:J:218:PRO:CB	1:J:246:PRO:HG2	2.28	0.59
1:A:23:LEU:HD22	1:A:74:VAL:HG13	1.85	0.59
1:E:489:ILE:HD13	1:E:494:LEU:HD21	1.85	0.59
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.82	0.59
1:D:242:LYS:C	1:D:244:GLY:H	2.03	0.59
1:F:90:THR:O	1:F:94:VAL:HG13	2.02	0.59
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.03	0.59
1:K:177:VAL:HG21	1:K:397:GLU:CG	2.32	0.59
1:M:349:ILE:HA	1:M:352:GLN:CG	2.32	0.59
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.85	0.59
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.02	0.59
1:M:206:ASN:HD21	1:M:214:GLU:H	1.51	0.59
1:B:449:ALA:HB1	6:B:2545:HOH:O	2.02	0.59
1:B:114:MET:HB3	6:B:2278:HOH:O	2.02	0.59
1:M:160:LYS:O	1:M:164:GLU:HG3	2.03	0.59
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.83	0.59
1:I:272:LYS:N	1:I:272:LYS:HD2	2.18	0.59
1:H:247:LEU:HB3	1:H:273:VAL:HG22	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.84	0.59
1:C:362:ARG:O	1:C:366:GLN:HG3	2.03	0.59
1:L:90:THR:O	1:L:94:VAL:HG13	2.03	0.59
1:L:205:ILE:HA	1:L:213:VAL:HG22	1.85	0.59
1:E:272:LYS:HD2	1:E:272:LYS:N	2.17	0.59
1:C:349:ILE:HA	1:C:352:GLN:CG	2.31	0.58
1:F:349:ILE:HA	1:F:352:GLN:CG	2.33	0.58
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.83	0.58
1:A:362:ARG:O	1:A:366:GLN:HG3	2.03	0.58
1:F:386:GLU:O	1:F:390:LYS:HG2	2.03	0.58
1:A:272:LYS:HD2	1:A:272:LYS:N	2.18	0.58
1:J:174:VAL:HG22	1:J:194:GLN:HE21	1.68	0.58
1:C:155:ASP:OD1	1:C:157:THR:HB	2.03	0.58
1:G:272:LYS:N	1:G:272:LYS:HD2	2.17	0.58
1:K:272:LYS:HD2	1:K:272:LYS:N	2.18	0.58
1:D:362:ARG:O	1:D:366:GLN:HG3	2.03	0.58
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.84	0.58
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.69	0.58
1:F:362:ARG:O	1:F:366:GLN:HG3	2.04	0.58
1:D:11:ASP:HB2	6:D:2704:HOH:O	2.02	0.58
1:I:200:LEU:O	1:I:201:SER:HB3	2.03	0.58
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.85	0.58
1:G:183:LEU:H	1:G:383:ALA:CB	2.08	0.58
1:H:218:PRO:CB	1:H:246:PRO:HG2	2.30	0.58
1:A:404:ARG:NH1	6:A:2654:HOH:O	2.36	0.58
1:I:183:LEU:HD12	1:I:184:GLN:HG3	1.85	0.58
1:H:183:LEU:O	1:H:184:GLN:HB2	2.03	0.58
1:K:218:PRO:CB	1:K:246:PRO:HG2	2.30	0.58
1:N:160:LYS:O	1:N:164:GLU:HG3	2.03	0.58
1:M:183:LEU:HD23	1:M:384:ALA:HB2	1.85	0.58
1:N:349:ILE:HA	1:N:352:GLN:CG	2.33	0.58
1:K:349:ILE:HA	1:K:352:GLN:CG	2.33	0.58
1:L:417:VAL:HG11	1:L:488:MET:HG3	1.84	0.58
1:C:206:ASN:HD21	1:C:214:GLU:H	1.50	0.58
1:H:272:LYS:N	1:H:272:LYS:HD2	2.19	0.58
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.68	0.58
1:E:183:LEU:O	1:E:184:GLN:HB2	2.04	0.57
1:F:200:LEU:O	1:F:201:SER:HB3	2.02	0.57
1:H:174:VAL:HG22	1:H:194:GLN:NE2	2.18	0.57
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.86	0.57
1:L:383:ALA:O	1:L:384:ALA:HB3	2.04	0.57
1:L:349:ILE:HA	1:L:352:GLN:CG	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:463:SER:HB2	6:D:2645:HOH:O	2.03	0.57
1:A:305:ILE:HD12	1:A:307:MET:HE2	1.85	0.57
1:A:382:GLY:O	1:A:389:MET:HG2	2.04	0.57
1:L:272:LYS:HD2	1:L:272:LYS:N	2.19	0.57
1:B:272:LYS:HD2	1:B:272:LYS:N	2.19	0.57
1:G:213:VAL:HB	1:G:325:ILE:HG13	1.86	0.57
1:E:183:LEU:H	1:E:383:ALA:CB	2.05	0.57
1:M:218:PRO:CB	1:M:246:PRO:HG2	2.27	0.57
1:G:382:GLY:O	1:G:389:MET:HG2	2.04	0.57
1:A:420:ILE:HD12	1:A:451:LEU:HD13	1.87	0.57
1:J:206:ASN:HD21	1:J:214:GLU:H	1.51	0.57
1:D:11:ASP:CB	6:D:2704:HOH:O	2.52	0.57
1:N:183:LEU:HD12	1:N:184:GLN:HG3	1.87	0.57
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.85	0.57
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.87	0.57
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.87	0.57
1:F:85:ALA:O	1:F:401:HIS:HE1	1.88	0.57
1:D:90:THR:O	1:D:94:VAL:HG13	2.05	0.57
1:K:183:LEU:HD12	1:K:184:GLN:HG3	1.87	0.57
1:H:360:TYR:OH	1:N:384:ALA:HA	2.04	0.57
1:N:183:LEU:CD1	1:N:184:GLN:HG3	2.34	0.57
1:I:349:ILE:HA	1:I:352:GLN:CG	2.33	0.57
1:A:326:ASN:HD22	1:A:329:THR:HB	1.70	0.57
1:N:247:LEU:HB3	1:N:273:VAL:HG22	1.86	0.57
1:L:386:GLU:O	1:L:390:LYS:HG2	2.04	0.57
1:N:362:ARG:O	1:N:366:GLN:HG3	2.05	0.57
1:I:183:LEU:O	1:I:184:GLN:HB2	2.05	0.57
1:A:235:PRO:CG	1:A:310:GLU:HA	2.29	0.57
1:A:218:PRO:CB	1:A:246:PRO:HG2	2.32	0.57
1:C:326:ASN:HD22	1:C:329:THR:HB	1.70	0.57
1:N:206:ASN:HD21	1:N:214:GLU:H	1.50	0.57
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.85	0.57
1:K:206:ASN:HD21	1:K:214:GLU:H	1.51	0.57
1:B:382:GLY:O	1:B:389:MET:HG2	2.05	0.57
1:E:200:LEU:O	1:E:201:SER:HB3	2.03	0.57
1:I:326:ASN:HD22	1:I:329:THR:HB	1.70	0.57
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.85	0.57
1:J:205:ILE:HA	1:J:213:VAL:HG22	1.85	0.57
1:L:242:LYS:C	1:L:244:GLY:H	2.06	0.57
1:A:16:MET:O	1:A:20:VAL:HG13	2.04	0.57
1:A:281:PHE:HZ	1:G:383:ALA:CB	2.15	0.57
1:E:218:PRO:CB	1:E:246:PRO:HG2	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:160:LYS:NZ	1:D:160:LYS:HB2	2.20	0.57
1:K:326:ASN:HD22	1:K:329:THR:HB	1.70	0.57
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.86	0.57
1:L:193:MET:CE	1:L:292:ILE:HG12	2.35	0.57
1:F:404:ARG:HH11	1:F:404:ARG:HG2	1.70	0.57
1:A:200:LEU:O	1:A:201:SER:HB3	2.04	0.56
1:A:155:ASP:OD1	1:A:157:THR:HB	2.04	0.56
1:N:183:LEU:O	1:N:184:GLN:HB2	2.05	0.56
1:A:46:ALA:HB2	1:B:76:GLU:HG3	1.87	0.56
6:B:1684:HOH:O	1:C:518:GLU:HG2	2.04	0.56
1:J:383:ALA:O	1:J:384:ALA:HB3	2.05	0.56
1:L:183:LEU:O	1:L:184:GLN:HB2	2.06	0.56
1:L:384:ALA:HA	1:M:360:TYR:OH	2.05	0.56
1:A:183:LEU:O	1:A:184:GLN:HB2	2.06	0.56
1:J:247:LEU:HB3	1:J:273:VAL:HG22	1.85	0.56
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.04	0.56
1:D:138:CYS:HB2	6:D:2989:HOH:O	2.05	0.56
1:E:155:ASP:OD1	1:E:157:THR:HB	2.03	0.56
1:D:386:GLU:O	1:D:390:LYS:HG2	2.05	0.56
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.88	0.56
1:L:160:LYS:O	1:L:164:GLU:HG3	2.05	0.56
1:N:242:LYS:C	1:N:244:GLY:H	2.07	0.56
1:M:220:ILE:HD12	1:M:296:THR:HG21	1.88	0.56
1:B:183:LEU:HD12	1:B:184:GLN:HG3	1.86	0.56
1:G:77:VAL:HG23	1:G:510:VAL:HG21	1.88	0.56
1:E:71:ALA:O	1:E:75:LYS:HB2	2.05	0.56
1:M:272:LYS:N	1:M:272:LYS:HD2	2.19	0.56
1:L:155:ASP:OD1	1:L:157:THR:HB	2.05	0.56
1:H:68:ASN:O	1:H:72:GLN:HG2	2.04	0.56
1:E:34:LYS:HG3	1:E:458:CYS:SG	2.46	0.56
1:A:282:GLY:HA3	1:G:181:THR:O	2.05	0.56
1:L:206:ASN:HD21	1:L:214:GLU:H	1.52	0.56
1:M:382:GLY:O	1:M:389:MET:HG2	2.06	0.56
1:B:155:ASP:OD1	1:B:157:THR:HB	2.05	0.56
1:J:242:LYS:C	1:J:244:GLY:H	2.09	0.56
1:E:300:VAL:HG22	6:E:2717:HOH:O	2.04	0.56
1:B:349:ILE:HA	1:B:352:GLN:CG	2.34	0.56
1:I:23:LEU:CD2	1:I:74:VAL:HG13	2.35	0.56
1:D:284:ARG:HH12	1:D:364:LYS:NZ	2.04	0.56
1:H:242:LYS:C	1:H:244:GLY:H	2.09	0.56
1:F:54:VAL:HG23	6:F:2017:HOH:O	2.06	0.56
1:E:301:ILE:HG21	1:E:309:LEU:HD23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:242:LYS:C	1:E:244:GLY:H	2.08	0.56
1:E:193:MET:CE	1:E:292:ILE:HG12	2.37	0.56
1:G:252:GLU:O	1:G:253:ASP:HB2	2.06	0.56
1:K:23:LEU:CD2	1:K:74:VAL:HG13	2.35	0.56
1:I:362:ARG:O	1:I:366:GLN:HG3	2.06	0.56
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.88	0.56
1:C:183:LEU:H	1:C:383:ALA:CB	2.08	0.55
1:F:326:ASN:HD22	1:F:329:THR:HB	1.71	0.55
1:L:181:THR:O	1:M:282:GLY:HA3	2.06	0.55
1:D:114:MET:HG2	6:D:2375:HOH:O	2.06	0.55
1:E:220:ILE:HD12	1:E:296:THR:HG21	1.88	0.55
1:M:462:PRO:HD2	6:M:2751:HOH:O	2.05	0.55
1:F:183:LEU:O	1:F:184:GLN:HB2	2.07	0.55
1:G:199:TYR:N	6:G:2628:HOH:O	2.39	0.55
1:H:205:ILE:HA	1:H:213:VAL:HG22	1.86	0.55
1:J:23:LEU:HD22	1:J:74:VAL:HG13	1.88	0.55
1:M:242:LYS:C	1:M:244:GLY:H	2.10	0.55
1:G:176:THR:HG21	1:G:322:ARG:HH12	1.72	0.55
1:K:383:ALA:HB1	1:L:281:PHE:CZ	2.39	0.55
1:M:235:PRO:CG	1:M:310:GLU:HA	2.32	0.55
1:J:326:ASN:HD22	1:J:329:THR:HB	1.71	0.55
1:H:23:LEU:CD2	1:H:74:VAL:HG13	2.37	0.55
1:H:386:GLU:O	1:H:390:LYS:HG2	2.07	0.55
1:K:242:LYS:C	1:K:244:GLY:H	2.08	0.55
1:J:183:LEU:CD1	1:J:184:GLN:HG3	2.36	0.55
1:J:235:PRO:CG	1:J:310:GLU:HA	2.32	0.55
1:J:180:GLY:HA3	1:J:381:VAL:O	2.07	0.55
1:I:266:THR:CG2	1:I:273:VAL:H	2.19	0.55
1:C:193:MET:CE	1:C:292:ILE:HG12	2.37	0.55
1:I:383:ALA:O	1:I:384:ALA:HB3	2.07	0.55
1:N:266:THR:CG2	1:N:273:VAL:H	2.19	0.55
1:J:362:ARG:O	1:J:366:GLN:HG3	2.06	0.55
1:I:155:ASP:OD1	1:I:157:THR:HB	2.06	0.55
1:K:155:ASP:OD1	1:K:157:THR:HB	2.06	0.55
1:A:183:LEU:HD12	1:A:184:GLN:HG3	1.89	0.55
1:D:218:PRO:CB	1:D:246:PRO:HG2	2.33	0.55
1:D:60:ILE:O	1:D:75:LYS:HE3	2.07	0.55
1:L:200:LEU:O	1:L:201:SER:HB3	2.07	0.55
1:G:200:LEU:O	1:G:201:SER:HB3	2.07	0.55
1:A:174:VAL:HG22	1:A:194:GLN:HE21	1.70	0.55
1:L:73:MET:O	1:L:76:GLU:HB2	2.07	0.55
1:K:272:LYS:NZ	1:L:229:ASN:HD21	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:193:MET:CE	1:I:292:ILE:HG12	2.36	0.55
1:A:206:ASN:HD21	1:A:214:GLU:H	1.54	0.55
1:G:310:GLU:OE1	1:G:310:GLU:N	2.40	0.55
1:E:453:GLN:NE2	2:E:4005:SO4:O1	2.40	0.55
1:K:386:GLU:O	1:K:390:LYS:HG2	2.07	0.55
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.07	0.55
1:B:183:LEU:O	1:B:184:GLN:HB2	2.06	0.55
1:M:180:GLY:HA3	1:M:381:VAL:O	2.07	0.55
1:E:326:ASN:HD22	1:E:329:THR:HB	1.72	0.55
1:E:160:LYS:O	1:E:164:GLU:HG3	2.07	0.55
1:G:183:LEU:CD1	1:G:184:GLN:HG3	2.37	0.55
1:N:60:ILE:O	1:N:75:LYS:HE3	2.07	0.55
1:C:178:GLU:OE2	1:C:322:ARG:HD3	2.07	0.55
1:D:54:VAL:HG23	6:D:1693:HOH:O	2.07	0.55
1:C:218:PRO:CB	1:C:246:PRO:HG2	2.35	0.55
1:A:331:THR:HG22	6:A:2839:HOH:O	2.06	0.55
1:K:362:ARG:O	1:K:366:GLN:HG3	2.07	0.55
1:B:362:ARG:O	1:B:366:GLN:HG3	2.07	0.55
1:G:386:GLU:O	1:G:390:LYS:HG2	2.07	0.55
1:G:23:LEU:HD22	1:G:74:VAL:HG13	1.89	0.55
1:B:384:ALA:O	1:B:385:THR:HG23	2.08	0.54
1:F:183:LEU:HD12	1:F:184:GLN:HG3	1.89	0.54
1:J:200:LEU:O	1:J:201:SER:HB3	2.05	0.54
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.06	0.54
1:G:418:ALA:N	6:G:2394:HOH:O	2.38	0.54
1:D:114:MET:HB3	6:D:2178:HOH:O	2.05	0.54
1:A:160:LYS:O	1:A:164:GLU:HG3	2.08	0.54
1:A:386:GLU:O	1:A:390:LYS:HG2	2.08	0.54
1:F:218:PRO:CB	1:F:246:PRO:HG2	2.31	0.54
1:N:382:GLY:O	1:N:389:MET:HG2	2.07	0.54
1:J:176:THR:HG21	1:J:322:ARG:HH12	1.71	0.54
1:B:386:GLU:O	1:B:390:LYS:HG2	2.07	0.54
1:C:260:ALA:O	1:C:264:VAL:HG23	2.07	0.54
1:C:183:LEU:CD1	1:C:184:GLN:HG3	2.38	0.54
1:B:218:PRO:CB	1:B:246:PRO:HG2	2.29	0.54
1:I:305:ILE:HB	1:I:307:MET:HE2	1.89	0.54
1:H:160:LYS:O	1:H:164:GLU:HG3	2.06	0.54
1:K:383:ALA:O	1:K:384:ALA:HB3	2.08	0.54
1:B:235:PRO:CG	1:B:310:GLU:HA	2.30	0.54
1:G:362:ARG:O	1:G:366:GLN:HG3	2.07	0.54
1:J:183:LEU:O	1:J:184:GLN:HB2	2.08	0.54
1:N:218:PRO:CB	1:N:246:PRO:HG2	2.34	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:200:LEU:O	1:H:201:SER:HB3	2.07	0.54
1:G:236:VAL:O	1:G:240:VAL:HG23	2.07	0.54
1:E:489:ILE:HD13	1:E:494:LEU:CD2	2.38	0.54
1:H:16:MET:O	1:H:20:VAL:HG13	2.07	0.54
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.90	0.54
1:H:193:MET:CE	1:H:292:ILE:HG12	2.38	0.54
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.07	0.54
1:H:305:ILE:O	1:H:305:ILE:HG22	2.08	0.54
1:J:259:LEU:O	1:J:263:VAL:HG23	2.08	0.54
1:I:16:MET:O	1:I:20:VAL:HG13	2.08	0.54
1:M:183:LEU:HD12	1:M:184:GLN:HG3	1.90	0.54
1:C:382:GLY:O	1:C:389:MET:HG2	2.08	0.54
1:E:382:GLY:O	1:E:389:MET:HG2	2.08	0.54
1:J:305:ILE:O	1:J:305:ILE:HG22	2.08	0.54
1:F:160:LYS:NZ	1:F:160:LYS:HB2	2.23	0.54
1:B:206:ASN:HD21	1:B:214:GLU:H	1.56	0.54
1:F:242:LYS:C	1:F:244:GLY:H	2.10	0.54
1:D:85:ALA:HB1	6:D:2188:HOH:O	2.07	0.54
1:H:176:THR:HG22	1:H:177:VAL:N	2.22	0.54
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.88	0.54
1:I:183:LEU:CD1	1:I:184:GLN:HG3	2.38	0.54
1:M:183:LEU:O	1:M:184:GLN:HB2	2.08	0.54
1:J:236:VAL:O	1:J:240:VAL:HG23	2.08	0.54
1:G:266:THR:CG2	1:G:273:VAL:H	2.21	0.54
1:B:383:ALA:O	1:B:384:ALA:HB3	2.08	0.53
1:B:85:ALA:O	1:B:401:HIS:HE1	1.90	0.53
1:H:382:GLY:O	1:H:389:MET:HG2	2.08	0.53
1:F:305:ILE:HG22	1:F:305:ILE:O	2.07	0.53
1:H:160:LYS:HB2	1:H:160:LYS:NZ	2.23	0.53
1:L:16:MET:O	1:L:20:VAL:HG13	2.08	0.53
1:N:221:LEU:HD23	1:N:249:ILE:HD12	1.90	0.53
1:B:242:LYS:C	1:B:244:GLY:H	2.11	0.53
1:I:90:THR:O	1:I:94:VAL:HG13	2.08	0.53
1:A:281:PHE:CZ	1:G:383:ALA:CB	2.89	0.53
1:G:218:PRO:CB	1:G:246:PRO:HG2	2.32	0.53
1:F:176:THR:HG22	1:F:177:VAL:N	2.23	0.53
1:H:73:MET:O	1:H:76:GLU:HB2	2.09	0.53
1:J:193:MET:CE	1:J:292:ILE:HG12	2.38	0.53
1:J:90:THR:O	1:J:94:VAL:HG13	2.09	0.53
1:D:16:MET:O	1:D:20:VAL:HG13	2.08	0.53
1:K:183:LEU:CD1	1:K:184:GLN:HG3	2.38	0.53
1:H:183:LEU:HD12	1:H:184:GLN:HG3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:383:ALA:O	1:C:384:ALA:HB3	2.08	0.53
1:M:183:LEU:CD1	1:M:184:GLN:HG3	2.38	0.53
1:I:174:VAL:HG22	1:I:194:GLN:HE21	1.73	0.53
1:M:176:THR:HG22	1:M:177:VAL:N	2.24	0.53
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.88	0.53
1:A:305:ILE:HG22	1:A:305:ILE:O	2.08	0.53
1:N:319:GLN:HB3	1:N:336:VAL:HG21	1.88	0.53
1:H:319:GLN:O	1:H:336:VAL:HG23	2.08	0.53
1:K:319:GLN:O	1:K:336:VAL:HG23	2.08	0.53
1:A:229:ASN:ND2	1:G:244:GLY:CA	2.71	0.53
1:G:349:ILE:HA	1:G:352:GLN:CG	2.37	0.53
1:H:129:GLU:HG2	6:H:1634:HOH:O	2.09	0.53
1:A:301:ILE:HG21	1:A:309:LEU:HD23	1.90	0.53
1:I:242:LYS:C	1:I:244:GLY:H	2.11	0.53
1:G:206:ASN:HD21	1:G:214:GLU:H	1.56	0.53
1:J:310:GLU:N	1:J:310:GLU:OE1	2.41	0.53
1:G:155:ASP:OD1	1:G:157:THR:HB	2.08	0.53
1:M:219:PHE:O	1:M:247:LEU:HD12	2.09	0.53
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.90	0.53
1:B:219:PHE:O	1:B:247:LEU:HD12	2.08	0.53
1:A:202:PRO:O	1:A:203:TYR:HB2	2.08	0.53
1:M:301:ILE:HG21	1:M:309:LEU:HD23	1.90	0.53
1:I:90:THR:OG1	5:I:1:AGS:S1G	2.65	0.53
1:B:183:LEU:CD1	1:B:184:GLN:HG3	2.38	0.53
1:M:183:LEU:H	1:M:383:ALA:CB	2.10	0.53
1:C:235:PRO:CG	1:C:310:GLU:HA	2.32	0.53
1:A:252:GLU:O	1:A:253:ASP:HB2	2.09	0.53
1:L:176:THR:HG21	1:L:322:ARG:HH12	1.74	0.53
1:N:326:ASN:HD22	1:N:329:THR:HB	1.74	0.53
1:E:362:ARG:O	1:E:366:GLN:HG3	2.09	0.53
1:M:155:ASP:OD1	1:M:157:THR:HB	2.08	0.53
1:N:23:LEU:CD2	1:N:74:VAL:HG13	2.38	0.53
1:L:319:GLN:O	1:L:336:VAL:HG23	2.09	0.53
1:D:247:LEU:HD21	1:D:249:ILE:HD11	1.90	0.53
1:H:23:LEU:HD22	1:H:74:VAL:HG13	1.89	0.53
1:B:301:ILE:HG21	1:B:309:LEU:HD23	1.91	0.53
1:B:239:ALA:O	1:B:314:LEU:HD11	2.09	0.53
1:E:386:GLU:O	1:E:390:LYS:HG2	2.09	0.53
1:B:319:GLN:O	1:B:336:VAL:HG23	2.08	0.53
1:C:236:VAL:O	1:C:240:VAL:HG23	2.09	0.53
1:D:383:ALA:O	1:D:384:ALA:HB3	2.09	0.53
1:L:183:LEU:CD1	1:L:184:GLN:HG3	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:325:ILE:HG22	1:G:330:THR:HA	1.91	0.53
1:G:183:LEU:HD12	1:G:184:GLN:HG3	1.90	0.53
1:C:176:THR:HG22	1:C:177:VAL:N	2.23	0.53
1:K:16:MET:O	1:K:20:VAL:HG13	2.09	0.53
1:J:155:ASP:OD1	1:J:157:THR:HB	2.09	0.53
1:K:239:ALA:O	1:K:314:LEU:HD11	2.08	0.53
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.74	0.53
1:F:183:LEU:CD1	1:F:184:GLN:HG3	2.39	0.53
1:B:310:GLU:OE1	1:B:310:GLU:N	2.42	0.53
1:H:266:THR:CG2	1:H:273:VAL:H	2.22	0.53
1:G:193:MET:CE	1:G:292:ILE:HG12	2.39	0.53
1:C:386:GLU:O	1:C:390:LYS:HG2	2.09	0.53
1:F:155:ASP:OD1	1:F:157:THR:HB	2.08	0.53
1:M:23:LEU:CD2	1:M:74:VAL:HG13	2.39	0.53
1:G:16:MET:O	1:G:20:VAL:HG13	2.09	0.53
1:E:383:ALA:O	1:E:384:ALA:HB3	2.09	0.52
1:M:383:ALA:O	1:M:384:ALA:HB3	2.09	0.52
1:I:382:GLY:O	1:I:389:MET:HG2	2.08	0.52
1:E:180:GLY:HA3	1:E:381:VAL:O	2.09	0.52
1:K:174:VAL:HG22	1:K:194:GLN:HE21	1.72	0.52
1:K:176:THR:HG22	1:K:177:VAL:N	2.24	0.52
1:B:176:THR:HG22	1:B:177:VAL:N	2.24	0.52
1:M:319:GLN:HB3	1:M:336:VAL:HG21	1.92	0.52
1:K:193:MET:CE	1:K:292:ILE:HG12	2.40	0.52
1:G:160:LYS:O	1:G:164:GLU:HG3	2.09	0.52
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.10	0.52
1:F:272:LYS:N	1:F:272:LYS:HD2	2.24	0.52
1:H:383:ALA:O	1:H:384:ALA:HB3	2.09	0.52
1:A:183:LEU:CD1	1:A:184:GLN:HG3	2.39	0.52
1:N:219:PHE:O	1:N:247:LEU:HD12	2.08	0.52
1:K:524:LEU:O	1:K:526:LYS:N	2.41	0.52
1:G:235:PRO:CG	1:G:310:GLU:HA	2.32	0.52
1:C:305:ILE:HG22	1:C:305:ILE:O	2.09	0.52
1:A:242:LYS:C	1:A:244:GLY:H	2.12	0.52
1:K:90:THR:O	1:K:94:VAL:HG13	2.09	0.52
1:I:310:GLU:OE1	1:I:310:GLU:N	2.42	0.52
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.92	0.52
1:M:23:LEU:HD22	1:M:74:VAL:HG13	1.90	0.52
1:G:160:LYS:HB2	1:G:160:LYS:NZ	2.25	0.52
1:C:242:LYS:C	1:C:244:GLY:H	2.11	0.52
1:B:90:THR:OG1	5:B:1:AGS:S1G	2.67	0.52
1:H:183:LEU:CD1	1:H:184:GLN:HG3	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.10	0.52
1:L:193:MET:HE2	1:L:292:ILE:HG12	1.90	0.52
1:C:239:ALA:O	1:C:314:LEU:HD11	2.10	0.52
1:F:202:PRO:O	1:F:203:TYR:HB2	2.10	0.52
1:K:254:VAL:HG12	1:K:259:LEU:HB2	1.92	0.52
1:B:160:LYS:NZ	1:B:160:LYS:HB2	2.24	0.52
1:B:470:LYS:HD3	6:B:2745:HOH:O	2.10	0.52
1:H:90:THR:OG1	5:H:1:AGS:S1G	2.63	0.52
1:J:252:GLU:O	1:J:253:ASP:HB2	2.10	0.52
1:N:193:MET:CE	1:N:292:ILE:HG12	2.39	0.52
1:J:496:PRO:HB2	1:J:499:VAL:CG1	2.40	0.52
1:M:90:THR:O	1:M:94:VAL:HG13	2.10	0.52
1:E:310:GLU:OE1	1:E:310:GLU:N	2.43	0.52
1:K:180:GLY:HA3	1:K:381:VAL:O	2.10	0.52
1:K:382:GLY:O	1:K:389:MET:HG2	2.10	0.52
1:F:271:VAL:HG12	1:F:273:VAL:HG23	1.92	0.52
1:M:134:LEU:HD21	1:M:425:LYS:NZ	2.25	0.52
1:I:235:PRO:CG	1:I:310:GLU:HA	2.33	0.52
1:E:69:MET:O	1:E:73:MET:HG3	2.09	0.52
1:J:386:GLU:O	1:J:390:LYS:HG2	2.10	0.52
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.92	0.52
1:C:180:GLY:HA3	1:C:381:VAL:O	2.10	0.52
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.92	0.52
1:E:193:MET:HE2	1:E:292:ILE:HG12	1.92	0.52
1:E:252:GLU:O	1:E:253:ASP:HB2	2.10	0.52
1:C:160:LYS:O	1:C:164:GLU:HG3	2.10	0.52
1:E:319:GLN:O	1:E:336:VAL:HG23	2.10	0.52
1:M:284:ARG:NH1	1:M:364:LYS:NZ	2.58	0.51
1:K:235:PRO:CG	1:K:310:GLU:HA	2.35	0.51
1:M:305:ILE:O	1:M:305:ILE:HG22	2.09	0.51
1:A:180:GLY:HA3	1:A:381:VAL:O	2.10	0.51
1:I:305:ILE:HG22	1:I:305:ILE:O	2.10	0.51
1:G:305:ILE:O	1:G:305:ILE:HG22	2.10	0.51
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.10	0.51
1:A:383:ALA:O	1:A:384:ALA:HB3	2.11	0.51
1:C:160:LYS:NZ	1:C:160:LYS:HB2	2.24	0.51
1:I:68:ASN:O	1:I:72:GLN:HG2	2.10	0.51
1:E:524:LEU:O	1:E:526:LYS:N	2.43	0.51
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.92	0.51
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.92	0.51
1:F:68:ASN:O	1:F:72:GLN:HG2	2.10	0.51
1:F:382:GLY:O	1:F:389:MET:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:310:GLU:N	1:A:310:GLU:OE1	2.44	0.51
1:E:174:VAL:HG22	1:E:194:GLN:HE21	1.74	0.51
1:C:266:THR:CG2	1:C:273:VAL:H	2.24	0.51
1:K:305:ILE:O	1:K:305:ILE:HG22	2.10	0.51
1:N:70:GLY:HA2	1:N:73:MET:HE3	1.93	0.51
1:C:134:LEU:HD21	1:C:425:LYS:NZ	2.25	0.51
1:I:239:ALA:O	1:I:314:LEU:HD11	2.10	0.51
1:B:193:MET:CE	1:B:292:ILE:HG12	2.40	0.51
1:D:384:ALA:HA	1:E:360:TYR:OH	2.11	0.51
1:E:183:LEU:CD1	1:E:184:GLN:HG3	2.40	0.51
1:C:384:ALA:O	1:C:385:THR:HG23	2.11	0.51
1:I:219:PHE:O	1:I:247:LEU:HD12	2.09	0.51
1:J:16:MET:O	1:J:20:VAL:HG13	2.11	0.51
1:A:54:VAL:HG23	6:A:2015:HOH:O	2.10	0.51
1:F:223:ALA:O	1:F:251:ALA:HA	2.10	0.51
1:E:305:ILE:O	1:E:305:ILE:HG22	2.10	0.51
1:A:160:LYS:HB2	1:A:160:LYS:NZ	2.26	0.51
1:L:305:ILE:O	1:L:305:ILE:HG22	2.10	0.51
1:B:305:ILE:O	1:B:305:ILE:HG22	2.11	0.51
1:L:266:THR:CG2	1:L:273:VAL:H	2.24	0.51
1:I:176:THR:HG22	1:I:177:VAL:N	2.25	0.51
1:M:287:ALA:HB1	1:M:368:ARG:NH1	2.25	0.51
1:F:239:ALA:O	1:F:314:LEU:HD11	2.10	0.51
1:A:193:MET:CE	1:A:292:ILE:HG12	2.41	0.51
1:M:252:GLU:O	1:M:253:ASP:HB2	2.10	0.51
1:I:23:LEU:HD22	1:I:74:VAL:HG13	1.92	0.51
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.93	0.51
1:M:16:MET:O	1:M:20:VAL:HG13	2.11	0.51
1:I:386:GLU:O	1:I:390:LYS:HG2	2.11	0.51
1:E:183:LEU:HD12	1:E:184:GLN:HG3	1.93	0.51
1:A:200:LEU:HG	1:A:276:VAL:HA	1.93	0.51
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.92	0.51
1:E:271:VAL:HG12	1:E:273:VAL:HG23	1.93	0.51
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.51	0.51
1:N:383:ALA:O	1:N:384:ALA:HB3	2.10	0.51
1:N:266:THR:HG22	1:N:271:VAL:O	2.11	0.51
1:A:176:THR:HG22	1:A:177:VAL:N	2.25	0.51
1:G:319:GLN:O	1:G:336:VAL:HG23	2.11	0.51
1:L:260:ALA:O	1:L:264:VAL:HG23	2.11	0.51
1:F:193:MET:CE	1:F:292:ILE:HG12	2.41	0.51
1:D:155:ASP:OD1	1:D:157:THR:HB	2.11	0.51
1:K:183:LEU:O	1:K:184:GLN:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:310:GLU:OE1	1:F:310:GLU:N	2.44	0.51
1:D:305:ILE:O	1:D:305:ILE:HG22	2.10	0.51
1:J:202:PRO:O	1:J:203:TYR:HB2	2.11	0.51
1:K:252:GLU:O	1:K:253:ASP:HB2	2.11	0.51
1:M:310:GLU:OE1	1:M:310:GLU:N	2.44	0.50
1:A:231:ARG:NH2	1:G:241:ALA:HB1	2.26	0.50
1:G:242:LYS:C	1:G:244:GLY:N	2.64	0.50
1:B:271:VAL:HG12	1:B:273:VAL:HG23	1.93	0.50
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.93	0.50
1:H:78:ALA:HB3	6:H:2660:HOH:O	2.11	0.50
1:G:90:THR:O	1:G:94:VAL:HG13	2.11	0.50
1:N:496:PRO:HD2	6:N:2145:HOH:O	2.10	0.50
1:E:383:ALA:HB1	1:F:281:PHE:HZ	1.75	0.50
1:N:305:ILE:O	1:N:305:ILE:HG22	2.11	0.50
1:N:23:LEU:HD22	1:N:74:VAL:HG13	1.93	0.50
1:I:54:VAL:HG23	6:I:2135:HOH:O	2.11	0.50
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.93	0.50
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.92	0.50
1:C:85:ALA:O	1:C:401:HIS:HE1	1.94	0.50
1:I:234:LEU:O	1:I:238:GLU:HG3	2.12	0.50
1:L:310:GLU:OE1	1:L:310:GLU:N	2.44	0.50
1:B:287:ALA:HB1	1:B:368:ARG:NH1	2.26	0.50
1:H:301:ILE:HG21	1:H:309:LEU:HD23	1.92	0.50
1:G:441:LYS:HE2	6:G:1481:HOH:O	2.11	0.50
1:M:496:PRO:HB2	1:M:499:VAL:CG1	2.41	0.50
1:J:271:VAL:HG12	1:J:273:VAL:HG23	1.92	0.50
1:E:413:ALA:CB	1:E:417:VAL:HG22	2.41	0.50
1:F:266:THR:CG2	1:F:273:VAL:H	2.25	0.50
1:N:319:GLN:O	1:N:336:VAL:HG23	2.12	0.50
1:K:193:MET:HE2	1:K:292:ILE:HG12	1.93	0.50
1:G:326:ASN:HD22	1:G:329:THR:HB	1.75	0.50
1:N:202:PRO:O	1:N:203:TYR:HB2	2.11	0.50
1:K:223:ALA:O	1:K:251:ALA:HA	2.12	0.50
1:D:183:LEU:CD1	1:D:184:GLN:HG3	2.40	0.50
1:L:183:LEU:HD12	1:L:184:GLN:HG3	1.93	0.50
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.94	0.50
1:K:236:VAL:O	1:K:240:VAL:HG23	2.11	0.50
1:K:266:THR:CG2	1:K:273:VAL:H	2.24	0.50
1:C:325:ILE:HG22	1:C:330:THR:HA	1.92	0.50
1:N:514:MET:SD	6:N:2800:HOH:O	2.60	0.50
1:H:90:THR:O	1:H:94:VAL:HG13	2.10	0.50
1:L:174:VAL:HG22	1:L:194:GLN:HE21	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:176:THR:HG21	1:I:322:ARG:HH12	1.76	0.50
1:I:206:ASN:OD1	1:I:207:LYS:HG3	2.11	0.50
1:D:260:ALA:O	1:D:264:VAL:HG23	2.11	0.50
1:L:23:LEU:HD22	1:L:74:VAL:HG13	1.93	0.50
1:D:180:GLY:HA3	1:D:381:VAL:O	2.12	0.50
1:D:381:VAL:O	1:D:382:GLY:O	2.30	0.50
1:H:252:GLU:O	1:H:253:ASP:HB2	2.12	0.50
1:F:301:ILE:HG21	1:F:309:LEU:HD23	1.93	0.50
1:M:209:GLU:OE1	1:M:209:GLU:N	2.44	0.50
1:K:310:GLU:OE1	1:K:310:GLU:N	2.44	0.50
1:N:310:GLU:OE1	1:N:310:GLU:N	2.45	0.50
1:L:180:GLY:HA3	1:L:381:VAL:O	2.11	0.50
1:K:271:VAL:HG12	1:K:273:VAL:HG23	1.93	0.50
1:M:266:THR:CG2	1:M:273:VAL:H	2.25	0.50
1:D:271:VAL:HG12	1:D:273:VAL:HG23	1.92	0.50
1:I:202:PRO:O	1:I:203:TYR:HB2	2.11	0.50
1:I:223:ALA:O	1:I:251:ALA:HA	2.12	0.50
1:G:383:ALA:O	1:G:384:ALA:HB3	2.12	0.50
1:J:266:THR:CG2	1:J:273:VAL:H	2.25	0.50
1:F:236:VAL:O	1:F:240:VAL:HG23	2.12	0.50
1:M:272:LYS:NZ	1:N:228:SER:HB2	2.27	0.50
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.94	0.49
1:M:413:ALA:HB3	1:M:417:VAL:HG22	1.94	0.49
1:E:176:THR:HG21	1:E:322:ARG:HH12	1.75	0.49
1:A:287:ALA:HB1	1:A:368:ARG:NH1	2.26	0.49
1:G:23:LEU:CD2	1:G:74:VAL:HG13	2.42	0.49
1:L:301:ILE:HG21	1:L:309:LEU:HD23	1.94	0.49
1:E:239:ALA:O	1:E:314:LEU:HD11	2.12	0.49
1:B:183:LEU:HD13	1:B:184:GLN:N	2.26	0.49
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.94	0.49
1:C:219:PHE:O	1:C:247:LEU:HD12	2.11	0.49
1:D:371:LYS:HG2	6:D:1228:HOH:O	2.11	0.49
1:I:160:LYS:HB2	1:I:160:LYS:NZ	2.27	0.49
1:M:236:VAL:O	1:M:240:VAL:HG23	2.12	0.49
1:A:319:GLN:O	1:A:336:VAL:HG23	2.12	0.49
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.94	0.49
1:N:348:GLN:O	1:N:352:GLN:HG2	2.13	0.49
1:L:252:GLU:O	1:L:253:ASP:HB2	2.11	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.92	0.49
1:D:78:ALA:HB1	1:D:89:THR:HB	1.94	0.49
1:F:174:VAL:HG22	1:F:194:GLN:HE21	1.77	0.49
1:H:325:ILE:HG22	1:H:330:THR:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:236:VAL:O	1:E:240:VAL:HG23	2.12	0.49
1:C:193:MET:HE1	1:C:292:ILE:HG12	1.93	0.49
1:G:202:PRO:O	1:G:203:TYR:HB2	2.12	0.49
1:H:176:THR:HG21	1:H:322:ARG:HH12	1.76	0.49
1:C:254:VAL:HG12	1:C:259:LEU:HB2	1.94	0.49
1:E:266:THR:CG2	1:E:273:VAL:H	2.25	0.49
1:F:23:LEU:HD22	1:F:74:VAL:HG13	1.94	0.49
1:E:90:THR:OG1	5:E:1:AGS:S1G	2.66	0.49
1:H:310:GLU:N	1:H:310:GLU:OE1	2.45	0.49
1:A:229:ASN:ND2	1:G:244:GLY:HA3	2.28	0.49
1:C:202:PRO:O	1:C:203:TYR:HB2	2.11	0.49
1:H:413:ALA:HB3	1:H:417:VAL:HG22	1.93	0.49
1:C:68:ASN:O	1:C:72:GLN:HG2	2.12	0.49
1:L:287:ALA:HB1	1:L:368:ARG:NH1	2.27	0.49
1:M:386:GLU:O	1:M:390:LYS:HG2	2.12	0.49
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.94	0.49
1:L:202:PRO:O	1:L:203:TYR:HB2	2.12	0.49
1:E:171:LYS:HB2	1:E:407:VAL:HG11	1.93	0.49
1:D:202:PRO:O	1:D:203:TYR:HB2	2.12	0.49
1:A:266:THR:CG2	1:A:273:VAL:H	2.26	0.49
1:B:202:PRO:O	1:B:203:TYR:HB2	2.12	0.49
1:L:223:ALA:O	1:L:251:ALA:HA	2.12	0.49
1:K:69:MET:O	1:K:73:MET:HG3	2.12	0.49
1:B:326:ASN:HD22	1:B:329:THR:HB	1.76	0.49
1:L:524:LEU:O	1:L:526:LYS:N	2.45	0.49
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.95	0.49
1:K:68:ASN:O	1:K:72:GLN:HG2	2.13	0.49
1:N:218:PRO:HD2	1:N:320:ALA:O	2.13	0.49
1:F:413:ALA:CB	1:F:417:VAL:HG22	2.42	0.49
1:J:382:GLY:O	1:J:389:MET:HG2	2.13	0.49
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.27	0.49
1:B:223:ALA:O	1:B:251:ALA:HA	2.13	0.49
1:B:525:PRO:HD3	6:B:1427:HOH:O	2.13	0.49
1:C:319:GLN:O	1:C:336:VAL:HG23	2.13	0.49
1:I:252:GLU:O	1:I:253:ASP:HB2	2.12	0.49
6:C:2466:HOH:O	1:D:518:GLU:HG2	2.12	0.49
1:B:5:ASP:HB2	1:B:524:LEU:HD12	1.95	0.49
1:N:234:LEU:O	1:N:238:GLU:HG3	2.13	0.49
1:A:60:ILE:O	1:A:75:LYS:HE3	2.13	0.49
1:M:271:VAL:HG12	1:M:273:VAL:HG23	1.95	0.49
1:A:271:VAL:HG12	1:A:273:VAL:HG23	1.94	0.49
1:E:287:ALA:HB1	1:E:368:ARG:NH1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:63:GLU:OE2	1:K:526:LYS:HE2	2.12	0.49
1:C:63:GLU:OE2	1:D:526:LYS:HE2	2.13	0.49
1:H:202:PRO:O	1:H:203:TYR:HB2	2.11	0.49
1:F:235:PRO:CG	1:F:310:GLU:HA	2.31	0.48
1:D:310:GLU:OE1	1:D:310:GLU:N	2.46	0.48
1:E:206:ASN:OD1	1:E:207:LYS:HG3	2.13	0.48
1:I:266:THR:HG22	1:I:271:VAL:O	2.13	0.48
1:I:319:GLN:O	1:I:336:VAL:HG23	2.13	0.48
1:M:223:ALA:O	1:M:251:ALA:HA	2.13	0.48
1:K:202:PRO:O	1:K:203:TYR:HB2	2.12	0.48
1:H:384:ALA:O	1:H:385:THR:HG23	2.13	0.48
1:G:259:LEU:O	1:G:263:VAL:HG23	2.13	0.48
1:D:259:LEU:O	1:D:263:VAL:HG23	2.13	0.48
1:D:325:ILE:HG22	1:D:330:THR:HA	1.94	0.48
1:L:326:ASN:HD22	1:L:329:THR:HB	1.77	0.48
1:N:413:ALA:HB3	1:N:417:VAL:HG22	1.94	0.48
1:L:69:MET:O	1:L:73:MET:HG3	2.13	0.48
1:B:179:ASP:HB3	1:B:389:MET:CE	2.44	0.48
1:L:23:LEU:CD2	1:L:74:VAL:HG13	2.42	0.48
1:H:171:LYS:HB2	1:H:407:VAL:HG11	1.95	0.48
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.78	0.48
1:E:202:PRO:O	1:E:203:TYR:HB2	2.13	0.48
1:M:202:PRO:O	1:M:203:TYR:HB2	2.13	0.48
1:G:69:MET:O	1:G:73:MET:HG3	2.13	0.48
1:C:183:LEU:O	1:C:184:GLN:HB2	2.14	0.48
1:H:234:LEU:O	1:H:238:GLU:HG3	2.13	0.48
1:F:73:MET:O	1:F:76:GLU:HB2	2.13	0.48
1:J:496:PRO:O	1:J:499:VAL:HG13	2.12	0.48
1:F:319:GLN:O	1:F:336:VAL:HG23	2.12	0.48
1:E:404:ARG:NH1	6:E:2208:HOH:O	2.45	0.48
1:B:77:VAL:HG11	1:B:510:VAL:CG2	2.43	0.48
1:L:384:ALA:O	1:L:385:THR:HG23	2.14	0.48
1:M:281:PHE:H	1:M:284:ARG:HD2	1.76	0.48
1:A:234:LEU:O	1:A:238:GLU:HG3	2.13	0.48
1:C:310:GLU:N	1:C:310:GLU:OE1	2.46	0.48
1:B:252:GLU:O	1:B:253:ASP:HB2	2.13	0.48
1:L:176:THR:HG22	1:L:177:VAL:N	2.28	0.48
1:J:206:ASN:OD1	1:J:207:LYS:HG3	2.13	0.48
1:J:496:PRO:HB2	1:J:499:VAL:HG12	1.94	0.48
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.78	0.48
6:E:1217:HOH:O	1:F:518:GLU:HG2	2.12	0.48
1:A:239:ALA:O	1:A:314:LEU:HD11	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:73:MET:O	1:I:76:GLU:HB2	2.13	0.48
1:G:425:LYS:NZ	6:G:2070:HOH:O	2.45	0.48
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.95	0.48
1:B:153:ASN:O	1:B:154:SER:HB2	2.14	0.48
1:K:160:LYS:O	1:K:164:GLU:HG3	2.12	0.48
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.96	0.48
1:C:524:LEU:O	1:C:526:LYS:N	2.45	0.48
1:M:193:MET:CE	1:M:292:ILE:HG12	2.43	0.48
1:E:235:PRO:CG	1:E:310:GLU:HA	2.32	0.48
1:M:200:LEU:HG	1:M:276:VAL:HA	1.95	0.48
1:M:266:THR:HG22	1:M:271:VAL:O	2.14	0.48
1:B:236:VAL:O	1:B:240:VAL:HG23	2.12	0.48
1:A:266:THR:HG22	1:A:271:VAL:O	2.13	0.48
1:N:499:VAL:HG11	6:N:2145:HOH:O	2.13	0.48
1:H:223:ALA:O	1:H:251:ALA:HA	2.12	0.48
1:D:384:ALA:O	1:D:385:THR:HG23	2.14	0.48
1:I:180:GLY:HA3	1:I:381:VAL:O	2.13	0.48
1:L:174:VAL:HG22	1:L:194:GLN:NE2	2.28	0.48
1:J:413:ALA:HB3	1:J:417:VAL:HG22	1.95	0.48
1:L:254:VAL:HG12	1:L:259:LEU:HB2	1.95	0.48
1:D:63:GLU:OE2	1:E:526:LYS:HE2	2.13	0.48
1:A:260:ALA:O	1:A:264:VAL:HG23	2.13	0.48
1:I:524:LEU:O	1:I:526:LYS:N	2.46	0.48
1:N:222:LEU:HB3	1:N:289:LEU:CD2	2.43	0.48
1:E:153:ASN:O	1:E:154:SER:HB2	2.13	0.48
1:B:200:LEU:HG	1:B:276:VAL:HA	1.96	0.48
1:L:219:PHE:O	1:L:247:LEU:HD12	2.13	0.48
1:A:46:ALA:HB2	1:B:76:GLU:HG2	1.93	0.48
1:A:176:THR:HG21	1:A:322:ARG:HH12	1.79	0.48
1:G:266:THR:HG22	1:G:271:VAL:O	2.14	0.48
1:A:206:ASN:OD1	1:A:207:LYS:HG3	2.13	0.48
1:G:362:ARG:HD2	6:G:1728:HOH:O	2.13	0.48
1:L:291:ASP:OD2	1:L:368:ARG:HD2	2.14	0.48
1:L:441:LYS:HE2	6:L:2814:HOH:O	2.13	0.48
1:N:16:MET:O	1:N:20:VAL:HG13	2.13	0.48
1:K:384:ALA:O	1:K:385:THR:HG23	2.14	0.48
1:M:174:VAL:HG22	1:M:194:GLN:HE21	1.77	0.48
1:N:325:ILE:HG22	1:N:330:THR:HA	1.96	0.48
1:E:353:ILE:HD13	1:E:366:GLN:HG2	1.96	0.48
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.44	0.48
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.95	0.48
1:J:319:GLN:O	1:J:336:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.95	0.48
1:L:209:GLU:OE1	1:L:209:GLU:N	2.47	0.48
1:F:180:GLY:HA3	1:F:381:VAL:O	2.13	0.48
1:F:252:GLU:O	1:F:253:ASP:HB2	2.14	0.48
1:C:266:THR:HG22	1:C:271:VAL:O	2.14	0.48
1:G:177:VAL:HG21	1:G:397:GLU:HG2	1.93	0.48
1:H:219:PHE:O	1:H:247:LEU:HD12	2.13	0.48
1:E:259:LEU:O	1:E:263:VAL:HG23	2.14	0.48
1:K:325:ILE:HG22	1:K:330:THR:HA	1.96	0.48
1:B:185:ASP:OD1	1:B:382:GLY:N	2.47	0.48
1:D:113:PRO:HD2	6:D:2375:HOH:O	2.14	0.48
1:D:524:LEU:O	1:D:526:LYS:N	2.46	0.48
1:N:386:GLU:O	1:N:390:LYS:HG2	2.14	0.48
1:N:223:ALA:O	1:N:251:ALA:HA	2.14	0.48
1:I:199:TYR:CZ	1:I:327:LYS:HA	2.49	0.48
1:G:254:VAL:HG12	1:G:259:LEU:HB2	1.96	0.48
1:H:266:THR:HG22	1:H:271:VAL:O	2.14	0.48
1:I:413:ALA:HB3	1:I:417:VAL:HG22	1.94	0.48
1:G:73:MET:O	1:G:76:GLU:HB2	2.13	0.48
1:F:222:LEU:HB3	1:F:289:LEU:CD2	2.44	0.48
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.96	0.48
1:H:180:GLY:HA3	1:H:381:VAL:O	2.14	0.47
1:D:85:ALA:O	1:D:401:HIS:HE1	1.95	0.47
1:A:223:ALA:O	1:A:251:ALA:HA	2.14	0.47
1:G:239:ALA:O	1:G:314:LEU:HD11	2.14	0.47
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.96	0.47
1:B:171:LYS:HB2	1:B:407:VAL:HG11	1.96	0.47
1:G:348:GLN:O	1:G:352:GLN:HG2	2.14	0.47
1:A:413:ALA:HB3	1:A:417:VAL:HG22	1.95	0.47
1:K:259:LEU:O	1:K:263:VAL:HG23	2.14	0.47
1:L:177:VAL:HG21	1:L:397:GLU:HG2	1.94	0.47
1:H:206:ASN:ND2	1:H:214:GLU:H	2.12	0.47
1:J:353:ILE:HD13	1:J:366:GLN:HG2	1.96	0.47
1:A:193:MET:HE2	1:A:292:ILE:HG12	1.96	0.47
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.95	0.47
1:B:260:ALA:O	1:B:264:VAL:HG23	2.15	0.47
1:C:259:LEU:O	1:C:263:VAL:HG23	2.14	0.47
1:D:23:LEU:CD2	1:D:74:VAL:HG13	2.44	0.47
1:I:236:VAL:O	1:I:240:VAL:HG23	2.14	0.47
1:I:271:VAL:HG12	1:I:273:VAL:HG23	1.95	0.47
1:J:325:ILE:HG22	1:J:330:THR:HA	1.97	0.47
1:M:366:GLN:O	1:M:369:VAL:HG22	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:206:ASN:OD1	1:K:207:LYS:HG3	2.13	0.47
1:K:287:ALA:HB1	1:K:368:ARG:NH1	2.28	0.47
1:K:37:ASN:HD21	1:K:51:LYS:HE3	1.80	0.47
1:B:220:ILE:HD12	1:B:296:THR:HG21	1.96	0.47
1:K:234:LEU:O	1:K:238:GLU:HG3	2.13	0.47
1:G:234:LEU:N	1:G:235:PRO:HD2	2.29	0.47
1:K:219:PHE:O	1:K:247:LEU:HD12	2.13	0.47
1:B:266:THR:CG2	1:B:273:VAL:H	2.27	0.47
1:J:287:ALA:HB1	1:J:368:ARG:NH1	2.29	0.47
1:L:206:ASN:OD1	1:L:207:LYS:HG3	2.15	0.47
1:I:287:ALA:HB1	1:I:368:ARG:NH1	2.29	0.47
1:F:524:LEU:O	1:F:526:LYS:N	2.46	0.47
1:N:199:TYR:CZ	1:N:327:LYS:HA	2.50	0.47
1:I:10:ASN:ND2	6:I:2045:HOH:O	2.47	0.47
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.97	0.47
1:H:209:GLU:OE1	1:H:209:GLU:N	2.46	0.47
1:G:209:GLU:OE1	1:G:209:GLU:N	2.44	0.47
1:B:234:LEU:N	1:B:235:PRO:HD2	2.29	0.47
1:A:231:ARG:NH1	1:G:242:LYS:HG2	2.28	0.47
1:D:217:SER:N	1:D:218:PRO:CD	2.78	0.47
1:H:271:VAL:HG12	1:H:273:VAL:HG23	1.96	0.47
1:L:78:ALA:HB1	1:L:89:THR:HB	1.97	0.47
1:N:160:LYS:HB2	1:N:160:LYS:NZ	2.29	0.47
1:B:206:ASN:OD1	1:B:207:LYS:HG3	2.13	0.47
1:H:239:ALA:O	1:H:314:LEU:HD11	2.15	0.47
1:M:524:LEU:O	1:M:526:LYS:N	2.46	0.47
1:A:209:GLU:OE1	1:A:209:GLU:N	2.44	0.47
1:B:383:ALA:HB1	1:C:281:PHE:CE2	2.49	0.47
1:L:234:LEU:O	1:L:238:GLU:HG3	2.15	0.47
1:N:236:VAL:O	1:N:240:VAL:HG23	2.14	0.47
1:F:177:VAL:HG21	1:F:397:GLU:HG2	1.96	0.47
1:D:89:THR:HG23	6:D:2757:HOH:O	2.13	0.47
1:A:305:ILE:HB	1:A:307:MET:HE2	1.95	0.47
1:I:220:ILE:HD12	1:I:296:THR:HG21	1.95	0.47
1:C:301:ILE:HG21	1:C:309:LEU:HD23	1.95	0.47
1:D:12:ALA:N	6:D:2704:HOH:O	2.47	0.47
1:N:183:LEU:HD13	1:N:184:GLN:N	2.29	0.47
1:A:183:LEU:CD2	1:A:384:ALA:HB2	2.44	0.47
1:I:234:LEU:N	1:I:235:PRO:HD2	2.29	0.47
1:L:234:LEU:N	1:L:235:PRO:HD2	2.30	0.47
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.95	0.47
1:J:266:THR:HG22	1:J:271:VAL:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:206:ASN:ND2	1:I:214:GLU:H	2.12	0.47
1:J:176:THR:HG22	1:J:177:VAL:N	2.29	0.47
1:G:302:SER:H	1:G:307:MET:CE	2.28	0.47
1:H:206:ASN:OD1	1:H:207:LYS:HG3	2.15	0.47
1:M:206:ASN:OD1	1:M:207:LYS:HG3	2.14	0.47
1:I:272:LYS:NZ	1:J:229:ASN:OD1	2.47	0.47
1:J:369:VAL:HG23	1:J:370:ALA:N	2.30	0.47
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.96	0.47
1:L:366:GLN:HA	1:L:369:VAL:HG22	1.95	0.47
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.50	0.47
1:M:260:ALA:O	1:M:264:VAL:HG23	2.15	0.47
1:D:252:GLU:O	1:D:253:ASP:HB2	2.15	0.47
1:K:183:LEU:CD2	1:K:384:ALA:HB2	2.43	0.47
1:H:185:ASP:OD1	1:H:382:GLY:N	2.46	0.47
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.96	0.47
1:D:382:GLY:O	1:D:389:MET:HG2	2.15	0.47
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.96	0.47
1:F:206:ASN:OD1	1:F:207:LYS:HG3	2.14	0.47
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.97	0.47
1:H:193:MET:HE1	1:H:292:ILE:HG12	1.97	0.47
1:A:134:LEU:HD21	1:A:425:LYS:NZ	2.30	0.47
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.50	0.47
1:J:525:PRO:HD3	6:J:2970:HOH:O	2.14	0.47
1:E:90:THR:O	1:E:94:VAL:HG13	2.14	0.47
1:C:183:LEU:HD13	1:C:184:GLN:N	2.30	0.47
1:L:325:ILE:HG22	1:L:330:THR:HA	1.97	0.47
1:M:160:LYS:NZ	1:M:160:LYS:HB2	2.29	0.47
1:K:160:LYS:HB2	1:K:160:LYS:NZ	2.30	0.47
1:E:260:ALA:O	1:E:264:VAL:HG23	2.15	0.47
1:L:236:VAL:O	1:L:240:VAL:HG23	2.15	0.47
1:J:111:MET:HG2	1:J:435:ASP:OD1	2.15	0.47
1:C:252:GLU:O	1:C:253:ASP:HB2	2.14	0.47
1:A:68:ASN:O	1:A:72:GLN:HG2	2.15	0.47
1:M:90:THR:OG1	5:M:1:AGS:S1G	2.63	0.47
1:J:234:LEU:O	1:J:238:GLU:HG3	2.13	0.47
1:C:23:LEU:CD2	1:C:74:VAL:HG13	2.45	0.47
1:D:302:SER:H	1:D:307:MET:HE1	1.80	0.47
1:L:271:VAL:HG12	1:L:273:VAL:HG23	1.96	0.47
1:A:236:VAL:O	1:A:240:VAL:HG23	2.15	0.47
1:D:206:ASN:HD21	1:D:214:GLU:H	1.63	0.47
1:M:269:GLY:O	1:N:229:ASN:OD1	2.33	0.47
1:C:223:ALA:O	1:C:251:ALA:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:384:ALA:O	1:F:385:THR:HG23	2.14	0.46
1:F:234:LEU:O	1:F:238:GLU:HG3	2.14	0.46
1:D:238:GLU:O	1:D:241:ALA:HB3	2.15	0.46
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.96	0.46
1:A:73:MET:O	1:A:76:GLU:HB2	2.15	0.46
1:L:242:LYS:C	1:L:244:GLY:N	2.69	0.46
1:H:199:TYR:CZ	1:H:327:LYS:HA	2.51	0.46
1:I:140:ASP:OD2	1:I:142:LYS:HB3	2.16	0.46
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.97	0.46
1:G:384:ALA:O	1:G:385:THR:HG23	2.15	0.46
1:C:60:ILE:O	1:C:75:LYS:HE3	2.15	0.46
1:I:325:ILE:HG22	1:I:330:THR:HA	1.98	0.46
1:I:254:VAL:HG12	1:I:259:LEU:HB2	1.97	0.46
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.81	0.46
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.98	0.46
1:A:169:VAL:HG13	1:A:377:ALA:HB2	1.97	0.46
1:N:155:ASP:OD1	1:N:157:THR:HB	2.14	0.46
1:I:260:ALA:O	1:I:264:VAL:HG23	2.14	0.46
1:M:63:GLU:OE2	1:N:526:LYS:HE2	2.15	0.46
5:G:1:AGS:O2G	5:G:1:AGS:S1G	2.53	0.46
1:C:234:LEU:N	1:C:235:PRO:HD2	2.30	0.46
1:G:78:ALA:HB1	1:G:89:THR:HB	1.96	0.46
1:M:239:ALA:O	1:M:314:LEU:HD11	2.15	0.46
1:M:323:VAL:HG12	1:M:332:ILE:HA	1.98	0.46
1:E:199:TYR:CZ	1:E:327:LYS:HA	2.50	0.46
1:I:463:SER:HB2	6:I:2586:HOH:O	2.14	0.46
1:E:451:LEU:HD23	1:E:451:LEU:C	2.35	0.46
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.46
1:F:381:VAL:O	1:F:382:GLY:O	2.33	0.46
1:K:183:LEU:HD13	1:K:184:GLN:N	2.30	0.46
1:G:218:PRO:HD2	1:G:320:ALA:O	2.15	0.46
1:B:325:ILE:HG22	1:B:330:THR:HA	1.96	0.46
1:G:180:GLY:HA3	1:G:381:VAL:O	2.16	0.46
1:F:353:ILE:HD13	1:F:366:GLN:HG2	1.98	0.46
1:A:171:LYS:HB2	1:A:407:VAL:HG11	1.98	0.46
1:N:122:LYS:HE2	1:N:429:LEU:HD11	1.97	0.46
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.98	0.46
1:B:169:VAL:CG1	1:B:377:ALA:HB2	2.45	0.46
1:D:209:GLU:N	1:D:209:GLU:OE1	2.45	0.46
1:M:234:LEU:N	1:M:235:PRO:HD2	2.30	0.46
1:H:234:LEU:N	1:H:235:PRO:HD2	2.30	0.46
1:I:381:VAL:O	1:I:382:GLY:O	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:60:ILE:O	1:K:75:LYS:HE3	2.16	0.46
1:K:325:ILE:HA	1:K:329:THR:O	2.15	0.46
1:N:366:GLN:HA	1:N:369:VAL:HG22	1.96	0.46
1:L:455:VAL:O	1:L:458:CYS:HB2	2.14	0.46
1:A:90:THR:O	1:A:94:VAL:HG13	2.14	0.46
1:K:144:ILE:HG23	1:K:403:THR:HG21	1.97	0.46
1:F:383:ALA:O	1:F:384:ALA:CB	2.63	0.46
1:A:182:GLY:HA2	1:A:383:ALA:HB3	1.97	0.46
1:F:234:LEU:N	1:F:235:PRO:HD2	2.30	0.46
1:J:234:LEU:N	1:J:235:PRO:HD2	2.31	0.46
1:M:234:LEU:O	1:M:238:GLU:HG3	2.14	0.46
1:D:235:PRO:CG	1:D:310:GLU:HA	2.34	0.46
1:H:404:ARG:CG	1:H:404:ARG:NH1	2.71	0.46
1:H:250:ILE:HG22	6:H:2938:HOH:O	2.15	0.46
1:F:200:LEU:HG	1:F:276:VAL:HA	1.98	0.46
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.96	0.46
1:E:223:ALA:O	1:E:251:ALA:HA	2.16	0.46
1:E:10:ASN:HB2	6:E:1989:HOH:O	2.14	0.46
1:C:209:GLU:OE1	1:C:209:GLU:N	2.45	0.46
1:G:60:ILE:O	1:G:75:LYS:HE3	2.16	0.46
1:J:174:VAL:HG22	1:J:194:GLN:NE2	2.31	0.46
1:D:266:THR:CG2	1:D:273:VAL:H	2.28	0.46
1:A:366:GLN:O	1:A:369:VAL:HG22	2.15	0.46
1:M:10:ASN:HA	6:M:2195:HOH:O	2.15	0.46
1:D:319:GLN:HB3	1:D:336:VAL:HG21	1.97	0.46
1:A:199:TYR:CZ	1:A:327:LYS:HA	2.51	0.46
1:J:384:ALA:O	1:J:385:THR:HG23	2.16	0.46
1:I:217:SER:N	1:I:218:PRO:CD	2.79	0.46
1:H:217:SER:N	1:H:218:PRO:CD	2.79	0.46
1:C:234:LEU:O	1:C:238:GLU:HG3	2.15	0.46
1:E:217:SER:N	1:E:218:PRO:HD3	2.31	0.46
1:F:217:SER:N	1:F:218:PRO:HD3	2.31	0.46
1:N:234:LEU:N	1:N:235:PRO:HD2	2.31	0.46
1:J:219:PHE:O	1:J:247:LEU:HD12	2.15	0.46
1:M:325:ILE:HA	1:M:329:THR:O	2.16	0.46
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.30	0.46
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.96	0.46
1:A:78:ALA:HB3	6:A:2430:HOH:O	2.15	0.46
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.98	0.46
1:M:438:VAL:O	1:M:442:VAL:HG23	2.16	0.46
1:J:223:ALA:O	1:J:251:ALA:HA	2.15	0.46
1:H:183:LEU:CD2	1:H:384:ALA:HB2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:234:LEU:N	1:E:235:PRO:HD2	2.31	0.46
1:B:180:GLY:HA3	1:B:381:VAL:O	2.15	0.46
1:H:353:ILE:HD13	1:H:366:GLN:HG2	1.98	0.46
1:J:319:GLN:HB3	1:J:336:VAL:HG21	1.97	0.46
1:G:171:LYS:HB2	1:G:407:VAL:HG11	1.98	0.46
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.97	0.46
1:C:290:GLN:HB3	1:C:345:ARG:NH2	2.31	0.46
1:I:301:ILE:HG21	1:I:309:LEU:HD23	1.97	0.46
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.98	0.46
1:K:78:ALA:HB1	1:K:89:THR:HB	1.98	0.46
1:L:68:ASN:O	1:L:72:GLN:HG2	2.16	0.46
1:K:234:LEU:N	1:K:235:PRO:HD2	2.31	0.46
1:A:325:ILE:HG22	1:A:330:THR:HA	1.98	0.46
1:I:69:MET:O	1:I:73:MET:HG3	2.15	0.46
1:A:524:LEU:O	1:A:526:LYS:N	2.48	0.46
1:K:210:THR:HG22	1:K:210:THR:O	2.16	0.46
1:K:302:SER:H	1:K:307:MET:HE1	1.81	0.45
1:K:177:VAL:HA	1:K:379:ILE:O	2.16	0.45
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.98	0.45
1:A:353:ILE:HD13	1:A:366:GLN:HG2	1.97	0.45
1:B:404:ARG:NH1	6:B:2253:HOH:O	2.48	0.45
1:L:171:LYS:HB2	1:L:407:VAL:HG11	1.98	0.45
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.57	0.45
1:A:101:THR:HG23	6:A:2971:HOH:O	2.16	0.45
1:J:183:LEU:HD13	1:J:184:GLN:N	2.30	0.45
1:B:183:LEU:CD2	1:B:384:ALA:HB2	2.43	0.45
1:H:235:PRO:CG	1:H:310:GLU:HA	2.35	0.45
1:G:234:LEU:O	1:G:238:GLU:HG3	2.17	0.45
1:N:271:VAL:HG12	1:N:273:VAL:HG23	1.97	0.45
1:I:353:ILE:HD13	1:I:366:GLN:HG2	1.98	0.45
1:I:369:VAL:HG23	1:I:370:ALA:N	2.31	0.45
1:K:369:VAL:HG23	1:K:370:ALA:N	2.31	0.45
1:N:215:LEU:HB2	1:N:323:VAL:CG2	2.47	0.45
1:D:319:GLN:O	1:D:336:VAL:HG23	2.17	0.45
1:C:324:VAL:O	1:C:331:THR:HG22	2.16	0.45
1:J:260:ALA:O	1:J:264:VAL:HG23	2.16	0.45
1:A:182:GLY:HA2	1:A:383:ALA:CB	2.46	0.45
1:F:217:SER:N	1:F:218:PRO:CD	2.79	0.45
1:I:60:ILE:O	1:I:75:LYS:HE3	2.16	0.45
1:E:325:ILE:HG22	1:E:330:THR:HA	1.97	0.45
1:N:266:THR:HG21	1:N:273:VAL:H	1.80	0.45
1:E:206:ASN:ND2	1:E:214:GLU:H	2.11	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:325:ILE:HG22	1:M:330:THR:HA	1.97	0.45
1:J:325:ILE:HA	1:J:329:THR:O	2.16	0.45
1:F:160:LYS:HB2	1:F:160:LYS:HZ2	1.81	0.45
1:E:219:PHE:O	1:E:247:LEU:HD12	2.16	0.45
1:F:193:MET:HE2	1:F:292:ILE:HG12	1.99	0.45
1:J:524:LEU:O	1:J:526:LYS:N	2.49	0.45
1:C:78:ALA:HB3	6:C:1582:HOH:O	2.16	0.45
1:D:301:ILE:HG21	1:D:309:LEU:HD23	1.98	0.45
1:A:384:ALA:O	1:A:385:THR:HG23	2.16	0.45
1:I:217:SER:N	1:I:218:PRO:HD3	2.31	0.45
1:K:217:SER:N	1:K:218:PRO:CD	2.80	0.45
1:L:224:ASP:HB3	1:L:302:SER:HB3	1.98	0.45
1:C:413:ALA:HB3	1:C:417:VAL:HG22	1.99	0.45
1:B:319:GLN:HB3	1:B:336:VAL:HG21	1.99	0.45
1:K:37:ASN:ND2	1:K:51:LYS:HE3	2.32	0.45
1:M:169:VAL:HG13	1:M:377:ALA:HB2	1.99	0.45
1:I:134:LEU:HD21	1:I:425:LYS:NZ	2.31	0.45
1:N:10:ASN:ND2	6:N:2158:HOH:O	2.49	0.45
1:E:290:GLN:HB3	1:E:345:ARG:NH2	2.31	0.45
1:G:68:ASN:O	1:G:72:GLN:HG2	2.16	0.45
1:I:183:LEU:CD2	1:I:384:ALA:HB2	2.45	0.45
1:E:182:GLY:O	1:E:183:LEU:O	2.35	0.45
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.99	0.45
1:F:219:PHE:O	1:F:247:LEU:HD12	2.16	0.45
1:E:369:VAL:HG23	1:E:370:ALA:N	2.30	0.45
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.99	0.45
1:J:301:ILE:HG21	1:J:309:LEU:HD23	1.97	0.45
1:K:301:ILE:HG21	1:K:309:LEU:HD23	1.97	0.45
1:F:171:LYS:HB2	1:F:407:VAL:HG11	1.98	0.45
1:D:90:THR:OG1	5:D:551:AGS:S1G	2.68	0.45
1:I:183:LEU:HD13	1:I:184:GLN:N	2.31	0.45
1:M:217:SER:N	1:M:218:PRO:HD3	2.32	0.45
1:E:217:SER:N	1:E:218:PRO:CD	2.79	0.45
1:J:197:ARG:HD2	1:J:277:LYS:HB2	1.98	0.45
1:A:185:ASP:OD1	1:A:382:GLY:N	2.48	0.45
1:L:438:VAL:O	1:L:442:VAL:HG23	2.17	0.45
1:H:524:LEU:O	1:H:526:LYS:N	2.49	0.45
1:G:238:GLU:O	1:G:241:ALA:HB3	2.16	0.45
1:E:158:VAL:HG22	6:E:2648:HOH:O	2.16	0.45
1:D:87:ASP:N	6:D:2757:HOH:O	2.49	0.45
1:A:369:VAL:HG23	1:A:370:ALA:N	2.32	0.45
1:C:206:ASN:OD1	1:C:207:LYS:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:524:LEU:HA	1:L:524:LEU:HD12	1.87	0.45
1:A:39:VAL:HG12	1:B:69:MET:CE	2.47	0.45
1:C:42:LYS:HE3	1:C:48:THR:OG1	2.17	0.45
1:M:222:LEU:HB3	1:M:289:LEU:CD2	2.47	0.45
1:L:222:LEU:HB3	1:L:289:LEU:CD2	2.46	0.45
1:M:218:PRO:HD2	1:M:320:ALA:O	2.17	0.45
1:N:238:GLU:O	1:N:241:ALA:HB3	2.17	0.45
1:F:325:ILE:HG22	1:F:330:THR:HA	1.98	0.45
1:N:174:VAL:HG22	1:N:194:GLN:HE21	1.82	0.45
1:F:366:GLN:O	1:F:369:VAL:HG22	2.16	0.45
1:H:242:LYS:C	1:H:244:GLY:N	2.70	0.45
1:N:90:THR:O	1:N:94:VAL:HG13	2.16	0.45
1:N:252:GLU:O	1:N:253:ASP:HB2	2.16	0.45
1:G:463:SER:O	1:G:467:ASN:HB2	2.17	0.45
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.47	0.45
1:E:210:THR:HG22	1:E:210:THR:O	2.17	0.45
1:K:88:GLY:HA2	5:K:1:AGS:PB	2.57	0.45
1:K:217:SER:N	1:K:218:PRO:HD3	2.31	0.45
1:B:217:SER:N	1:B:218:PRO:HD3	2.32	0.45
1:A:217:SER:N	1:A:218:PRO:CD	2.80	0.45
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.98	0.45
1:K:174:VAL:HG22	1:K:194:GLN:NE2	2.32	0.45
1:F:325:ILE:HA	1:F:329:THR:O	2.17	0.45
1:J:160:LYS:NZ	1:J:160:LYS:HB2	2.32	0.45
1:J:272:LYS:NZ	1:K:229:ASN:OD1	2.50	0.45
1:D:242:LYS:C	1:D:244:GLY:N	2.67	0.45
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.29	0.45
1:N:242:LYS:C	1:N:244:GLY:N	2.69	0.45
1:C:239:ALA:C	1:C:314:LEU:HD21	2.38	0.45
1:L:369:VAL:HG23	1:L:370:ALA:N	2.32	0.45
1:K:260:ALA:O	1:K:264:VAL:HG23	2.16	0.45
1:K:342:ILE:O	1:K:346:VAL:HG23	2.16	0.45
1:J:239:ALA:O	1:J:314:LEU:HD11	2.16	0.45
1:B:210:THR:HG22	1:B:210:THR:O	2.16	0.45
1:L:90:THR:OG1	5:L:1:AGS:S1G	2.65	0.45
1:J:183:LEU:CD2	1:J:384:ALA:HB2	2.44	0.45
1:A:217:SER:N	1:A:218:PRO:HD3	2.32	0.45
1:M:238:GLU:O	1:M:241:ALA:HB3	2.17	0.45
1:B:39:VAL:HG12	1:C:69:MET:CE	2.47	0.45
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.98	0.45
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.57	0.45
1:B:342:ILE:O	1:B:346:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:141:SER:HB3	6:E:2603:HOH:O	2.17	0.45
1:A:392:LYS:O	1:A:396:VAL:HG23	2.17	0.45
1:C:210:THR:HG22	1:C:210:THR:O	2.17	0.45
1:C:182:GLY:HA2	1:C:383:ALA:HB3	1.97	0.44
1:C:381:VAL:O	1:C:382:GLY:O	2.36	0.44
1:C:305:ILE:HB	1:C:307:MET:HE2	1.98	0.44
1:L:266:THR:HG22	1:L:271:VAL:O	2.16	0.44
1:D:73:MET:O	1:D:76:GLU:HB2	2.17	0.44
1:H:284:ARG:HH12	1:H:364:LYS:NZ	2.14	0.44
1:J:37:ASN:HD21	1:J:51:LYS:HE3	1.80	0.44
1:K:209:GLU:OE1	1:K:209:GLU:N	2.47	0.44
1:B:384:ALA:HA	1:C:360:TYR:OH	2.17	0.44
1:A:234:LEU:N	1:A:235:PRO:HD2	2.32	0.44
1:I:174:VAL:HG22	1:I:194:GLN:NE2	2.32	0.44
1:F:194:GLN:HG3	1:F:331:THR:HB	1.99	0.44
1:D:247:LEU:CD2	1:D:249:ILE:HD11	2.47	0.44
1:N:353:ILE:HD13	1:N:366:GLN:HG2	1.99	0.44
1:B:455:VAL:O	1:B:458:CYS:HB2	2.17	0.44
1:I:70:GLY:HA2	1:I:73:MET:HE3	2.00	0.44
1:N:301:ILE:HG21	1:N:309:LEU:HD23	1.99	0.44
1:I:191:GLU:O	1:I:334:ASP:HA	2.16	0.44
1:D:358:SER:HB3	1:D:361:ASP:OD1	2.16	0.44
1:B:209:GLU:OE1	1:B:209:GLU:N	2.48	0.44
1:K:182:GLY:HA2	1:K:383:ALA:HB3	1.99	0.44
1:E:381:VAL:O	1:E:382:GLY:O	2.36	0.44
1:E:325:ILE:HA	1:E:329:THR:O	2.18	0.44
1:G:302:SER:O	1:G:307:MET:HE3	2.17	0.44
1:I:366:GLN:O	1:I:369:VAL:HG22	2.16	0.44
1:N:496:PRO:HB2	1:N:499:VAL:CG1	2.47	0.44
1:C:319:GLN:HB3	1:C:336:VAL:HG21	2.00	0.44
1:I:222:LEU:HB3	1:I:289:LEU:CD2	2.47	0.44
1:D:183:LEU:HD12	1:D:184:GLN:HG3	1.99	0.44
1:J:463:SER:O	1:J:467:ASN:HB2	2.18	0.44
1:L:302:SER:H	1:L:307:MET:HE1	1.83	0.44
1:I:325:ILE:HA	1:I:329:THR:O	2.17	0.44
1:E:413:ALA:HB3	1:E:417:VAL:HG22	1.99	0.44
1:K:266:THR:HG22	1:K:271:VAL:O	2.17	0.44
1:G:305:ILE:HB	1:G:307:MET:HE2	1.98	0.44
1:C:287:ALA:HB1	1:C:368:ARG:NH1	2.32	0.44
1:H:336:VAL:O	1:H:337:GLY:C	2.56	0.44
1:H:155:ASP:OD1	1:H:157:THR:HB	2.18	0.44
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:222:LEU:HB3	1:K:289:LEU:CD2	2.48	0.44
1:D:288:MET:HG2	1:D:368:ARG:HD3	1.99	0.44
1:H:236:VAL:O	1:H:240:VAL:HG23	2.16	0.44
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.99	0.44
1:N:325:ILE:HG22	1:N:330:THR:HG23	1.99	0.44
1:B:524:LEU:C	1:B:526:LYS:H	2.20	0.44
1:J:460:GLU:O	1:J:462:PRO:HD3	2.18	0.44
5:K:1:AGS:S1G	5:K:1:AGS:O2G	2.55	0.44
1:N:384:ALA:O	1:N:385:THR:HG23	2.17	0.44
1:J:217:SER:N	1:J:218:PRO:HD3	2.32	0.44
1:D:218:PRO:HD2	1:D:320:ALA:O	2.18	0.44
1:I:348:GLN:O	1:I:352:GLN:HG2	2.18	0.44
1:B:302:SER:O	1:B:307:MET:HE3	2.18	0.44
1:K:413:ALA:HB3	1:K:417:VAL:HG22	1.98	0.44
1:N:193:MET:HE2	1:N:292:ILE:HG12	1.99	0.44
1:M:73:MET:HB3	6:M:2221:HOH:O	2.18	0.44
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.99	0.44
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.99	0.44
1:C:369:VAL:HG23	1:C:370:ALA:N	2.32	0.44
1:M:290:GLN:HB3	1:M:345:ARG:NH2	2.31	0.44
1:K:134:LEU:HD21	1:K:425:LYS:NZ	2.32	0.44
1:J:324:VAL:O	1:J:331:THR:HG22	2.18	0.44
1:E:323:VAL:HG12	1:E:332:ILE:HA	1.99	0.44
1:G:210:THR:O	1:G:210:THR:HG22	2.17	0.44
1:F:183:LEU:CD2	1:F:384:ALA:HB2	2.47	0.44
1:E:384:ALA:O	1:E:385:THR:HG23	2.17	0.44
1:M:182:GLY:HA2	1:M:383:ALA:HB3	2.00	0.44
1:J:217:SER:N	1:J:218:PRO:CD	2.81	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:L:253:ASP:OD1	1:L:277:LYS:HE2	2.18	0.44
1:H:176:THR:HG22	1:H:177:VAL:H	1.82	0.44
1:D:413:ALA:HB3	1:D:417:VAL:HG22	1.98	0.44
1:C:325:ILE:HA	1:C:329:THR:O	2.17	0.44
1:A:69:MET:CE	1:G:39:VAL:HG12	2.47	0.44
1:F:369:VAL:HG23	1:F:370:ALA:N	2.32	0.44
1:K:23:LEU:HD22	1:K:74:VAL:HG13	1.99	0.44
1:H:215:LEU:HB2	1:H:323:VAL:HG22	2.00	0.44
1:J:68:ASN:O	1:J:72:GLN:HG2	2.17	0.44
1:F:210:THR:O	1:F:210:THR:HG22	2.17	0.44
1:I:384:ALA:O	1:I:385:THR:HG23	2.18	0.44
1:A:218:PRO:HD2	1:A:320:ALA:O	2.17	0.44
1:D:234:LEU:N	1:D:235:PRO:HD2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:217:SER:N	1:C:218:PRO:CD	2.81	0.44
1:I:496:PRO:O	1:I:499:VAL:HG13	2.17	0.44
1:H:392:LYS:O	1:H:396:VAL:HG23	2.18	0.44
1:N:153:ASN:O	1:N:154:SER:HB2	2.18	0.44
1:J:224:ASP:HB3	1:J:302:SER:HB3	2.00	0.44
1:C:16:MET:O	1:C:20:VAL:HG13	2.17	0.44
1:F:389:MET:N	6:F:2746:HOH:O	2.50	0.44
1:E:234:LEU:O	1:E:238:GLU:HG3	2.17	0.44
1:N:217:SER:N	1:N:218:PRO:CD	2.81	0.44
1:C:179:ASP:HB3	1:C:389:MET:CE	2.48	0.44
1:M:369:VAL:HG23	1:M:370:ALA:N	2.32	0.44
1:E:242:LYS:C	1:E:244:GLY:N	2.71	0.44
1:K:242:LYS:C	1:K:244:GLY:N	2.71	0.44
1:G:336:VAL:O	1:G:337:GLY:C	2.55	0.44
1:N:42:LYS:HE3	1:N:48:THR:OG1	2.18	0.44
1:H:217:SER:N	1:H:218:PRO:HD3	2.33	0.43
1:B:217:SER:N	1:B:218:PRO:CD	2.80	0.43
1:B:325:ILE:HA	1:B:329:THR:O	2.18	0.43
1:G:381:VAL:O	1:G:382:GLY:O	2.36	0.43
1:D:200:LEU:HD13	1:D:254:VAL:HB	2.00	0.43
1:B:259:LEU:O	1:B:263:VAL:HG23	2.18	0.43
1:H:302:SER:H	1:H:307:MET:HE1	1.83	0.43
1:B:413:ALA:HB3	1:B:417:VAL:HG22	2.00	0.43
1:I:266:THR:HG22	1:I:273:VAL:H	1.82	0.43
1:G:70:GLY:HA2	1:G:73:MET:HE3	2.01	0.43
1:L:63:GLU:OE2	1:M:526:LYS:HE2	2.17	0.43
1:F:260:ALA:O	1:F:264:VAL:HG23	2.18	0.43
1:F:199:TYR:CZ	1:F:327:LYS:HA	2.53	0.43
1:M:210:THR:HG22	1:M:210:THR:O	2.18	0.43
1:C:183:LEU:CD2	1:C:384:ALA:HB2	2.47	0.43
1:C:348:GLN:O	1:C:352:GLN:HG2	2.18	0.43
1:E:200:LEU:HG	1:E:276:VAL:HA	2.01	0.43
1:L:417:VAL:CG1	6:L:2905:HOH:O	2.66	0.43
1:L:417:VAL:HB	6:L:2905:HOH:O	2.18	0.43
1:C:177:VAL:HG21	1:C:397:GLU:HG2	1.98	0.43
1:J:242:LYS:C	1:J:244:GLY:N	2.71	0.43
1:F:342:ILE:O	1:F:346:VAL:HG23	2.18	0.43
1:H:144:ILE:HG23	1:H:403:THR:HG21	1.99	0.43
1:H:518:GLU:HG2	6:N:1187:HOH:O	2.18	0.43
1:G:260:ALA:O	1:G:264:VAL:HG23	2.18	0.43
1:L:199:TYR:CZ	1:L:327:LYS:HA	2.53	0.43
1:D:236:VAL:O	1:D:240:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:451:LEU:HD23	1:B:451:LEU:C	2.39	0.43
1:L:421:ARG:CZ	1:L:473:ASP:HA	2.48	0.43
1:N:217:SER:N	1:N:218:PRO:HD3	2.33	0.43
1:A:348:GLN:O	1:A:352:GLN:HG2	2.17	0.43
1:K:348:GLN:O	1:K:352:GLN:HG2	2.19	0.43
1:L:325:ILE:HA	1:L:329:THR:O	2.18	0.43
1:E:73:MET:O	1:E:76:GLU:HB2	2.18	0.43
1:B:242:LYS:O	1:B:243:ALA:HB3	2.19	0.43
1:G:351:GLN:HA	1:G:354:GLU:HG2	1.99	0.43
1:N:525:PRO:HD3	6:N:2033:HOH:O	2.18	0.43
1:H:260:ALA:O	1:H:264:VAL:HG23	2.18	0.43
1:N:210:THR:HG22	1:N:210:THR:O	2.18	0.43
1:A:526:LYS:HE2	1:G:63:GLU:OE2	2.19	0.43
1:N:171:LYS:HB2	1:N:407:VAL:HG11	2.01	0.43
1:I:409:GLU:OE2	1:I:498:LYS:HG3	2.19	0.43
1:A:210:THR:HG22	1:A:210:THR:O	2.18	0.43
1:H:384:ALA:C	1:H:385:THR:HG23	2.39	0.43
1:M:217:SER:N	1:M:218:PRO:CD	2.82	0.43
1:B:218:PRO:HD2	1:B:320:ALA:O	2.18	0.43
1:N:180:GLY:HA3	1:N:381:VAL:O	2.18	0.43
1:N:381:VAL:O	1:N:382:GLY:O	2.37	0.43
1:D:193:MET:HG3	1:D:371:LYS:HB3	2.01	0.43
1:B:266:THR:HG22	1:B:271:VAL:O	2.19	0.43
1:G:224:ASP:HB3	1:G:302:SER:HB3	2.00	0.43
1:J:69:MET:O	1:J:73:MET:HG3	2.19	0.43
1:N:366:GLN:O	1:N:369:VAL:HG22	2.18	0.43
1:J:199:TYR:CZ	1:J:327:LYS:HA	2.54	0.43
1:A:191:GLU:O	1:A:334:ASP:HA	2.18	0.43
1:N:284:ARG:O	1:N:288:MET:HG3	2.19	0.43
1:H:183:LEU:HD13	1:H:184:GLN:N	2.33	0.43
1:D:325:ILE:HG22	1:D:330:THR:HG23	1.99	0.43
1:M:259:LEU:O	1:M:263:VAL:HG23	2.19	0.43
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.99	0.43
1:F:240:VAL:HG11	1:F:247:LEU:HB2	2.00	0.43
1:F:178:GLU:OE2	1:F:322:ARG:NH1	2.51	0.43
1:K:205:ILE:CA	1:K:213:VAL:HG22	2.49	0.43
1:B:369:VAL:HG23	1:B:370:ALA:N	2.33	0.43
1:C:242:LYS:C	1:C:244:GLY:N	2.72	0.43
1:N:82:ASN:O	1:N:86:GLY:N	2.49	0.43
1:H:409:GLU:OE2	1:H:498:LYS:HG3	2.19	0.43
1:J:449:ALA:HB3	1:J:450:PRO:HD3	2.01	0.43
1:N:37:ASN:HD21	1:N:51:LYS:HE3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:210:THR:HG22	1:I:210:THR:O	2.19	0.43
1:J:210:THR:O	1:J:210:THR:HG22	2.18	0.43
1:F:383:ALA:HA	6:F:2746:HOH:O	2.19	0.43
1:A:384:ALA:O	1:A:385:THR:OG1	2.33	0.43
1:B:234:LEU:O	1:B:238:GLU:HG3	2.18	0.43
1:E:218:PRO:HD2	1:E:320:ALA:O	2.19	0.43
1:A:194:GLN:OE1	1:A:329:THR:HG21	2.18	0.43
1:E:176:THR:HG22	1:E:177:VAL:N	2.33	0.43
1:G:132:LYS:HG3	6:G:1971:HOH:O	2.19	0.43
1:H:369:VAL:HG23	1:H:370:ALA:N	2.34	0.43
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.52	0.43
1:L:85:ALA:O	1:L:401:HIS:HE1	2.01	0.43
1:J:209:GLU:N	1:J:209:GLU:OE1	2.47	0.43
1:D:349:ILE:CG2	1:D:369:VAL:HG13	2.48	0.43
1:I:259:LEU:O	1:I:263:VAL:HG23	2.18	0.43
1:A:69:MET:HE2	1:G:39:VAL:HG12	2.01	0.43
1:C:272:LYS:NZ	1:D:228:SER:HB2	2.34	0.43
1:B:215:LEU:HB2	1:B:323:VAL:CG2	2.48	0.43
1:K:144:ILE:HG23	1:K:403:THR:CG2	2.49	0.43
1:G:223:ALA:O	1:G:251:ALA:HA	2.19	0.43
1:K:449:ALA:HB3	1:K:450:PRO:HD3	2.00	0.43
1:H:37:ASN:ND2	1:H:51:LYS:HE3	2.34	0.43
1:B:463:SER:O	1:B:467:ASN:HB2	2.19	0.43
1:E:324:VAL:O	1:E:331:THR:HG22	2.17	0.43
1:L:239:ALA:O	1:L:314:LEU:HD11	2.18	0.43
1:L:217:SER:N	1:L:218:PRO:CD	2.82	0.43
1:G:217:SER:N	1:G:218:PRO:CD	2.82	0.43
1:F:348:GLN:O	1:F:352:GLN:HG2	2.18	0.43
1:L:381:VAL:O	1:L:382:GLY:O	2.37	0.43
1:F:420:ILE:CD1	1:F:451:LEU:HD13	2.49	0.43
1:N:222:LEU:HB3	1:N:289:LEU:HD21	2.01	0.43
1:C:70:GLY:HA2	1:C:73:MET:HE3	2.01	0.43
1:E:65:LYS:HE3	1:E:522:THR:OG1	2.19	0.43
1:M:68:ASN:O	1:M:72:GLN:HG2	2.18	0.43
1:F:209:GLU:OE1	1:F:209:GLU:N	2.49	0.43
1:B:384:ALA:C	1:B:385:THR:HG23	2.38	0.43
1:L:217:SER:N	1:L:218:PRO:HD3	2.33	0.43
1:D:234:LEU:O	1:D:238:GLU:HG3	2.18	0.43
1:A:417:VAL:HG11	1:A:488:MET:HG3	2.00	0.43
1:E:177:VAL:HG21	1:E:397:GLU:HG2	1.99	0.43
1:K:220:ILE:CD1	1:K:296:THR:HG21	2.49	0.43
1:N:524:LEU:O	1:N:526:LYS:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:496:PRO:HB2	1:I:499:VAL:CG1	2.49	0.43
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.43
1:D:65:LYS:HG2	6:D:1200:HOH:O	2.19	0.43
1:B:241:ALA:HB1	1:C:231:ARG:NH1	2.33	0.43
1:M:27:VAL:HG12	1:M:90:THR:HG23	2.00	0.42
5:N:1:AGS:O2G	5:N:1:AGS:S1G	2.54	0.42
1:L:383:ALA:O	1:L:384:ALA:CB	2.66	0.42
1:M:284:ARG:HH11	1:M:364:LYS:CE	2.32	0.42
1:K:182:GLY:HA2	1:K:383:ALA:CB	2.49	0.42
1:J:179:ASP:HB3	1:J:389:MET:CE	2.48	0.42
1:L:60:ILE:O	1:L:75:LYS:HE3	2.19	0.42
1:A:329:THR:HG22	6:A:2839:HOH:O	2.18	0.42
1:F:266:THR:HG22	1:F:271:VAL:O	2.18	0.42
1:E:177:VAL:HA	1:E:379:ILE:O	2.19	0.42
1:B:353:ILE:HD13	1:B:366:GLN:HG2	2.01	0.42
1:K:70:GLY:HA2	1:K:73:MET:HE3	2.01	0.42
1:F:191:GLU:O	1:F:334:ASP:HA	2.18	0.42
1:C:421:ARG:CZ	1:C:473:ASP:HA	2.49	0.42
1:K:384:ALA:C	1:K:385:THR:HG23	2.39	0.42
1:G:302:SER:H	1:G:307:MET:HE1	1.83	0.42
1:E:240:VAL:HG11	1:E:247:LEU:HB2	2.00	0.42
1:A:366:GLN:HA	1:A:369:VAL:HG22	2.00	0.42
1:K:319:GLN:HB3	1:K:336:VAL:HG21	2.00	0.42
1:M:496:PRO:O	1:M:499:VAL:HG13	2.19	0.42
1:J:222:LEU:HB3	1:J:289:LEU:CD2	2.50	0.42
1:I:466:ALA:O	1:I:470:LYS:HG3	2.19	0.42
1:I:238:GLU:O	1:I:241:ALA:HB3	2.19	0.42
1:J:200:LEU:HG	1:J:276:VAL:HA	2.01	0.42
1:A:253:ASP:OD1	1:A:277:LYS:HE2	2.19	0.42
1:L:324:VAL:O	1:L:331:THR:HG22	2.19	0.42
1:D:284:ARG:O	1:D:288:MET:HG3	2.19	0.42
1:N:272:LYS:CD	1:N:272:LYS:N	2.83	0.42
1:E:220:ILE:CD1	1:E:296:THR:HG21	2.48	0.42
1:N:336:VAL:O	1:N:337:GLY:C	2.58	0.42
1:B:193:MET:HE3	1:B:292:ILE:HG12	2.02	0.42
1:I:496:PRO:HD2	1:I:499:VAL:CG1	2.49	0.42
1:K:438:VAL:O	1:K:442:VAL:HG23	2.18	0.42
1:D:37:ASN:HD21	1:D:51:LYS:HE3	1.84	0.42
1:C:496:PRO:O	1:C:499:VAL:HG13	2.19	0.42
1:K:421:ARG:CZ	1:K:473:ASP:HA	2.49	0.42
1:L:94:VAL:HB	6:L:2642:HOH:O	2.20	0.42
1:F:384:ALA:C	1:F:385:THR:HG23	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:348:GLN:O	1:E:352:GLN:HG2	2.19	0.42
1:I:200:LEU:HG	1:I:276:VAL:HA	2.00	0.42
1:F:253:ASP:OD1	1:F:277:LYS:HE2	2.19	0.42
1:C:271:VAL:HG12	1:C:273:VAL:HG23	2.00	0.42
1:N:193:MET:HE1	1:N:292:ILE:HG12	2.01	0.42
1:A:177:VAL:HA	1:A:379:ILE:O	2.19	0.42
1:M:325:ILE:HG22	1:M:330:THR:HG23	2.01	0.42
1:N:206:ASN:ND2	1:N:214:GLU:H	2.16	0.42
1:M:288:MET:HA	1:M:291:ASP:OD2	2.19	0.42
1:D:206:ASN:OD1	1:D:207:LYS:HG3	2.19	0.42
1:B:169:VAL:HG13	1:B:377:ALA:HB2	2.00	0.42
1:G:524:LEU:O	1:G:526:LYS:N	2.52	0.42
1:I:224:ASP:HB3	1:I:302:SER:HB3	2.02	0.42
1:A:8:PHE:HB3	6:A:1960:HOH:O	2.20	0.42
1:D:36:ARG:HG3	1:E:518:GLU:HG2	2.00	0.42
1:G:85:ALA:O	1:G:401:HIS:HE1	2.02	0.42
1:L:183:LEU:HD13	1:L:184:GLN:N	2.34	0.42
1:M:284:ARG:HH11	1:M:364:LYS:NZ	2.18	0.42
1:F:183:LEU:HD13	1:F:184:GLN:N	2.34	0.42
1:A:183:LEU:HD13	1:A:184:GLN:N	2.34	0.42
1:J:238:GLU:O	1:J:241:ALA:HB3	2.20	0.42
1:F:60:ILE:O	1:F:75:LYS:HE3	2.19	0.42
1:C:23:LEU:HD13	1:C:75:LYS:HD2	2.01	0.42
1:C:27:VAL:HG12	1:C:90:THR:HG23	2.01	0.42
1:A:240:VAL:HG11	1:A:247:LEU:HB2	2.00	0.42
1:L:202:PRO:O	1:L:204:PHE:N	2.46	0.42
1:J:215:LEU:HB2	1:J:323:VAL:CG2	2.50	0.42
1:G:134:LEU:HD22	6:G:2213:HOH:O	2.19	0.42
6:I:2009:HOH:O	1:J:117:LYS:HE3	2.18	0.42
1:H:342:ILE:O	1:H:346:VAL:HG23	2.19	0.42
1:D:445:ARG:HD3	6:D:2123:HOH:O	2.19	0.42
1:J:182:GLY:HA2	1:J:383:ALA:HB3	2.02	0.42
1:G:242:LYS:O	1:G:244:GLY:N	2.52	0.42
6:C:2549:HOH:O	1:J:463:SER:HB2	2.19	0.42
1:J:348:GLN:O	1:J:352:GLN:HG2	2.19	0.42
1:N:259:LEU:O	1:N:263:VAL:HG23	2.20	0.42
1:L:259:LEU:O	1:L:263:VAL:HG23	2.19	0.42
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.02	0.42
1:D:404:ARG:HH11	1:D:404:ARG:CG	2.27	0.42
1:N:194:GLN:HG3	1:N:331:THR:HB	2.00	0.42
1:E:266:THR:HG22	1:E:271:VAL:O	2.19	0.42
1:G:266:THR:HG21	1:G:273:VAL:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:220:ILE:CD1	1:M:296:THR:HG21	2.48	0.42
1:H:160:LYS:HB2	1:H:160:LYS:HZ3	1.84	0.42
1:F:319:GLN:HB3	1:F:336:VAL:HG21	2.02	0.42
1:G:131:LEU:HD13	1:G:422:VAL:HG21	2.02	0.42
1:K:460:GLU:O	1:K:462:PRO:HD3	2.18	0.42
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.60	0.42
1:G:112:ASN:HA	1:G:113:PRO:HD3	1.91	0.42
1:E:209:GLU:OE1	1:E:209:GLU:N	2.49	0.42
1:D:182:GLY:HA2	1:D:383:ALA:CB	2.50	0.42
1:H:182:GLY:HA2	1:H:383:ALA:HB3	2.02	0.42
1:I:179:ASP:HB3	1:I:389:MET:CE	2.49	0.42
1:J:206:ASN:ND2	1:J:214:GLU:H	2.17	0.42
1:M:242:LYS:O	1:M:243:ALA:HB3	2.20	0.42
1:I:336:VAL:O	1:I:337:GLY:C	2.58	0.42
1:B:144:ILE:HG23	1:B:403:THR:HG21	2.02	0.42
1:C:191:GLU:O	1:C:334:ASP:HA	2.20	0.42
1:N:111:MET:HG2	1:N:435:ASP:OD1	2.19	0.42
1:K:496:PRO:O	1:K:499:VAL:HG13	2.19	0.42
1:B:197:ARG:HD2	1:B:277:LYS:HB2	2.01	0.42
1:H:381:VAL:O	1:H:382:GLY:O	2.38	0.42
1:J:305:ILE:HB	1:J:307:MET:HE2	2.01	0.42
1:H:325:ILE:HA	1:H:329:THR:O	2.19	0.42
1:I:266:THR:HG21	1:I:273:VAL:H	1.84	0.42
1:G:193:MET:HE2	1:G:292:ILE:HG12	2.00	0.42
1:F:206:ASN:ND2	1:F:214:GLU:H	2.16	0.42
1:A:302:SER:O	1:A:307:MET:HE3	2.20	0.42
1:M:179:ASP:HB3	1:M:389:MET:CE	2.50	0.42
1:H:319:GLN:HB3	1:H:336:VAL:HG21	2.01	0.42
1:B:140:ASP:O	1:B:144:ILE:HG13	2.20	0.42
1:M:524:LEU:HA	1:M:524:LEU:HD12	1.87	0.42
1:J:331:THR:HG23	1:J:331:THR:O	2.20	0.42
1:M:144:ILE:HG23	1:M:403:THR:HG21	2.01	0.42
1:H:210:THR:HG22	1:H:210:THR:O	2.20	0.42
1:B:77:VAL:HG11	1:B:506:TYR:O	2.18	0.42
1:M:348:GLN:O	1:M:352:GLN:HG2	2.20	0.42
1:L:382:GLY:O	1:L:389:MET:HG2	2.20	0.42
1:B:324:VAL:O	1:B:331:THR:HG22	2.20	0.42
1:N:305:ILE:HB	1:N:307:MET:HE2	2.01	0.42
1:N:369:VAL:HG23	1:N:370:ALA:N	2.35	0.42
1:L:206:ASN:ND2	1:L:214:GLU:H	2.18	0.42
1:I:366:GLN:HA	1:I:369:VAL:HG22	2.01	0.42
1:A:4:LYS:HG3	1:G:59:GLU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:384:ALA:C	1:C:385:THR:HG23	2.39	0.42
1:F:259:LEU:O	1:F:263:VAL:HG23	2.19	0.42
1:H:240:VAL:HG11	1:H:247:LEU:HB2	2.01	0.42
1:G:219:PHE:O	1:G:247:LEU:HD12	2.19	0.42
1:E:76:GLU:HG3	6:E:2322:HOH:O	2.20	0.42
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.91	0.42
1:N:37:ASN:ND2	1:N:51:LYS:HE3	2.35	0.42
1:L:33:PRO:CG	1:L:480:ALA:HB3	2.50	0.42
1:D:223:ALA:O	1:D:251:ALA:HA	2.20	0.42
1:N:183:LEU:CD2	1:N:384:ALA:HB2	2.49	0.41
1:B:305:ILE:HB	1:B:307:MET:HE2	2.02	0.41
1:I:177:VAL:HG21	1:I:397:GLU:HG2	1.99	0.41
1:N:325:ILE:HA	1:N:329:THR:O	2.18	0.41
1:G:417:VAL:HG13	6:G:2394:HOH:O	2.20	0.41
1:F:242:LYS:C	1:F:244:GLY:N	2.73	0.41
1:A:336:VAL:O	1:A:337:GLY:C	2.59	0.41
1:J:37:ASN:ND2	1:J:51:LYS:HE3	2.34	0.41
1:F:510:VAL:CG2	6:F:2556:HOH:O	2.67	0.41
1:D:191:GLU:O	1:D:334:ASP:HA	2.20	0.41
1:C:222:LEU:HB3	1:C:289:LEU:CD2	2.50	0.41
1:H:220:ILE:HD12	1:H:296:THR:HG21	2.02	0.41
5:L:1:AGS:O2G	5:L:1:AGS:S1G	2.55	0.41
1:C:200:LEU:HG	1:C:276:VAL:HA	2.02	0.41
1:D:177:VAL:HA	1:D:379:ILE:O	2.20	0.41
1:D:160:LYS:HZ2	1:D:160:LYS:HB2	1.84	0.41
1:A:176:THR:HG22	1:A:177:VAL:H	1.84	0.41
1:M:242:LYS:C	1:M:244:GLY:N	2.72	0.41
1:B:366:GLN:HA	1:B:369:VAL:HG22	2.02	0.41
1:G:353:ILE:HD13	1:G:366:GLN:HG2	2.02	0.41
1:M:496:PRO:HB2	1:M:499:VAL:HG12	2.02	0.41
1:L:97:GLN:HG2	6:L:2018:HOH:O	2.19	0.41
1:F:487:ASN:O	1:F:491:MET:HG3	2.20	0.41
1:M:171:LYS:HB2	1:M:407:VAL:HG11	2.02	0.41
1:G:409:GLU:OE2	1:G:498:LYS:HG3	2.20	0.41
1:F:182:GLY:HA2	1:F:383:ALA:HB3	2.01	0.41
1:E:183:LEU:CD2	1:E:384:ALA:HB2	2.50	0.41
1:G:384:ALA:C	1:G:385:THR:HG23	2.40	0.41
1:E:238:GLU:O	1:E:241:ALA:HB3	2.19	0.41
1:D:217:SER:N	1:D:218:PRO:HD3	2.34	0.41
1:B:194:GLN:OE1	1:B:329:THR:HG21	2.20	0.41
1:C:353:ILE:HD13	1:C:366:GLN:HG2	2.01	0.41
1:K:239:ALA:C	1:K:314:LEU:HD21	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:69:MET:O	1:N:73:MET:HG3	2.19	0.41
1:M:193:MET:HE2	1:M:292:ILE:HG12	2.02	0.41
1:J:336:VAL:O	1:J:337:GLY:C	2.58	0.41
1:N:524:LEU:HA	1:N:524:LEU:HD12	1.91	0.41
1:G:222:LEU:HB3	1:G:289:LEU:CD2	2.50	0.41
1:L:122:LYS:HE2	1:L:429:LEU:HD11	2.02	0.41
1:A:220:ILE:HD12	1:A:296:THR:HG21	2.02	0.41
1:A:140:ASP:OD2	1:A:142:LYS:HB3	2.21	0.41
1:B:222:LEU:HB3	1:B:289:LEU:CD2	2.49	0.41
1:A:153:ASN:O	1:A:154:SER:HB2	2.19	0.41
1:C:224:ASP:HB3	1:C:302:SER:HB3	2.02	0.41
1:E:191:GLU:O	1:E:334:ASP:HA	2.20	0.41
1:N:209:GLU:N	1:N:209:GLU:OE1	2.48	0.41
1:L:210:THR:O	1:L:210:THR:HG22	2.20	0.41
1:I:217:SER:HA	1:I:320:ALA:O	2.20	0.41
1:N:176:THR:HG22	1:N:177:VAL:N	2.35	0.41
1:B:240:VAL:HG11	1:B:247:LEU:HB2	2.01	0.41
1:J:177:VAL:HA	1:J:379:ILE:O	2.20	0.41
1:K:366:GLN:HA	1:K:369:VAL:HG22	2.01	0.41
1:H:16:MET:HE3	6:H:2854:HOH:O	2.21	0.41
1:B:242:LYS:C	1:B:244:GLY:N	2.73	0.41
1:G:351:GLN:HA	1:G:354:GLU:CG	2.49	0.41
1:K:171:LYS:HB2	1:K:407:VAL:HG11	2.02	0.41
1:J:295:LEU:HD13	1:J:295:LEU:O	2.20	0.41
1:D:182:GLY:HA2	1:D:383:ALA:HB3	2.03	0.41
1:A:182:GLY:O	1:A:183:LEU:O	2.39	0.41
1:E:182:GLY:HA2	1:E:383:ALA:HB3	2.02	0.41
1:B:325:ILE:HG22	1:B:330:THR:HG23	2.03	0.41
1:D:284:ARG:NH1	1:D:364:LYS:NZ	2.67	0.41
1:E:325:ILE:HG22	1:E:330:THR:HG23	2.02	0.41
1:A:219:PHE:O	1:A:247:LEU:HD12	2.20	0.41
1:C:177:VAL:HA	1:C:379:ILE:O	2.20	0.41
1:E:28:LYS:HD2	1:E:453:GLN:NE2	2.36	0.41
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.87	0.41
1:M:63:GLU:HB2	1:N:524:LEU:CD2	2.50	0.41
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.50	0.41
1:C:460:GLU:O	1:C:462:PRO:HD3	2.21	0.41
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.60	0.41
1:E:178:GLU:OE1	1:E:378:VAL:HG11	2.20	0.41
1:H:153:ASN:O	1:H:154:SER:HB2	2.20	0.41
1:L:461:GLU:HA	1:L:462:PRO:HD3	1.91	0.41
1:J:134:LEU:HD21	1:J:425:LYS:NZ	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:54:VAL:HG23	6:M:2164:HOH:O	2.20	0.41
1:N:463:SER:O	1:N:467:ASN:HB2	2.19	0.41
1:H:295:LEU:C	1:H:295:LEU:HD13	2.41	0.41
1:C:182:GLY:HA2	1:C:383:ALA:CB	2.50	0.41
1:I:324:VAL:O	1:I:331:THR:HG22	2.21	0.41
1:L:477:GLY:CA	6:L:2905:HOH:O	2.68	0.41
1:D:200:LEU:HG	1:D:276:VAL:HA	2.01	0.41
1:K:204:PHE:C	1:K:213:VAL:HG22	2.41	0.41
1:C:272:LYS:HZ3	1:D:228:SER:HB2	1.85	0.41
1:K:366:GLN:O	1:K:369:VAL:HG22	2.20	0.41
1:B:336:VAL:O	1:B:337:GLY:C	2.59	0.41
1:B:193:MET:HE1	1:B:292:ILE:HG12	2.02	0.41
1:M:215:LEU:HB2	1:M:323:VAL:HG22	2.03	0.41
1:H:85:ALA:O	1:H:401:HIS:HE1	2.03	0.41
1:K:199:TYR:CZ	1:K:327:LYS:HA	2.56	0.41
1:F:140:ASP:OD2	1:F:142:LYS:HB3	2.20	0.41
1:K:295:LEU:HD13	1:K:295:LEU:O	2.20	0.41
1:D:210:THR:HG22	1:D:210:THR:O	2.19	0.41
1:M:136:VAL:HA	1:M:137:PRO:HD3	1.87	0.41
1:A:231:ARG:NH1	1:G:242:LYS:HA	2.35	0.41
1:A:266:THR:HG21	1:A:273:VAL:H	1.86	0.41
1:E:305:ILE:HB	1:E:307:MET:HE2	2.02	0.41
1:A:242:LYS:C	1:A:244:GLY:N	2.73	0.41
1:B:69:MET:O	1:B:73:MET:HG3	2.20	0.41
1:N:455:VAL:O	1:N:458:CYS:HB2	2.21	0.41
1:G:183:LEU:CD2	1:G:384:ALA:HB2	2.48	0.41
1:F:238:GLU:O	1:F:241:ALA:HB3	2.20	0.41
1:D:348:GLN:O	1:D:352:GLN:HG2	2.21	0.41
1:K:381:VAL:O	1:K:382:GLY:O	2.39	0.41
1:D:201:SER:O	1:D:202:PRO:O	2.39	0.41
1:B:302:SER:H	1:B:307:MET:HE1	1.85	0.41
1:L:194:GLN:HG3	1:L:331:THR:HB	2.03	0.41
1:G:266:THR:HG22	1:G:273:VAL:H	1.86	0.41
1:I:242:LYS:O	1:I:243:ALA:HB3	2.20	0.41
1:E:336:VAL:O	1:E:337:GLY:C	2.58	0.41
1:G:202:PRO:C	1:G:204:PHE:H	2.23	0.41
1:E:39:VAL:HG12	1:F:69:MET:CE	2.51	0.41
1:N:260:ALA:O	1:N:264:VAL:HG23	2.21	0.41
1:J:140:ASP:OD2	1:J:142:LYS:HB3	2.21	0.41
1:D:324:VAL:HB	1:D:331:THR:CG2	2.51	0.41
1:E:85:ALA:O	1:E:401:HIS:HE1	2.03	0.41
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:153:ASN:O	1:K:154:SER:HB2	2.20	0.41
1:B:77:VAL:CB	1:B:510:VAL:HG22	2.51	0.41
1:J:182:GLY:HA2	1:J:383:ALA:CB	2.50	0.41
1:L:183:LEU:CD2	1:L:384:ALA:HB2	2.49	0.41
1:L:384:ALA:C	1:L:385:THR:HG23	2.40	0.41
1:L:235:PRO:CG	1:L:310:GLU:HA	2.34	0.41
1:M:253:ASP:OD1	1:M:277:LYS:HE2	2.20	0.41
1:L:200:LEU:HG	1:L:276:VAL:HA	2.02	0.41
1:J:381:VAL:O	1:J:382:GLY:O	2.39	0.41
1:G:200:LEU:HG	1:G:276:VAL:HA	2.02	0.41
1:L:477:GLY:HA2	6:L:2905:HOH:O	2.20	0.41
1:B:194:GLN:HG3	1:B:331:THR:HB	2.03	0.41
1:B:174:VAL:HG22	1:B:194:GLN:NE2	2.36	0.41
1:B:205:ILE:CA	1:B:213:VAL:HG22	2.50	0.41
1:H:177:VAL:HG21	1:H:397:GLU:HG2	2.00	0.41
1:A:194:GLN:HG3	1:A:331:THR:HB	2.02	0.41
1:B:177:VAL:HA	1:B:379:ILE:O	2.21	0.41
1:N:194:GLN:OE1	1:N:329:THR:HG21	2.21	0.41
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.34	0.41
1:D:39:VAL:HG12	1:E:69:MET:CE	2.50	0.41
1:G:77:VAL:CG2	1:G:510:VAL:HG21	2.51	0.41
1:J:242:LYS:O	1:J:243:ALA:HB3	2.20	0.41
1:E:160:LYS:HB2	1:E:160:LYS:NZ	2.36	0.41
1:K:353:ILE:HD13	1:K:366:GLN:HG2	2.01	0.41
1:G:366:GLN:HA	1:G:369:VAL:HG22	2.03	0.41
1:E:366:GLN:HA	1:E:369:VAL:HG22	2.03	0.41
1:K:524:LEU:HD12	1:K:524:LEU:HA	1.87	0.41
1:I:63:GLU:HB2	1:J:524:LEU:CD2	2.50	0.41
1:C:496:PRO:HB2	1:C:499:VAL:CG1	2.50	0.41
1:L:215:LEU:HB2	1:L:323:VAL:HG22	2.03	0.41
1:L:351:GLN:HA	1:L:354:GLU:HG2	2.02	0.41
1:F:421:ARG:CZ	1:F:473:ASP:HA	2.51	0.41
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.60	0.41
1:H:191:GLU:O	1:H:334:ASP:HA	2.19	0.41
1:L:290:GLN:HB3	1:L:345:ARG:NH2	2.35	0.41
1:N:85:ALA:O	1:N:401:HIS:HE1	2.03	0.41
1:N:134:LEU:HD21	1:N:425:LYS:NZ	2.35	0.41
1:H:324:VAL:O	1:H:331:THR:HG22	2.21	0.41
1:I:171:LYS:HB2	1:I:407:VAL:HG11	2.02	0.41
1:M:449:ALA:HB3	1:M:450:PRO:HD3	2.03	0.41
1:L:46:ALA:HA	1:L:47:PRO:HD3	1.93	0.41
1:G:284:ARG:HH12	1:G:364:LYS:NZ	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:284:ARG:O	1:G:288:MET:HG3	2.21	0.41
1:I:421:ARG:CZ	1:I:473:ASP:HA	2.51	0.41
1:E:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.41
1:A:325:ILE:HA	1:A:329:THR:O	2.20	0.41
1:N:193:MET:HG3	1:N:371:LYS:HB3	2.03	0.41
1:F:23:LEU:CD2	1:F:74:VAL:HG13	2.51	0.41
1:E:202:PRO:C	1:E:204:PHE:H	2.23	0.41
1:M:102:GLU:HB2	1:M:442:VAL:HG13	2.03	0.41
1:C:153:ASN:O	1:C:154:SER:HB2	2.21	0.41
1:E:224:ASP:HB3	1:E:302:SER:HB3	2.01	0.41
1:M:384:ALA:C	1:M:385:THR:HG23	2.42	0.40
1:M:205:ILE:CA	1:M:213:VAL:HG22	2.48	0.40
1:L:160:LYS:NZ	1:L:160:LYS:HB2	2.36	0.40
1:H:77:VAL:HG23	1:H:510:VAL:HG21	2.03	0.40
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.51	0.40
1:K:46:ALA:HA	1:K:47:PRO:HD3	1.88	0.40
1:A:466:ALA:O	1:A:470:LYS:HG3	2.21	0.40
1:N:384:ALA:C	1:N:385:THR:HG23	2.41	0.40
1:G:182:GLY:HA2	1:G:383:ALA:HB3	2.04	0.40
1:K:451:LEU:C	1:K:451:LEU:HD23	2.41	0.40
1:M:197:ARG:HD2	1:M:277:LYS:HB2	2.04	0.40
1:H:200:LEU:HG	1:H:276:VAL:HA	2.02	0.40
1:D:224:ASP:HB3	1:D:302:SER:HB3	2.04	0.40
1:F:302:SER:O	1:F:307:MET:HE3	2.21	0.40
1:I:325:ILE:HG22	1:I:330:THR:HG23	2.02	0.40
1:K:224:ASP:HB3	1:K:302:SER:HB3	2.03	0.40
1:K:194:GLN:OE1	1:K:329:THR:HG21	2.21	0.40
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.31	0.40
1:E:242:LYS:O	1:E:243:ALA:HB3	2.21	0.40
1:J:366:GLN:O	1:J:369:VAL:HG22	2.20	0.40
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.03	0.40
1:K:215:LEU:HB2	1:K:323:VAL:CG2	2.51	0.40
1:I:496:PRO:HD2	1:I:499:VAL:HG11	2.03	0.40
1:K:7:LYS:HE2	1:K:66:PHE:CE2	2.56	0.40
1:C:284:ARG:HH12	1:C:364:LYS:NZ	2.19	0.40
1:M:183:LEU:HD13	1:M:184:GLN:N	2.35	0.40
1:C:174:VAL:HG22	1:C:194:GLN:HE21	1.87	0.40
1:I:240:VAL:HG11	1:I:247:LEU:HB2	2.02	0.40
1:I:242:LYS:C	1:I:244:GLY:N	2.73	0.40
1:C:336:VAL:O	1:C:337:GLY:C	2.60	0.40
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.51	0.40
1:K:284:ARG:HH12	1:K:364:LYS:NZ	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:342:ILE:O	1:M:346:VAL:HG23	2.22	0.40
1:A:342:ILE:O	1:A:346:VAL:HG23	2.21	0.40
1:C:199:TYR:CZ	1:C:327:LYS:HA	2.56	0.40
1:H:455:VAL:HG13	1:H:460:GLU:HB2	2.02	0.40
1:I:295:LEU:HD13	1:I:295:LEU:C	2.42	0.40
1:C:295:LEU:O	1:C:295:LEU:HD13	2.21	0.40
1:I:384:ALA:C	1:I:385:THR:HG23	2.41	0.40
1:N:182:GLY:O	1:N:183:LEU:O	2.40	0.40
1:E:384:ALA:C	1:E:385:THR:HG23	2.42	0.40
1:D:369:VAL:HG23	1:D:370:ALA:N	2.36	0.40
1:C:201:SER:O	1:C:202:PRO:O	2.40	0.40
1:B:253:ASP:OD1	1:B:277:LYS:HE2	2.21	0.40
1:K:200:LEU:HG	1:K:276:VAL:HA	2.03	0.40
1:N:179:ASP:HB3	1:N:389:MET:CE	2.51	0.40
1:I:194:GLN:HG3	1:I:331:THR:HB	2.02	0.40
1:C:266:THR:HG21	1:C:273:VAL:H	1.86	0.40
1:K:240:VAL:HG11	1:K:247:LEU:HB2	2.02	0.40
1:C:160:LYS:HB2	1:C:160:LYS:HZ2	1.87	0.40
1:H:202:PRO:C	1:H:204:PHE:H	2.24	0.40
1:C:524:LEU:HA	1:C:524:LEU:HD12	1.92	0.40
1:I:524:LEU:HA	1:I:524:LEU:HD12	1.93	0.40
1:N:10:ASN:HA	6:N:2143:HOH:O	2.21	0.40
1:L:361:ASP:O	1:L:365:LEU:HG	2.20	0.40
1:D:118:ARG:HD2	1:D:436:GLN:NE2	2.36	0.40
1:K:392:LYS:O	1:K:396:VAL:HG23	2.22	0.40
1:B:111:MET:SD	1:B:438:VAL:HG21	2.62	0.40
1:C:46:ALA:HA	1:C:47:PRO:HD3	1.94	0.40
1:I:438:VAL:O	1:I:442:VAL:HG23	2.21	0.40
1:F:215:LEU:HB2	1:F:323:VAL:HG22	2.03	0.40
1:C:34:LYS:HG3	1:C:458:CYS:SG	2.62	0.40
1:A:295:LEU:HD13	1:A:295:LEU:C	2.42	0.40
5:M:1:AGS:O2G	5:M:1:AGS:S1G	2.54	0.40
1:H:182:GLY:HA2	1:H:383:ALA:CB	2.51	0.40
1:K:217:SER:HA	1:K:320:ALA:O	2.21	0.40
1:H:216:GLU:C	1:H:218:PRO:HD3	2.41	0.40
1:J:253:ASP:OD1	1:J:277:LYS:HE2	2.22	0.40
1:L:348:GLN:O	1:L:352:GLN:HG2	2.21	0.40
1:M:194:GLN:HG3	1:M:331:THR:HB	2.03	0.40
1:H:266:THR:HG21	1:H:273:VAL:H	1.85	0.40
1:K:302:SER:O	1:K:307:MET:HE3	2.22	0.40
1:D:404:ARG:HG2	1:D:404:ARG:NH1	2.33	0.40
1:K:194:GLN:HG3	1:K:331:THR:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:326:ASN:HD22	1:H:329:THR:HB	1.86	0.40
1:C:206:ASN:ND2	1:C:214:GLU:H	2.18	0.40
1:C:331:THR:O	1:C:331:THR:HG23	2.22	0.40
1:I:85:ALA:O	1:I:401:HIS:HE1	2.04	0.40
1:I:132:LYS:HE2	6:I:1912:HOH:O	2.21	0.40
1:G:174:VAL:HG12	1:G:376:VAL:HG13	2.04	0.40
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.95	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:315:GLU:OE2	1:N:338:GLU:OE1[1_554]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	A	523/547 (96%)	487 (93%)	27 (5%)	9 (2%)	14	5
1	B	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	10	3
1	C	523/547 (96%)	488 (93%)	24 (5%)	11 (2%)	11	3
1	D	523/547 (96%)	492 (94%)	22 (4%)	9 (2%)	14	5
1	E	523/547 (96%)	485 (93%)	27 (5%)	11 (2%)	11	3
1	F	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	10	3
1	G	523/547 (96%)	489 (94%)	23 (4%)	11 (2%)	11	3
1	H	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	10	3
1	I	523/547 (96%)	486 (93%)	27 (5%)	10 (2%)	12	4
1	J	523/547 (96%)	486 (93%)	25 (5%)	12 (2%)	10	3
1	K	523/547 (96%)	484 (92%)	29 (6%)	10 (2%)	12	4
1	L	523/547 (96%)	488 (93%)	23 (4%)	12 (2%)	10	3
1	M	523/547 (96%)	487 (93%)	25 (5%)	11 (2%)	11	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	523/547 (96%)	487 (93%)	26 (5%)	10 (2%)	12	4
All	All	7322/7658 (96%)	6820 (93%)	350 (5%)	152 (2%)	11	3

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	LEU
1	E	183	LEU
1	A	183	LEU
1	A	256	GLY
1	A	271	VAL
1	B	256	GLY
1	B	385	THR
1	C	183	LEU
1	C	256	GLY
1	D	183	LEU
1	D	256	GLY
1	D	382	GLY
1	E	256	GLY
1	F	183	LEU
1	F	256	GLY
1	F	271	VAL
1	F	382	GLY
1	G	183	LEU
1	G	256	GLY
1	G	382	GLY
1	H	183	LEU
1	H	256	GLY
1	H	382	GLY
1	I	183	LEU
1	I	256	GLY
1	I	382	GLY
1	J	183	LEU
1	J	256	GLY
1	K	183	LEU
1	K	256	GLY
1	L	183	LEU
1	L	256	GLY
1	L	382	GLY
1	M	183	LEU
1	M	256	GLY
1	M	271	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	183	LEU
1	N	256	GLY
1	N	382	GLY
1	A	202	PRO
1	A	385	THR
1	B	202	PRO
1	B	271	VAL
1	C	202	PRO
1	C	271	VAL
1	C	382	GLY
1	C	385	THR
1	D	202	PRO
1	D	271	VAL
1	D	385	THR
1	E	202	PRO
1	E	271	VAL
1	E	382	GLY
1	E	385	THR
1	F	202	PRO
1	F	384	ALA
1	F	385	THR
1	G	202	PRO
1	G	271	VAL
1	G	385	THR
1	H	202	PRO
1	H	271	VAL
1	H	385	THR
1	I	202	PRO
1	I	271	VAL
1	I	385	THR
1	J	202	PRO
1	J	271	VAL
1	J	382	GLY
1	J	385	THR
1	K	202	PRO
1	K	271	VAL
1	K	385	THR
1	L	202	PRO
1	L	271	VAL
1	L	384	ALA
1	L	385	THR
1	M	202	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	385	THR
1	N	202	PRO
1	N	271	VAL
1	N	385	THR
1	A	253	ASP
1	B	382	GLY
1	B	384	ALA
1	C	184	GLN
1	C	201	SER
1	C	383	ALA
1	D	201	SER
1	D	383	ALA
1	E	253	ASP
1	F	334	ASP
1	F	383	ALA
1	G	253	ASP
1	G	337	GLY
1	I	253	ASP
1	I	383	ALA
1	J	253	ASP
1	J	383	ALA
1	J	384	ALA
1	K	184	GLN
1	K	201	SER
1	K	253	ASP
1	K	382	GLY
1	L	253	ASP
1	L	383	ALA
1	M	201	SER
1	M	253	ASP
1	M	382	GLY
1	B	184	GLN
1	B	201	SER
1	B	253	ASP
1	B	383	ALA
1	C	253	ASP
1	C	334	ASP
1	E	184	GLN
1	E	334	ASP
1	E	383	ALA
1	F	184	GLN
1	F	201	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	253	ASP
1	G	184	GLN
1	H	337	GLY
1	H	383	ALA
1	I	184	GLN
1	J	184	GLN
1	J	334	ASP
1	K	383	ALA
1	L	184	GLN
1	M	334	ASP
1	M	383	ALA
1	N	184	GLN
1	N	201	SER
1	N	383	ALA
1	A	184	GLN
1	A	201	SER
1	B	334	ASP
1	D	184	GLN
1	E	201	SER
1	G	201	SER
1	G	383	ALA
1	H	184	GLN
1	H	253	ASP
1	H	384	ALA
1	I	201	SER
1	J	201	SER
1	M	184	GLN
1	A	382	GLY
1	N	337	GLY
1	H	201	SER
1	L	201	SER
1	L	337	GLY

5.3.2 Protein sidechains ⓘ

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	Percentiles
1	A	404/413 (98%)	394 (98%)	10 (2%)	60 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	404/413 (98%)	397 (98%)	7 (2%)	73	75
1	C	404/413 (98%)	396 (98%)	8 (2%)	68	69
1	D	404/413 (98%)	394 (98%)	10 (2%)	60	59
1	E	404/413 (98%)	397 (98%)	7 (2%)	73	75
1	F	404/413 (98%)	396 (98%)	8 (2%)	68	69
1	G	404/413 (98%)	395 (98%)	9 (2%)	64	65
1	H	404/413 (98%)	397 (98%)	7 (2%)	73	75
1	I	404/413 (98%)	395 (98%)	9 (2%)	64	65
1	J	404/413 (98%)	397 (98%)	7 (2%)	73	75
1	K	404/413 (98%)	396 (98%)	8 (2%)	68	69
1	L	404/413 (98%)	394 (98%)	10 (2%)	60	59
1	M	404/413 (98%)	396 (98%)	8 (2%)	68	69
1	N	404/413 (98%)	396 (98%)	8 (2%)	68	69
All	All	5656/5782 (98%)	5540 (98%)	116 (2%)	66	67

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	20	VAL
1	A	75	LYS
1	A	94	VAL
1	A	183	LEU
1	A	289	LEU
1	A	310	GLU
1	A	328	ASP
1	A	404	ARG
1	A	499	VAL
1	B	75	LYS
1	B	183	LEU
1	B	289	LEU
1	B	310	GLU
1	B	404	ARG
1	B	499	VAL
1	B	510	VAL
1	C	20	VAL
1	C	75	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	94	VAL
1	C	183	LEU
1	C	289	LEU
1	C	328	ASP
1	C	404	ARG
1	C	499	VAL
1	D	20	VAL
1	D	23	LEU
1	D	75	LYS
1	D	94	VAL
1	D	183	LEU
1	D	289	LEU
1	D	310	GLU
1	D	404	ARG
1	D	473	ASP
1	D	499	VAL
1	E	94	VAL
1	E	183	LEU
1	E	310	GLU
1	E	328	ASP
1	E	404	ARG
1	E	499	VAL
1	E	514	MET
1	F	20	VAL
1	F	75	LYS
1	F	94	VAL
1	F	183	LEU
1	F	310	GLU
1	F	328	ASP
1	F	404	ARG
1	F	499	VAL
1	G	10	ASN
1	G	20	VAL
1	G	75	LYS
1	G	183	LEU
1	G	289	LEU
1	G	310	GLU
1	G	328	ASP
1	G	404	ARG
1	G	499	VAL
1	H	20	VAL
1	H	75	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	94	VAL
1	H	183	LEU
1	H	289	LEU
1	H	404	ARG
1	H	499	VAL
1	I	10	ASN
1	I	20	VAL
1	I	75	LYS
1	I	94	VAL
1	I	183	LEU
1	I	289	LEU
1	I	310	GLU
1	I	404	ARG
1	I	499	VAL
1	J	20	VAL
1	J	75	LYS
1	J	94	VAL
1	J	183	LEU
1	J	310	GLU
1	J	404	ARG
1	J	499	VAL
1	K	20	VAL
1	K	75	LYS
1	K	94	VAL
1	K	183	LEU
1	K	289	LEU
1	K	328	ASP
1	K	404	ARG
1	K	499	VAL
1	L	20	VAL
1	L	75	LYS
1	L	94	VAL
1	L	183	LEU
1	L	289	LEU
1	L	310	GLU
1	L	328	ASP
1	L	404	ARG
1	L	417	VAL
1	L	499	VAL
1	M	20	VAL
1	M	75	LYS
1	M	94	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	183	LEU
1	M	284	ARG
1	M	310	GLU
1	M	404	ARG
1	M	499	VAL
1	N	20	VAL
1	N	75	LYS
1	N	94	VAL
1	N	183	LEU
1	N	289	LEU
1	N	310	GLU
1	N	404	ARG
1	N	499	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	146	GLN
1	A	229	ASN
1	A	265	ASN
1	A	319	GLN
1	A	326	ASN
1	A	348	GLN
1	A	351	GLN
1	B	146	GLN
1	B	265	ASN
1	B	319	GLN
1	B	326	ASN
1	B	348	GLN
1	B	351	GLN
1	B	366	GLN
1	B	401	HIS
1	B	475	ASN
1	C	37	ASN
1	C	146	GLN
1	C	265	ASN
1	C	319	GLN
1	C	326	ASN
1	C	348	GLN
1	C	351	GLN
1	C	366	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	401	HIS
1	D	37	ASN
1	D	146	GLN
1	D	229	ASN
1	D	265	ASN
1	D	319	GLN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	366	GLN
1	D	401	HIS
1	D	453	GLN
1	D	475	ASN
1	E	37	ASN
1	E	146	GLN
1	E	265	ASN
1	E	319	GLN
1	E	326	ASN
1	E	348	GLN
1	E	351	GLN
1	E	401	HIS
1	E	453	GLN
1	E	475	ASN
1	F	146	GLN
1	F	265	ASN
1	F	319	GLN
1	F	326	ASN
1	F	348	GLN
1	F	351	GLN
1	F	401	HIS
1	G	37	ASN
1	G	146	GLN
1	G	265	ASN
1	G	319	GLN
1	G	326	ASN
1	G	348	GLN
1	G	351	GLN
1	G	401	HIS
1	G	453	GLN
1	G	475	ASN
1	H	37	ASN
1	H	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	265	ASN
1	H	319	GLN
1	H	326	ASN
1	H	348	GLN
1	H	351	GLN
1	H	401	HIS
1	I	37	ASN
1	I	146	GLN
1	I	265	ASN
1	I	319	GLN
1	I	326	ASN
1	I	348	GLN
1	I	351	GLN
1	I	401	HIS
1	J	37	ASN
1	J	146	GLN
1	J	265	ASN
1	J	319	GLN
1	J	326	ASN
1	J	348	GLN
1	J	351	GLN
1	J	453	GLN
1	K	37	ASN
1	K	146	GLN
1	K	265	ASN
1	K	319	GLN
1	K	326	ASN
1	K	348	GLN
1	K	351	GLN
1	K	401	HIS
1	L	37	ASN
1	L	146	GLN
1	L	229	ASN
1	L	265	ASN
1	L	319	GLN
1	L	326	ASN
1	L	348	GLN
1	L	351	GLN
1	L	401	HIS
1	L	453	GLN
1	M	37	ASN
1	M	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	229	ASN
1	M	265	ASN
1	M	319	GLN
1	M	326	ASN
1	M	348	GLN
1	M	351	GLN
1	M	401	HIS
1	M	453	GLN
1	N	37	ASN
1	N	146	GLN
1	N	265	ASN
1	N	319	GLN
1	N	326	ASN
1	N	348	GLN
1	N	351	GLN
1	N	401	HIS
1	N	453	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 66 ligands modelled in this entry, 30 are monoatomic - leaving 36 for Mogul analysis.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	AGS	A	1	3,4	33,33,33	4.04	4 (12%)	52,52,52	3.07	6 (11%)
2	SO4	A	4001	-	4,4,4	2.37	1 (25%)	6,6,6	0.86	0
2	SO4	A	4007	-	4,4,4	2.32	1 (25%)	6,6,6	0.89	0
2	SO4	A	4008	-	4,4,4	2.37	1 (25%)	6,6,6	0.84	0
5	AGS	B	1	3,4	33,33,33	4.08	5 (15%)	52,52,52	2.93	5 (9%)
2	SO4	B	4009	-	4,4,4	2.36	1 (25%)	6,6,6	0.88	0
2	SO4	B	4010	-	4,4,4	2.41	1 (25%)	6,6,6	0.86	0
5	AGS	C	1	3,4	33,33,33	4.12	3 (9%)	52,52,52	3.19	5 (9%)
2	SO4	C	4011	-	4,4,4	2.38	1 (25%)	6,6,6	0.87	0
2	SO4	C	4012	-	4,4,4	2.45	1 (25%)	6,6,6	0.90	0
5	AGS	D	551	3,4	33,33,33	4.19	4 (12%)	52,52,52	3.21	5 (9%)
5	AGS	E	1	3,4	33,33,33	4.23	4 (12%)	52,52,52	3.14	5 (9%)
2	SO4	E	4005	-	4,4,4	2.22	1 (25%)	6,6,6	0.92	0
2	SO4	E	4006	-	4,4,4	2.38	1 (25%)	6,6,6	0.84	0
5	AGS	F	1	3,4	33,33,33	4.08	3 (9%)	52,52,52	2.95	5 (9%)
2	SO4	F	4004	-	4,4,4	2.26	1 (25%)	6,6,6	0.89	0
5	AGS	G	1	3,4	33,33,33	4.23	4 (12%)	52,52,52	3.26	7 (13%)
2	SO4	G	4002	-	4,4,4	2.37	1 (25%)	6,6,6	0.88	0
5	AGS	H	1	3,4	33,33,33	4.11	4 (12%)	52,52,52	3.39	5 (9%)
2	SO4	H	4017	-	4,4,4	2.39	1 (25%)	6,6,6	0.88	0
2	SO4	H	4018	-	4,4,4	2.38	1 (25%)	6,6,6	0.87	0
5	AGS	I	1	3,4	33,33,33	4.13	3 (9%)	52,52,52	3.07	5 (9%)
5	AGS	J	1	3,4	33,33,33	4.11	3 (9%)	52,52,52	3.24	7 (13%)
2	SO4	J	4019	-	4,4,4	2.38	1 (25%)	6,6,6	0.89	0
2	SO4	J	4020	-	4,4,4	2.39	1 (25%)	6,6,6	0.86	0
5	AGS	K	1	3,4	33,33,33	4.12	4 (12%)	52,52,52	2.83	7 (13%)
2	SO4	K	4021	-	4,4,4	2.44	1 (25%)	6,6,6	0.85	0
2	SO4	K	4022	-	4,4,4	2.36	1 (25%)	6,6,6	0.88	0
5	AGS	L	1	3,4	33,33,33	4.08	5 (15%)	52,52,52	2.75	5 (9%)
2	SO4	L	4003	-	4,4,4	2.37	1 (25%)	6,6,6	0.90	0
5	AGS	M	1	3,4	33,33,33	4.12	3 (9%)	52,52,52	2.86	5 (9%)
2	SO4	M	4013	-	4,4,4	2.49	1 (25%)	6,6,6	0.87	0
2	SO4	M	4014	-	4,4,4	2.41	1 (25%)	6,6,6	0.85	0
5	AGS	N	1	3,4	33,33,33	4.16	4 (12%)	52,52,52	2.77	6 (11%)
2	SO4	N	4015	-	4,4,4	2.40	1 (25%)	6,6,6	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	N	4016	-	4,4,4	2.38	1 (25%)	6,6,6	0.87	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
5	AGS	A	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	A	4001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4007	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4008	-	-	0/0/0/0	0/0/0/0
5	AGS	B	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	B	4009	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4010	-	-	0/0/0/0	0/0/0/0
5	AGS	C	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	C	4011	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4012	-	-	0/0/0/0	0/0/0/0
5	AGS	D	551	3,4	-	0/21/38/38	0/1/3/3
5	AGS	E	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	E	4005	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4006	-	-	0/0/0/0	0/0/0/0
5	AGS	F	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	F	4004	-	-	0/0/0/0	0/0/0/0
5	AGS	G	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	G	4002	-	-	0/0/0/0	0/0/0/0
5	AGS	H	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	H	4017	-	-	0/0/0/0	0/0/0/0
2	SO4	H	4018	-	-	0/0/0/0	0/0/0/0
5	AGS	I	1	3,4	-	0/21/38/38	0/1/3/3
5	AGS	J	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	J	4019	-	-	0/0/0/0	0/0/0/0
2	SO4	J	4020	-	-	0/0/0/0	0/0/0/0
5	AGS	K	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	K	4021	-	-	0/0/0/0	0/0/0/0
2	SO4	K	4022	-	-	0/0/0/0	0/0/0/0
5	AGS	L	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	L	4003	-	-	0/0/0/0	0/0/0/0
5	AGS	M	1	3,4	-	0/21/38/38	0/1/3/3
2	SO4	M	4013	-	-	0/0/0/0	0/0/0/0
2	SO4	M	4014	-	-	0/0/0/0	0/0/0/0
5	AGS	N	1	3,4	-	0/21/38/38	0/1/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	N	4015	-	-	0/0/0/0	0/0/0/0
2	SO4	N	4016	-	-	0/0/0/0	0/0/0/0

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	AGS	PG-S1G	-23.20	1.48	1.90
5	E	1	AGS	PG-S1G	-23.11	1.48	1.90
5	D	551	AGS	PG-S1G	-22.99	1.48	1.90
5	N	1	AGS	PG-S1G	-22.64	1.49	1.90
5	I	1	AGS	PG-S1G	-22.64	1.49	1.90
5	H	1	AGS	PG-S1G	-22.52	1.49	1.90
5	C	1	AGS	PG-S1G	-22.51	1.49	1.90
5	J	1	AGS	PG-S1G	-22.49	1.49	1.90
5	K	1	AGS	PG-S1G	-22.47	1.49	1.90
5	M	1	AGS	PG-S1G	-22.43	1.49	1.90
5	F	1	AGS	PG-S1G	-22.33	1.49	1.90
5	L	1	AGS	PG-S1G	-22.32	1.49	1.90
5	B	1	AGS	PG-S1G	-22.13	1.50	1.90
5	A	1	AGS	PG-S1G	-22.00	1.50	1.90
2	M	4013	SO4	O1-S	4.80	1.62	1.47
2	K	4021	SO4	O1-S	4.70	1.62	1.47
2	C	4012	SO4	O1-S	4.68	1.62	1.47
2	B	4010	SO4	O1-S	4.66	1.62	1.47
2	M	4014	SO4	O1-S	4.66	1.62	1.47
2	N	4015	SO4	O1-S	4.64	1.62	1.47
2	C	4011	SO4	O1-S	4.63	1.62	1.47
2	H	4018	SO4	O1-S	4.62	1.62	1.47
2	E	4006	SO4	O1-S	4.62	1.62	1.47
2	J	4019	SO4	O1-S	4.62	1.62	1.47
2	J	4020	SO4	O1-S	4.62	1.62	1.47
2	H	4017	SO4	O1-S	4.61	1.62	1.47
2	B	4009	SO4	O1-S	4.60	1.62	1.47
2	A	4008	SO4	O1-S	4.60	1.62	1.47
2	N	4016	SO4	O1-S	4.60	1.62	1.47
2	A	4001	SO4	O1-S	4.59	1.62	1.47
2	G	4002	SO4	O1-S	4.58	1.62	1.47
2	L	4003	SO4	O1-S	4.56	1.61	1.47
2	K	4022	SO4	O1-S	4.55	1.61	1.47
2	A	4007	SO4	O1-S	4.49	1.61	1.47
2	F	4004	SO4	O1-S	4.36	1.61	1.47
2	E	4005	SO4	O1-S	4.28	1.61	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	AGS	PG-O3G	-4.16	1.47	1.56
5	D	551	AGS	PG-O3G	-3.98	1.48	1.56
5	E	1	AGS	PG-O3G	-3.96	1.48	1.56
5	J	1	AGS	PG-O3G	-3.91	1.48	1.56
5	C	1	AGS	PG-O3G	-3.90	1.48	1.56
5	B	1	AGS	PG-O3G	-3.89	1.48	1.56
5	N	1	AGS	PG-O3G	-3.89	1.48	1.56
5	K	1	AGS	PG-O3G	-3.88	1.48	1.56
5	M	1	AGS	PG-O3G	-3.78	1.48	1.56
5	I	1	AGS	PG-O3G	-3.78	1.48	1.56
5	G	1	AGS	PG-O3G	-3.69	1.48	1.56
5	A	1	AGS	PG-O3G	-3.66	1.48	1.56
5	H	1	AGS	PG-O3G	-3.61	1.49	1.56
5	L	1	AGS	PG-O3G	-3.39	1.49	1.56
5	J	1	AGS	PG-O2G	-3.35	1.49	1.56
5	M	1	AGS	PG-O2G	-3.24	1.49	1.56
5	G	1	AGS	PG-O2G	-3.20	1.49	1.56
5	N	1	AGS	PG-O2G	-3.16	1.50	1.56
5	A	1	AGS	PG-O2G	-3.05	1.50	1.56
5	I	1	AGS	PG-O2G	-3.03	1.50	1.56
5	B	1	AGS	PG-O2G	-2.99	1.50	1.56
5	L	1	AGS	PG-O2G	-2.96	1.50	1.56
5	K	1	AGS	PG-O2G	-2.82	1.50	1.56
5	C	1	AGS	PG-O2G	-2.77	1.50	1.56
5	F	1	AGS	PG-O2G	-2.76	1.50	1.56
5	D	551	AGS	PG-O2G	-2.75	1.50	1.56
5	H	1	AGS	PG-O2G	-2.73	1.50	1.56
5	K	1	AGS	O4'-C1'	2.67	1.45	1.41
5	A	1	AGS	PA-O3A	2.49	1.64	1.59
5	E	1	AGS	PG-O2G	-2.42	1.51	1.56
5	B	1	AGS	PB-O3A	2.24	1.63	1.59
5	D	551	AGS	C2'-C1'	-2.22	1.50	1.53
5	E	1	AGS	PG-O3B	2.13	1.62	1.60
5	H	1	AGS	PA-O3A	2.10	1.63	1.59
5	G	1	AGS	C8-N9	2.08	1.39	1.36
5	L	1	AGS	PB-O3A	2.07	1.63	1.59
5	L	1	AGS	C2'-C1'	-2.06	1.50	1.53
5	N	1	AGS	PG-O3B	2.02	1.62	1.60
5	B	1	AGS	PA-O3A	2.01	1.63	1.59

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	AGS	O3B-PG-S1G	-21.71	104.90	114.53
5	J	1	AGS	O3B-PG-S1G	-21.16	105.14	114.53
5	G	1	AGS	O3B-PG-S1G	-20.92	105.25	114.53
5	D	551	AGS	O3B-PG-S1G	-20.68	105.35	114.53
5	C	1	AGS	O3B-PG-S1G	-20.08	105.62	114.53
5	A	1	AGS	O3B-PG-S1G	-19.50	105.88	114.53
5	E	1	AGS	O3B-PG-S1G	-19.45	105.90	114.53
5	I	1	AGS	O3B-PG-S1G	-19.35	105.94	114.53
5	F	1	AGS	O3B-PG-S1G	-18.78	106.20	114.53
5	M	1	AGS	O3B-PG-S1G	-17.78	106.64	114.53
5	B	1	AGS	O3B-PG-S1G	-17.78	106.64	114.53
5	K	1	AGS	O3B-PG-S1G	-17.46	106.78	114.53
5	N	1	AGS	O3B-PG-S1G	-17.46	106.78	114.53
5	L	1	AGS	O3B-PG-S1G	-16.74	107.10	114.53
5	E	1	AGS	O4'-C1'-N9	7.75	115.64	108.44
5	B	1	AGS	O4'-C1'-N9	7.23	115.17	108.44
5	C	1	AGS	O4'-C1'-N9	6.71	114.68	108.44
5	H	1	AGS	O4'-C1'-N9	6.62	114.59	108.44
5	L	1	AGS	O4'-C1'-N9	6.54	114.53	108.44
5	I	1	AGS	O4'-C1'-N9	6.34	114.34	108.44
5	D	551	AGS	O4'-C1'-N9	6.28	114.28	108.44
5	G	1	AGS	O4'-C1'-N9	6.21	114.22	108.44
5	M	1	AGS	O4'-C1'-N9	6.16	114.17	108.44
5	K	1	AGS	O4'-C1'-N9	6.07	114.09	108.44
5	F	1	AGS	O4'-C1'-N9	5.56	113.61	108.44
5	A	1	AGS	O4'-C1'-N9	5.13	113.21	108.44
5	N	1	AGS	O4'-C1'-N9	5.02	113.11	108.44
5	J	1	AGS	O4'-C1'-N9	4.97	113.06	108.44
5	H	1	AGS	O2G-PG-S1G	4.75	117.73	112.73
5	A	1	AGS	O2G-PG-S1G	4.67	117.65	112.73
5	B	1	AGS	O2G-PG-S1G	4.53	117.50	112.73
5	C	1	AGS	O2G-PG-S1G	4.50	117.47	112.73
5	I	1	AGS	O2G-PG-S1G	4.39	117.35	112.73
5	E	1	AGS	O2G-PG-S1G	4.30	117.25	112.73
5	G	1	AGS	O2G-PG-S1G	4.09	117.04	112.73
5	D	551	AGS	O2G-PG-S1G	4.08	117.03	112.73
5	F	1	AGS	O2G-PG-S1G	4.06	117.00	112.73
5	J	1	AGS	O2G-PG-S1G	3.99	116.93	112.73
5	N	1	AGS	O2G-PG-S1G	3.83	116.76	112.73
5	L	1	AGS	O2G-PG-S1G	3.81	116.75	112.73
5	K	1	AGS	O2G-PG-S1G	3.76	116.69	112.73
5	M	1	AGS	O2G-PG-S1G	3.54	116.45	112.73
5	K	1	AGS	C8-N9-C4	-3.53	104.20	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1	AGS	C8-N9-C4	-3.31	104.37	106.90
5	C	1	AGS	C8-N9-C4	-3.15	104.50	106.90
5	H	1	AGS	C8-N9-C4	-2.96	104.64	106.90
5	F	1	AGS	C8-N9-C4	-2.93	104.66	106.90
5	M	1	AGS	C8-N9-C4	-2.91	104.68	106.90
5	I	1	AGS	C8-N9-C4	-2.90	104.68	106.90
5	N	1	AGS	C8-N9-C4	-2.90	104.69	106.90
5	E	1	AGS	C8-N9-C4	-2.89	104.69	106.90
5	M	1	AGS	C8-N9-C1'	2.84	131.99	126.38
5	B	1	AGS	C8-N9-C4	-2.82	104.74	106.90
5	A	1	AGS	C8-N9-C4	-2.82	104.75	106.90
5	G	1	AGS	C8-N9-C4	-2.71	104.83	106.90
5	A	1	AGS	C8-N9-C1'	2.67	131.64	126.38
5	J	1	AGS	O3A-PB-O3B	2.63	107.01	101.66
5	H	1	AGS	C8-N9-C1'	2.59	131.49	126.38
5	K	1	AGS	O4'-C1'-C2'	-2.56	102.84	106.77
5	C	1	AGS	C8-N9-C1'	2.56	131.43	126.38
5	L	1	AGS	C8-N9-C1'	2.55	131.41	126.38
5	L	1	AGS	C8-N9-C4	-2.55	104.95	106.90
5	G	1	AGS	C8-N9-C1'	2.53	131.36	126.38
5	K	1	AGS	O3A-PB-O3B	2.50	106.76	101.66
5	B	1	AGS	C8-N9-C1'	2.50	131.31	126.38
5	I	1	AGS	C8-N9-C1'	2.49	131.29	126.38
5	E	1	AGS	C8-N9-C1'	2.48	131.26	126.38
5	K	1	AGS	C8-N9-C1'	2.45	131.21	126.38
5	J	1	AGS	O4'-C1'-C2'	-2.44	103.04	106.77
5	N	1	AGS	C8-N9-C1'	2.42	131.16	126.38
5	D	551	AGS	C8-N9-C1'	2.42	131.15	126.38
5	D	551	AGS	C8-N9-C4	-2.38	105.08	106.90
5	G	1	AGS	O4'-C1'-C2'	-2.38	103.13	106.77
5	F	1	AGS	C8-N9-C1'	2.33	130.98	126.38
5	A	1	AGS	O4'-C1'-C2'	-2.31	103.23	106.77
5	N	1	AGS	O4'-C1'-C2'	-2.15	103.48	106.77
5	J	1	AGS	C8-N9-C1'	2.14	130.61	126.38
5	G	1	AGS	O3A-PB-O3B	2.05	105.84	101.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	525/547 (95%)	0.68	64 (12%) 5 4	28, 64, 121, 132	0
1	B	525/547 (95%)	1.22	120 (22%) 1 2	24, 59, 149, 159	0
1	C	525/547 (95%)	1.12	111 (21%) 1 2	29, 71, 141, 152	0
1	D	525/547 (95%)	0.46	28 (5%) 25 25	25, 48, 99, 115	0
1	E	525/547 (95%)	0.92	88 (16%) 2 2	23, 55, 134, 145	0
1	F	525/547 (95%)	1.23	115 (21%) 1 2	27, 66, 150, 159	0
1	G	525/547 (95%)	0.55	40 (7%) 14 13	26, 50, 113, 126	0
1	H	525/547 (95%)	0.59	50 (9%) 8 8	26, 56, 118, 130	0
1	I	525/547 (95%)	0.89	70 (13%) 4 4	31, 69, 132, 143	0
1	J	525/547 (95%)	0.96	81 (15%) 3 3	31, 73, 138, 146	0
1	K	525/547 (95%)	1.39	135 (25%) 1 1	31, 78, 151, 159	0
1	L	525/547 (95%)	0.88	80 (15%) 3 3	29, 66, 136, 149	0
1	M	525/547 (95%)	1.31	131 (24%) 1 1	30, 77, 152, 160	0
1	N	525/547 (95%)	0.68	53 (10%) 7 7	28, 65, 118, 129	0
All	All	7350/7658 (95%)	0.92	1166 (15%) 3 3	23, 60, 140, 160	0

All (1166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	309	LEU	12.4
1	C	349	ILE	12.2
1	F	233	MET	12.1
1	K	271	VAL	11.2
1	F	314	LEU	10.9
1	K	349	ILE	10.8
1	M	270	ILE	10.8
1	K	237	LEU	10.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	233	MET	10.5
1	F	240	VAL	10.5
1	K	309	LEU	10.3
1	E	309	LEU	10.2
1	M	272	LYS	10.1
1	M	353	ILE	10.1
1	J	271	VAL	10.1
1	K	305	ILE	10.0
1	K	236	VAL	10.0
1	F	259	LEU	10.0
1	B	356	ALA	9.7
1	M	271	VAL	9.6
1	F	353	ILE	9.6
1	K	270	ILE	9.6
1	C	270	ILE	9.5
1	J	356	ALA	9.5
1	B	353	ILE	9.4
1	K	260	ALA	9.4
1	C	356	ALA	9.3
1	F	349	ILE	9.3
1	B	349	ILE	9.2
1	K	259	LEU	9.2
1	K	233	MET	9.1
1	M	259	LEU	9.1
1	J	270	ILE	9.1
1	M	237	LEU	9.0
1	E	356	ALA	8.9
1	B	233	MET	8.8
1	E	353	ILE	8.6
1	J	309	LEU	8.5
1	E	271	VAL	8.5
1	M	314	LEU	8.5
1	N	349	ILE	8.4
1	M	223	ALA	8.4
1	C	353	ILE	8.4
1	I	270	ILE	8.3
1	J	233	MET	8.2
1	M	240	VAL	8.1
1	B	301	ILE	8.1
1	M	349	ILE	8.1
1	L	266	THR	8.0
1	J	268	ARG	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	271	VAL	8.0
1	K	360	TYR	7.9
1	K	268	ARG	7.9
1	M	309	LEU	7.9
1	M	221	LEU	7.8
1	B	309	LEU	7.7
1	B	230	ILE	7.7
1	J	349	ILE	7.7
1	E	223	ALA	7.6
1	K	264	VAL	7.6
1	K	356	ALA	7.5
1	F	270	ILE	7.5
1	M	357	THR	7.5
1	K	203	TYR	7.4
1	B	281	PHE	7.3
1	D	271	VAL	7.3
1	M	273	VAL	7.2
1	L	305	ILE	7.2
1	M	268	ARG	7.2
1	J	357	THR	7.1
1	J	269	GLY	7.1
1	K	353	ILE	7.1
1	F	360	TYR	7.0
1	K	240	VAL	7.0
1	K	231	ARG	7.0
1	K	267	MET	7.0
1	A	353	ILE	7.0
1	L	231	ARG	6.9
1	M	356	ALA	6.9
1	L	270	ILE	6.9
1	B	264	VAL	6.9
1	L	271	VAL	6.8
1	C	274	ALA	6.8
1	F	342	ILE	6.8
1	M	267	MET	6.8
1	C	268	ARG	6.8
1	K	340	ALA	6.8
1	M	266	THR	6.7
1	K	227	ILE	6.7
1	B	227	ILE	6.6
1	E	233	MET	6.6
1	L	264	VAL	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	239	ALA	6.6
1	E	234	LEU	6.5
1	K	230	ILE	6.5
1	F	237	LEU	6.4
1	A	270	ILE	6.4
1	I	305	ILE	6.4
1	E	230	ILE	6.4
1	C	233	MET	6.4
1	B	357	THR	6.3
1	F	272	LYS	6.3
1	F	203	TYR	6.3
1	B	258	ALA	6.3
1	E	270	ILE	6.3
1	A	356	ALA	6.3
1	M	358	SER	6.2
1	I	268	ARG	6.2
1	J	526	LYS	6.2
1	F	230	ILE	6.2
1	M	251	ALA	6.2
1	C	263	VAL	6.2
1	H	309	LEU	6.2
1	J	264	VAL	6.2
1	K	265	ASN	6.2
1	B	268	ARG	6.2
1	L	383	ALA	6.2
1	I	349	ILE	6.2
1	B	365	LEU	6.1
1	J	44	PHE	6.1
1	F	219	PHE	6.1
1	B	257	GLU	6.0
1	N	230	ILE	6.0
1	M	203	TYR	6.0
1	E	349	ILE	5.9
1	F	268	ARG	5.9
1	F	227	ILE	5.9
1	N	270	ILE	5.8
1	B	271	VAL	5.8
1	B	229	ASN	5.8
1	I	271	VAL	5.7
1	C	259	LEU	5.7
1	K	234	LEU	5.7
1	K	228	SER	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	264	VAL	5.7
1	F	231	ARG	5.6
1	I	353	ILE	5.6
1	J	353	ILE	5.6
1	C	244	GLY	5.6
1	I	265	ASN	5.6
1	C	369	VAL	5.6
1	K	223	ALA	5.6
1	F	336	VAL	5.6
1	K	241	ALA	5.6
1	M	244	GLY	5.6
1	M	336	VAL	5.6
1	B	259	LEU	5.6
1	J	266	THR	5.6
1	F	267	MET	5.5
1	E	203	TYR	5.5
1	C	249	ILE	5.5
1	J	317	LEU	5.5
1	M	305	ILE	5.5
1	C	256	GLY	5.5
1	I	264	VAL	5.5
1	M	263	VAL	5.5
1	F	305	ILE	5.5
1	L	230	ILE	5.5
1	J	237	LEU	5.5
1	J	305	ILE	5.4
1	N	263	VAL	5.4
1	F	222	LEU	5.4
1	L	227	ILE	5.4
1	M	342	ILE	5.4
1	B	203	TYR	5.4
1	K	232	GLU	5.4
1	F	357	THR	5.4
1	B	286	LYS	5.4
1	C	230	ILE	5.3
1	I	230	ILE	5.3
1	E	268	ARG	5.3
1	I	356	ALA	5.3
1	H	243	ALA	5.3
1	B	231	ARG	5.3
1	M	262	LEU	5.3
1	C	237	LEU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	236	VAL	5.3
1	F	271	VAL	5.3
1	M	249	ILE	5.3
1	I	234	LEU	5.2
1	B	526	LYS	5.2
1	K	273	VAL	5.2
1	F	273	VAL	5.2
1	I	352	GLN	5.1
1	I	526	LYS	5.1
1	I	309	LEU	5.1
1	B	240	VAL	5.1
1	L	268	ARG	5.1
1	K	219	PHE	5.1
1	I	203	TYR	5.1
1	C	357	THR	5.1
1	M	317	LEU	5.1
1	B	250	ILE	5.1
1	H	526	LYS	5.1
1	B	307	MET	5.0
1	G	230	ILE	5.0
1	K	306	GLY	5.0
1	N	264	VAL	5.0
1	A	349	ILE	5.0
1	M	219	PHE	5.0
1	K	275	ALA	5.0
1	L	267	MET	5.0
1	K	269	GLY	5.0
1	E	357	THR	5.0
1	C	372	LEU	4.9
1	J	263	VAL	4.9
1	E	305	ILE	4.9
1	F	317	LEU	4.9
1	J	262	LEU	4.9
1	B	355	GLU	4.9
1	F	44	PHE	4.9
1	L	309	LEU	4.9
1	L	275	ALA	4.9
1	C	44	PHE	4.9
1	E	300	VAL	4.9
1	G	259	LEU	4.9
1	M	186	GLU	4.9
1	J	231	ARG	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	260	ALA	4.9
1	F	221	LEU	4.8
1	L	203	TYR	4.8
1	G	44	PHE	4.8
1	K	44	PHE	4.8
1	H	233	MET	4.8
1	A	263	VAL	4.8
1	M	365	LEU	4.8
1	B	273	VAL	4.8
1	B	305	ILE	4.8
1	H	234	LEU	4.8
1	M	265	ASN	4.8
1	C	360	TYR	4.8
1	B	342	ILE	4.8
1	L	234	LEU	4.8
1	A	44	PHE	4.8
1	J	229	ASN	4.8
1	C	273	VAL	4.7
1	H	356	ALA	4.7
1	C	261	THR	4.7
1	C	333	ILE	4.7
1	D	270	ILE	4.7
1	G	271	VAL	4.7
1	B	251	ALA	4.7
1	C	292	ILE	4.7
1	C	332	ILE	4.7
1	L	258	ALA	4.7
1	B	262	LEU	4.7
1	K	204	PHE	4.7
1	M	230	ILE	4.7
1	G	383	ALA	4.7
1	B	306	GLY	4.7
1	C	264	VAL	4.7
1	C	295	LEU	4.7
1	F	264	VAL	4.7
1	F	255	GLU	4.6
1	I	243	ALA	4.6
1	I	258	ALA	4.6
1	F	355	GLU	4.6
1	H	44	PHE	4.6
1	I	233	MET	4.6
1	L	526	LYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	351	GLN	4.6
1	M	204	PHE	4.6
1	C	342	ILE	4.6
1	B	300	VAL	4.6
1	J	256	GLY	4.6
1	J	219	PHE	4.6
1	G	270	ILE	4.6
1	E	312	ALA	4.6
1	E	355	GLU	4.6
1	K	256	GLY	4.6
1	B	223	ALA	4.6
1	K	383	ALA	4.6
1	M	335	GLY	4.6
1	F	234	LEU	4.6
1	K	372	LEU	4.6
1	B	44	PHE	4.6
1	M	195	PHE	4.6
1	L	244	GLY	4.5
1	F	249	ILE	4.5
1	L	259	LEU	4.5
1	L	233	MET	4.5
1	E	266	THR	4.5
1	F	263	VAL	4.5
1	C	272	LYS	4.5
1	G	233	MET	4.5
1	F	245	LYS	4.5
1	K	281	PHE	4.5
1	C	231	ARG	4.5
1	H	305	ILE	4.5
1	C	266	THR	4.5
1	F	365	LEU	4.5
1	I	355	GLU	4.5
1	K	160	LYS	4.5
1	M	258	ALA	4.4
1	D	230	ILE	4.4
1	I	272	LYS	4.4
1	J	358	SER	4.4
1	E	351	GLN	4.4
1	L	269	GLY	4.4
1	E	265	ASN	4.4
1	B	266	THR	4.4
1	E	301	ILE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	237	LEU	4.4
1	G	258	ALA	4.4
1	K	346	VAL	4.4
1	C	181	THR	4.4
1	H	357	THR	4.4
1	F	389	MET	4.4
1	F	241	ALA	4.4
1	B	351	GLN	4.4
1	I	231	ARG	4.3
1	M	236	VAL	4.3
1	B	224	ASP	4.3
1	B	282	GLY	4.3
1	K	272	LYS	4.3
1	J	333	ILE	4.3
1	C	365	LEU	4.3
1	D	44	PHE	4.3
1	B	243	ALA	4.3
1	B	237	LEU	4.3
1	K	247	LEU	4.3
1	A	271	VAL	4.3
1	F	306	GLY	4.3
1	F	346	VAL	4.3
1	K	357	THR	4.3
1	E	231	ARG	4.3
1	H	268	ARG	4.3
1	B	295	LEU	4.3
1	J	265	ASN	4.3
1	J	204	PHE	4.3
1	B	180	GLY	4.3
1	M	218	PRO	4.3
1	L	255	GLU	4.2
1	L	185	ASP	4.2
1	B	289	LEU	4.2
1	D	526	LYS	4.2
1	E	272	LYS	4.2
1	F	300	VAL	4.2
1	A	182	GLY	4.2
1	M	340	ALA	4.2
1	F	261	THR	4.2
1	B	221	LEU	4.2
1	I	384	ALA	4.2
1	M	351	GLN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	270	ILE	4.2
1	C	340	ALA	4.2
1	H	229	ASN	4.2
1	E	44	PHE	4.2
1	F	396	VAL	4.2
1	K	299	THR	4.1
1	G	229	ASN	4.1
1	K	224	ASP	4.1
1	M	238	GLU	4.1
1	E	242	LYS	4.1
1	L	44	PHE	4.1
1	M	222	LEU	4.1
1	F	369	VAL	4.1
1	I	267	MET	4.1
1	L	314	LEU	4.1
1	F	243	ALA	4.1
1	K	222	LEU	4.1
1	K	365	LEU	4.1
1	J	360	TYR	4.1
1	K	332	ILE	4.1
1	K	334	ASP	4.0
1	L	229	ASN	4.0
1	K	283	ASP	4.0
1	B	354	GLU	4.0
1	E	295	LEU	4.0
1	H	353	ILE	4.0
1	G	265	ASN	4.0
1	M	161	LEU	4.0
1	K	358	SER	4.0
1	K	369	VAL	4.0
1	M	355	GLU	4.0
1	H	383	ALA	4.0
1	N	526	LYS	4.0
1	E	263	VAL	4.0
1	E	273	VAL	4.0
1	F	315	GLU	4.0
1	C	350	ARG	4.0
1	C	526	LYS	4.0
1	I	44	PHE	4.0
1	E	346	VAL	3.9
1	N	256	GLY	3.9
1	M	295	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	186	GLU	3.9
1	C	362	ARG	3.9
1	K	250	ILE	3.9
1	E	360	TYR	3.9
1	K	263	VAL	3.9
1	B	234	LEU	3.9
1	F	242	LYS	3.9
1	G	267	MET	3.9
1	M	250	ILE	3.9
1	C	309	LEU	3.9
1	L	224	ASP	3.9
1	C	161	LEU	3.9
1	L	317	LEU	3.9
1	K	355	GLU	3.9
1	M	261	THR	3.9
1	C	336	VAL	3.8
1	B	383	ALA	3.8
1	F	258	ALA	3.8
1	F	260	ALA	3.8
1	B	372	LEU	3.8
1	G	262	LEU	3.8
1	K	304	GLU	3.8
1	K	311	LYS	3.8
1	B	270	ILE	3.8
1	A	257	GLU	3.8
1	F	186	GLU	3.8
1	M	384	ALA	3.8
1	M	526	LYS	3.8
1	F	248	LEU	3.8
1	L	247	LEU	3.8
1	F	337	GLY	3.8
1	M	350	ARG	3.8
1	B	265	ASN	3.8
1	L	228	SER	3.8
1	F	356	ALA	3.8
1	N	44	PHE	3.8
1	F	381	VAL	3.8
1	J	383	ALA	3.8
1	L	356	ALA	3.8
1	N	203	TYR	3.8
1	C	355	GLU	3.8
1	F	266	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	266	THR	3.8
1	M	231	ARG	3.8
1	E	264	VAL	3.8
1	I	360	TYR	3.8
1	M	180	GLY	3.8
1	F	214	GLU	3.7
1	M	224	ASP	3.7
1	F	244	GLY	3.7
1	F	269	GLY	3.7
1	B	293	ALA	3.7
1	E	383	ALA	3.7
1	B	311	LYS	3.7
1	M	168	LYS	3.7
1	B	317	LEU	3.7
1	B	191	GLU	3.7
1	K	312	ALA	3.7
1	K	331	THR	3.7
1	A	187	LEU	3.7
1	F	180	GLY	3.7
1	B	249	ILE	3.7
1	C	304	GLU	3.7
1	D	281	PHE	3.7
1	K	335	GLY	3.7
1	J	319	GLN	3.7
1	K	301	ILE	3.7
1	E	247	LEU	3.7
1	K	351	GLN	3.7
1	C	334	ASP	3.7
1	F	228	SER	3.7
1	M	333	ILE	3.7
1	L	219	PHE	3.7
1	M	347	ALA	3.6
1	B	269	GLY	3.6
1	C	229	ASN	3.6
1	E	354	GLU	3.6
1	F	178	GLU	3.6
1	B	332	ILE	3.6
1	G	325	ILE	3.6
1	M	346	VAL	3.6
1	K	362	ARG	3.6
1	M	188	ASP	3.6
1	K	307	MET	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	342	ILE	3.6
1	F	332	ILE	3.6
1	B	222	LEU	3.6
1	H	355	GLU	3.6
1	F	358	SER	3.6
1	K	350	ARG	3.6
1	K	274	ALA	3.6
1	B	209	GLU	3.6
1	I	263	VAL	3.6
1	K	310	GLU	3.6
1	C	284	ARG	3.6
1	B	358	SER	3.6
1	B	188	ASP	3.6
1	C	346	VAL	3.6
1	M	183	LEU	3.6
1	D	266	THR	3.6
1	J	203	TYR	3.6
1	M	274	ALA	3.6
1	C	265	ASN	3.5
1	F	236	VAL	3.5
1	E	384	ALA	3.5
1	K	242	LYS	3.5
1	M	269	GLY	3.5
1	B	363	GLU	3.5
1	J	281	PHE	3.5
1	J	248	LEU	3.5
1	C	347	ALA	3.5
1	J	355	GLU	3.5
1	K	345	ARG	3.5
1	M	286	LYS	3.5
1	A	276	VAL	3.5
1	J	273	VAL	3.5
1	K	297	GLY	3.5
1	C	351	GLN	3.5
1	I	184	GLN	3.5
1	M	343	GLN	3.5
1	B	254	VAL	3.5
1	G	264	VAL	3.5
1	J	381	VAL	3.5
1	L	262	LEU	3.5
1	C	203	TYR	3.5
1	A	357	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	300	VAL	3.5
1	B	244	GLY	3.4
1	C	204	PHE	3.4
1	B	284	ARG	3.4
1	M	220	ILE	3.4
1	I	363	GLU	3.4
1	K	188	ASP	3.4
1	M	217	SER	3.4
1	A	260	ALA	3.4
1	J	260	ALA	3.4
1	M	44	PHE	3.4
1	J	365	LEU	3.4
1	K	288	MET	3.4
1	M	160	LYS	3.4
1	F	351	GLN	3.4
1	E	292	ILE	3.4
1	A	358	SER	3.4
1	F	340	ALA	3.4
1	I	237	LEU	3.4
1	B	346	VAL	3.4
1	B	241	ALA	3.4
1	E	274	ALA	3.4
1	B	219	PHE	3.4
1	B	304	GLU	3.3
1	C	248	LEU	3.3
1	B	225	LYS	3.3
1	F	265	ASN	3.3
1	D	264	VAL	3.3
1	L	381	VAL	3.3
1	F	224	ASP	3.3
1	F	256	GLY	3.3
1	K	352	GLN	3.3
1	C	247	LEU	3.3
1	I	259	LEU	3.3
1	J	342	ILE	3.3
1	B	360	TYR	3.3
1	F	225	LYS	3.3
1	A	384	ALA	3.3
1	B	274	ALA	3.3
1	C	223	ALA	3.3
1	C	219	PHE	3.3
1	A	231	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	181	THR	3.3
1	L	272	LYS	3.3
1	L	304	GLU	3.3
1	K	258	ALA	3.3
1	E	304	GLU	3.3
1	H	346	VAL	3.3
1	G	306	GLY	3.3
1	N	281	PHE	3.3
1	B	215	LEU	3.3
1	L	161	LEU	3.3
1	A	268	ARG	3.3
1	A	304	GLU	3.3
1	K	386	GLU	3.3
1	J	250	ILE	3.3
1	F	372	LEU	3.3
1	J	221	LEU	3.3
1	A	361	ASP	3.3
1	C	220	ILE	3.2
1	I	351	GLN	3.2
1	A	203	TYR	3.2
1	H	360	TYR	3.2
1	I	357	THR	3.2
1	K	181	THR	3.2
1	C	267	MET	3.2
1	M	319	GLN	3.2
1	D	268	ARG	3.2
1	L	382	GLY	3.2
1	K	243	ALA	3.2
1	M	320	ALA	3.2
1	E	229	ASN	3.2
1	C	317	LEU	3.2
1	K	221	LEU	3.2
1	J	257	GLU	3.2
1	L	239	ALA	3.2
1	N	258	ALA	3.2
1	F	181	THR	3.2
1	C	281	PHE	3.2
1	G	268	ARG	3.2
1	L	200	LEU	3.2
1	J	361	ASP	3.2
1	E	220	ILE	3.2
1	H	349	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	269	GLY	3.2
1	L	222	LEU	3.2
1	N	365	LEU	3.2
1	E	255	GLU	3.2
1	F	232	GLU	3.2
1	I	336	VAL	3.2
1	L	240	VAL	3.2
1	J	362	ARG	3.2
1	D	325	ILE	3.2
1	J	184	GLN	3.2
1	N	231	ARG	3.2
1	C	337	GLY	3.1
1	E	526	LYS	3.1
1	M	304	GLU	3.1
1	K	302	SER	3.1
1	I	369	VAL	3.1
1	L	273	VAL	3.1
1	B	298	GLY	3.1
1	E	382	GLY	3.1
1	L	353	ILE	3.1
1	M	360	TYR	3.1
1	B	248	LEU	3.1
1	F	361	ASP	3.1
1	M	383	ALA	3.1
1	A	381	VAL	3.1
1	C	300	VAL	3.1
1	C	322	ARG	3.1
1	D	231	ARG	3.1
1	J	267	MET	3.1
1	K	276	VAL	3.1
1	N	325	ILE	3.1
1	K	361	ASP	3.1
1	E	237	LEU	3.1
1	K	191	GLU	3.1
1	N	363	GLU	3.1
1	K	253	ASP	3.1
1	L	249	ILE	3.1
1	E	358	SER	3.1
1	I	211	GLY	3.1
1	J	234	LEU	3.1
1	A	265	ASN	3.1
1	H	286	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	304	GLU	3.1
1	N	259	LEU	3.1
1	E	257	GLU	3.1
1	F	354	GLU	3.1
1	I	245	LYS	3.1
1	M	323	VAL	3.1
1	C	180	GLY	3.1
1	A	295	LEU	3.0
1	F	161	LEU	3.0
1	L	307	MET	3.0
1	M	234	LEU	3.0
1	J	367	GLU	3.0
1	L	311	LYS	3.0
1	N	254	VAL	3.0
1	D	305	ILE	3.0
1	L	333	ILE	3.0
1	J	303	GLU	3.0
1	M	307	MET	3.0
1	A	183	LEU	3.0
1	B	247	LEU	3.0
1	D	323	VAL	3.0
1	B	187	LEU	3.0
1	G	182	GLY	3.0
1	A	388	GLU	3.0
1	A	281	PHE	3.0
1	K	342	ILE	3.0
1	F	347	ALA	3.0
1	H	314	LEU	3.0
1	H	269	GLY	3.0
1	K	239	ALA	3.0
1	M	235	PRO	3.0
1	J	272	LYS	3.0
1	M	308	GLU	3.0
1	E	249	ILE	3.0
1	E	284	ARG	3.0
1	G	234	LEU	3.0
1	H	259	LEU	3.0
1	I	334	ASP	3.0
1	D	236	VAL	3.0
1	A	261	THR	3.0
1	L	349	ILE	3.0
1	M	184	GLN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	251	ALA	3.0
1	B	183	LEU	3.0
1	L	237	LEU	3.0
1	N	360	TYR	2.9
1	B	267	MET	2.9
1	H	265	ASN	2.9
1	E	250	ILE	2.9
1	C	221	LEU	2.9
1	H	361	ASP	2.9
1	L	184	GLN	2.9
1	B	308	GLU	2.9
1	G	257	GLU	2.9
1	K	526	LYS	2.9
1	H	300	VAL	2.9
1	I	332	ILE	2.9
1	B	525	PRO	2.9
1	F	215	LEU	2.9
1	K	255	GLU	2.9
1	G	231	ARG	2.9
1	B	260	ALA	2.9
1	F	384	ALA	2.9
1	K	152	ALA	2.9
1	N	351	GLN	2.9
1	A	209	GLU	2.9
1	H	325	ILE	2.9
1	K	317	LEU	2.9
1	H	284	ARG	2.9
1	N	284	ARG	2.9
1	B	302	SER	2.9
1	G	266	THR	2.9
1	K	257	GLU	2.9
1	M	369	VAL	2.9
1	N	275	ALA	2.9
1	A	273	VAL	2.9
1	B	336	VAL	2.9
1	M	254	VAL	2.9
1	D	262	LEU	2.9
1	K	248	LEU	2.9
1	B	181	THR	2.9
1	L	206	ASN	2.9
1	B	350	ARG	2.8
1	H	242	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	252	GLU	2.8
1	H	351	GLN	2.8
1	A	259	LEU	2.8
1	F	295	LEU	2.8
1	K	295	LEU	2.8
1	M	248	LEU	2.8
1	M	334	ASP	2.8
1	I	310	GLU	2.8
1	M	322	ARG	2.8
1	C	319	GLN	2.8
1	F	352	GLN	2.8
1	I	340	ALA	2.8
1	I	383	ALA	2.8
1	E	240	VAL	2.8
1	C	286	LYS	2.8
1	A	250	ILE	2.8
1	J	288	MET	2.8
1	E	345	ARG	2.8
1	I	257	GLU	2.8
1	L	324	VAL	2.8
1	B	314	LEU	2.8
1	C	222	LEU	2.8
1	G	221	LEU	2.8
1	J	280	GLY	2.8
1	M	299	THR	2.8
1	K	325	ILE	2.8
1	C	363	GLU	2.8
1	B	352	GLN	2.8
1	C	352	GLN	2.8
1	A	382	GLY	2.8
1	J	181	THR	2.8
1	I	314	LEU	2.8
1	K	215	LEU	2.8
1	K	308	GLU	2.8
1	A	188	ASP	2.8
1	C	358	SER	2.8
1	C	258	ALA	2.8
1	J	223	ALA	2.8
1	N	356	ALA	2.8
1	F	350	ARG	2.8
1	M	354	GLU	2.8
1	B	381	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	376	VAL	2.7
1	D	229	ASN	2.7
1	C	269	GLY	2.7
1	E	267	MET	2.7
1	M	247	LEU	2.7
1	D	257	GLU	2.7
1	F	238	GLU	2.7
1	A	181	THR	2.7
1	B	348	GLN	2.7
1	N	369	VAL	2.7
1	C	301	ILE	2.7
1	L	325	ILE	2.7
1	L	332	ILE	2.7
1	C	212	ALA	2.7
1	F	343	GLN	2.7
1	L	302	SER	2.7
1	C	240	VAL	2.7
1	D	273	VAL	2.7
1	N	134	LEU	2.7
1	K	341	ALA	2.7
1	J	240	VAL	2.7
1	K	381	VAL	2.7
1	F	251	ALA	2.7
1	M	301	ILE	2.7
1	B	261	THR	2.7
1	M	279	PRO	2.7
1	A	526	LYS	2.7
1	C	242	LYS	2.7
1	E	339	GLU	2.7
1	G	311	LYS	2.7
1	J	354	GLU	2.7
1	K	286	LYS	2.7
1	L	201	SER	2.7
1	M	252	GLU	2.7
1	I	256	GLY	2.7
1	E	184	GLN	2.7
1	G	314	LEU	2.7
1	C	186	GLU	2.6
1	F	155	ASP	2.6
1	F	250	ILE	2.6
1	B	322	ARG	2.6
1	A	242	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	209	GLU	2.6
1	M	315	GLU	2.6
1	E	341	ALA	2.6
1	A	284	ARG	2.6
1	C	325	ILE	2.6
1	A	363	GLU	2.6
1	F	339	GLU	2.6
1	L	310	GLU	2.6
1	A	365	LEU	2.6
1	C	378	VAL	2.6
1	M	300	VAL	2.6
1	L	284	ARG	2.6
1	B	275	ALA	2.6
1	B	280	GLY	2.6
1	J	261	THR	2.6
1	N	357	THR	2.6
1	K	245	LYS	2.6
1	N	354	GLU	2.6
1	K	202	PRO	2.6
1	K	284	ARG	2.6
1	I	215	LEU	2.6
1	N	311	LYS	2.6
1	J	243	ALA	2.6
1	M	256	GLY	2.6
1	K	266	THR	2.6
1	A	305	ILE	2.6
1	B	292	ILE	2.6
1	K	229	ASN	2.6
1	N	283	ASP	2.6
1	F	204	PHE	2.6
1	I	204	PHE	2.6
1	G	269	GLY	2.6
1	K	139	SER	2.6
1	M	182	GLY	2.6
1	M	193	MET	2.6
1	I	372	LEU	2.6
1	N	240	VAL	2.6
1	B	361	ASP	2.6
1	A	266	THR	2.6
1	C	260	ALA	2.6
1	C	275	ALA	2.6
1	D	383	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	213	VAL	2.6
1	F	313	THR	2.6
1	N	257	GLU	2.6
1	B	205	ILE	2.5
1	N	382	GLY	2.5
1	M	389	MET	2.5
1	K	326	ASN	2.5
1	N	242	LYS	2.5
1	A	300	VAL	2.5
1	A	309	LEU	2.5
1	D	203	TYR	2.5
1	E	215	LEU	2.5
1	F	319	GLN	2.5
1	A	346	VAL	2.5
1	C	396	VAL	2.5
1	F	385	THR	2.5
1	L	336	VAL	2.5
1	M	187	LEU	2.5
1	M	215	LEU	2.5
1	J	332	ILE	2.5
1	F	321	LYS	2.5
1	E	365	LEU	2.5
1	I	276	VAL	2.5
1	D	284	ARG	2.5
1	J	363	GLU	2.5
1	H	358	SER	2.5
1	A	204	PHE	2.5
1	L	204	PHE	2.5
1	E	299	THR	2.5
1	G	309	LEU	2.5
1	K	371	LYS	2.5
1	N	161	LEU	2.5
1	J	177	VAL	2.5
1	N	77	VAL	2.5
1	B	256	GLY	2.5
1	I	358	SER	2.5
1	I	250	ILE	2.5
1	I	286	LYS	2.5
1	K	164	GLU	2.5
1	C	215	LEU	2.5
1	D	382	GLY	2.5
1	I	365	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	302	SER	2.5
1	L	236	VAL	2.5
1	M	324	VAL	2.5
1	N	273	VAL	2.5
1	D	267	MET	2.5
1	I	193	MET	2.5
1	K	321	LYS	2.5
1	C	250	ILE	2.5
1	I	249	ILE	2.5
1	A	233	MET	2.5
1	A	264	VAL	2.5
1	C	172	GLU	2.5
1	C	354	GLU	2.5
1	E	381	VAL	2.5
1	E	224	ASP	2.5
1	E	219	PHE	2.4
1	E	256	GLY	2.4
1	H	313	THR	2.4
1	C	178	GLU	2.4
1	C	341	ALA	2.4
1	G	243	ALA	2.4
1	M	191	GLU	2.4
1	M	216	GLU	2.4
1	F	322	ARG	2.4
1	N	309	LEU	2.4
1	F	288	MET	2.4
1	N	346	VAL	2.4
1	B	186	GLU	2.4
1	L	306	GLY	2.4
1	N	362	ARG	2.4
1	E	258	ALA	2.4
1	G	384	ALA	2.4
1	M	243	ALA	2.4
1	A	200	LEU	2.4
1	H	365	LEU	2.4
1	C	160	LYS	2.4
1	H	273	VAL	2.4
1	K	226	LYS	2.4
1	K	323	VAL	2.4
1	L	462	PRO	2.4
1	F	362	ARG	2.4
1	M	181	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	334	ASP	2.4
1	I	341	ALA	2.4
1	G	237	LEU	2.4
1	M	164	GLU	2.4
1	E	334	ASP	2.4
1	M	329	THR	2.4
1	F	160	LYS	2.4
1	B	333	ILE	2.4
1	H	363	GLU	2.4
1	C	85	ALA	2.4
1	K	278	ALA	2.4
1	N	350	ARG	2.4
1	D	269	GLY	2.4
1	E	318	GLY	2.4
1	M	337	GLY	2.4
1	C	214	GLU	2.4
1	M	232	GLU	2.4
1	M	330	THR	2.4
1	D	233	MET	2.4
1	B	238	GLU	2.4
1	C	391	GLU	2.4
1	B	263	VAL	2.4
1	C	201	SER	2.4
1	B	285	ARG	2.4
1	M	345	ARG	2.4
1	K	320	ALA	2.4
1	L	223	ALA	2.4
1	C	315	GLU	2.4
1	K	175	ILE	2.4
1	K	220	ILE	2.4
1	K	183	LEU	2.3
1	L	221	LEU	2.3
1	F	299	THR	2.3
1	I	346	VAL	2.3
1	E	338	GLU	2.3
1	K	401	HIS	2.3
1	N	304	GLU	2.3
1	B	400	LEU	2.3
1	E	289	LEU	2.3
1	H	317	LEU	2.3
1	J	215	LEU	2.3
1	G	283	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	271	VAL	2.3
1	F	333	ILE	2.3
1	J	302	SER	2.3
1	C	216	GLU	2.3
1	C	367	GLU	2.3
1	I	255	GLU	2.3
1	G	295	LEU	2.3
1	N	372	LEU	2.3
1	C	299	THR	2.3
1	A	184	GLN	2.3
1	C	236	VAL	2.3
1	K	213	VAL	2.3
1	B	272	LYS	2.3
1	D	258	ALA	2.3
1	F	341	ALA	2.3
1	H	315	GLU	2.3
1	B	299	THR	2.3
1	D	184	GLN	2.3
1	N	265	ASN	2.3
1	A	256	GLY	2.3
1	I	284	ARG	2.3
1	K	368	ARG	2.3
1	I	240	VAL	2.3
1	F	188	ASP	2.3
1	J	200	LEU	2.3
1	N	186	GLU	2.3
1	I	236	VAL	2.3
1	F	223	ALA	2.3
1	J	152	ALA	2.3
1	B	242	LYS	2.3
1	G	526	LYS	2.3
1	A	355	GLU	2.3
1	F	281	PHE	2.3
1	I	304	GLU	2.3
1	M	294	THR	2.3
1	A	262	LEU	2.3
1	E	287	ALA	2.2
1	E	363	GLU	2.2
1	J	275	ALA	2.2
1	E	188	ASP	2.2
1	A	301	ILE	2.2
1	A	245	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	348	GLN	2.2
1	E	222	LEU	2.2
1	J	220	ILE	2.2
1	L	372	LEU	2.2
1	M	325	ILE	2.2
1	N	317	LEU	2.2
1	A	350	ARG	2.2
1	L	315	GLU	2.2
1	L	384	ALA	2.2
1	M	278	ALA	2.2
1	B	182	GLY	2.2
1	C	305	ILE	2.2
1	G	220	ILE	2.2
1	B	239	ALA	2.2
1	C	306	GLY	2.2
1	H	335	GLY	2.2
1	I	260	ALA	2.2
1	A	286	LYS	2.2
1	C	323	VAL	2.2
1	E	369	VAL	2.2
1	F	254	VAL	2.2
1	J	323	VAL	2.2
1	L	321	LYS	2.2
1	H	184	GLN	2.2
1	J	345	ARG	2.2
1	L	351	GLN	2.2
1	N	268	ARG	2.2
1	B	390	LYS	2.2
1	D	253	ASP	2.2
1	M	363	GLU	2.2
1	E	340	ALA	2.2
1	N	383	ALA	2.2
1	K	254	VAL	2.2
1	N	266	THR	2.2
1	E	372	LEU	2.2
1	J	230	ILE	2.2
1	K	161	LEU	2.2
1	K	292	ILE	2.2
1	N	353	ILE	2.2
1	C	226	LYS	2.2
1	B	206	ASN	2.2
1	G	326	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	339	GLU	2.2
1	E	259	LEU	2.2
1	N	262	LEU	2.2
1	J	249	ILE	2.2
1	J	242	LYS	2.2
1	G	255	GLU	2.2
1	L	265	ASN	2.2
1	G	236	VAL	2.2
1	L	361	ASP	2.2
1	M	302	SER	2.2
1	F	285	ARG	2.1
1	H	281	PHE	2.1
1	A	311	LYS	2.1
1	F	311	LYS	2.1
1	F	310	GLU	2.1
1	H	332	ILE	2.1
1	I	361	ASP	2.1
1	M	275	ALA	2.1
1	E	313	THR	2.1
1	N	184	GLN	2.1
1	A	236	VAL	2.1
1	E	236	VAL	2.1
1	L	369	VAL	2.1
1	G	308	GLU	2.1
1	J	232	GLU	2.1
1	A	288	MET	2.1
1	K	249	ILE	2.1
1	K	251	ALA	2.1
1	C	311	LYS	2.1
1	G	228	SER	2.1
1	K	364	LYS	2.1
1	F	308	GLU	2.1
1	H	297	GLY	2.1
1	N	391	GLU	2.1
1	J	376	VAL	2.1
1	C	155	ASP	2.1
1	C	188	ASP	2.1
1	M	316	ASP	2.1
1	A	229	ASN	2.1
1	M	200	LEU	2.1
1	C	217	SER	2.1
1	E	227	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	312	ALA	2.1
1	K	315	GLU	2.1
1	N	223	ALA	2.1
1	A	362	ARG	2.1
1	H	236	VAL	2.1
1	L	190	VAL	2.1
1	M	362	ARG	2.1
1	K	290	GLN	2.1
1	M	281	PHE	2.1
1	C	134	LEU	2.1
1	J	161	LEU	2.1
1	N	314	LEU	2.1
1	K	333	ILE	2.1
1	A	351	GLN	2.1
1	E	366	GLN	2.1
1	M	311	LYS	2.1
1	E	232	GLU	2.1
1	F	363	GLU	2.1
1	L	281	PHE	2.1
1	B	228	SER	2.1
1	L	274	ALA	2.1
1	B	313	THR	2.1
1	K	168	LYS	2.1
1	M	142	LYS	2.1
1	E	333	ILE	2.1
1	I	301	ILE	2.1
1	J	325	ILE	2.1
1	K	367	GLU	2.1
1	M	379	ILE	2.1
1	E	160	LYS	2.1
1	E	350	ARG	2.1
1	H	306	GLY	2.1
1	M	284	ARG	2.1
1	C	234	LEU	2.0
1	C	262	LEU	2.0
1	J	384	ALA	2.0
1	L	215	LEU	2.0
1	H	230	ILE	2.0
1	H	333	ILE	2.0
1	B	369	VAL	2.0
1	F	158	VAL	2.0
1	J	369	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	255	GLU	2.0
1	B	310	GLU	2.0
1	H	319	GLN	2.0
1	F	183	LEU	2.0
1	I	161	LEU	2.0
1	J	259	LEU	2.0
1	B	220	ILE	2.0
1	E	168	LYS	2.0
1	G	305	ILE	2.0
1	M	332	ILE	2.0
1	F	257	GLU	2.0
1	K	214	GLU	2.0
1	E	297	GLY	2.0
1	K	343	GLN	2.0
1	B	324	VAL	2.0
1	C	381	VAL	2.0
1	M	376	VAL	2.0
1	F	157	THR	2.0
1	H	266	THR	2.0
1	I	311	LYS	2.0
1	L	313	THR	2.0
1	M	388	GLU	2.0
1	A	205	ILE	2.0
1	E	43	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	G	550	1/1	0.18	59.00	29,29,29,29	0
3	MG	B	550	1/1	0.13	28.00	31,31,31,31	0
3	MG	D	550	1/1	0.13	19.00	29,29,29,29	0
2	SO4	E	4006	5/5	0.33	18.75	118,119,119,120	0
2	SO4	K	4021	5/5	0.43	15.20	137,138,139,139	0
2	SO4	A	4008	5/5	0.37	13.18	150,150,150,150	0
2	SO4	J	4020	5/5	0.47	11.89	160,160,160,160	0
2	SO4	B	4009	5/5	0.28	11.71	118,119,119,120	0
2	SO4	J	4019	5/5	0.22	11.36	123,124,124,124	0
2	SO4	F	4004	5/5	0.29	10.36	137,138,138,138	0
2	SO4	B	4010	5/5	0.29	9.97	137,137,137,138	0
2	SO4	N	4015	5/5	0.25	9.40	132,133,133,133	0
2	SO4	H	4018	5/5	0.33	9.33	125,125,126,126	0
2	SO4	E	4005	5/5	0.35	9.09	140,141,141,141	0
2	SO4	C	4011	5/5	0.31	8.55	137,137,137,138	0
2	SO4	C	4012	5/5	0.29	7.59	141,141,141,142	0
2	SO4	A	4007	5/5	0.27	7.34	128,129,129,129	0
2	SO4	N	4016	5/5	0.27	6.96	137,137,137,138	0
2	SO4	M	4014	5/5	0.24	6.72	142,142,143,143	0
2	SO4	H	4017	5/5	0.33	6.68	145,146,146,146	0
2	SO4	A	4001	5/5	0.24	5.74	119,120,120,120	0
2	SO4	L	4003	5/5	0.26	5.54	130,131,132,132	0
2	SO4	K	4022	5/5	0.28	4.91	145,146,146,146	0
2	SO4	M	4013	5/5	0.23	4.41	126,126,127,127	0
3	MG	J	550	1/1	0.12	4.33	37,37,37,37	0
3	MG	N	550	1/1	0.19	4.20	34,34,34,34	0
3	MG	A	550	1/1	0.17	4.08	31,31,31,31	0
2	SO4	G	4002	5/5	0.26	3.70	128,128,129,129	0
3	MG	M	550	1/1	0.19	3.47	38,38,38,38	0
3	MG	H	550	1/1	0.16	2.32	26,26,26,26	0
3	MG	K	550	1/1	0.12	1.71	35,35,35,35	0
5	AGS	D	551	31/31	0.15	1.20	25,31,39,41	0
3	MG	C	550	1/1	0.14	1.00	36,36,36,36	0
3	MG	L	550	1/1	0.12	1.00	31,31,31,31	0
4	K	M	549	1/1	0.14	0.90	45,45,45,45	0
5	AGS	C	1	31/31	0.14	0.81	37,41,49,52	0
4	K	J	549	1/1	0.15	0.79	47,47,47,47	0
4	K	H	549	1/1	0.14	0.75	41,41,41,41	0
5	AGS	M	1	31/31	0.14	0.71	38,42,50,52	0
5	AGS	J	1	31/31	0.14	0.63	39,42,53,54	0
4	K	I	549	1/1	0.17	0.63	43,43,43,43	0
5	AGS	N	1	31/31	0.14	0.58	35,39,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	K	G	549	1/1	0.15	0.46	39,39,39,39	0
5	AGS	L	1	31/31	0.14	0.44	34,37,45,48	0
4	K	D	549	1/1	0.14	0.40	34,34,34,34	0
5	AGS	G	1	31/31	0.13	0.36	25,32,40,41	0
5	AGS	E	1	31/31	0.12	0.24	27,30,34,37	0
4	K	N	549	1/1	0.13	0.22	41,41,41,41	0
5	AGS	K	1	31/31	0.12	0.18	37,40,51,54	0
5	AGS	H	1	31/31	0.13	0.16	30,34,38,42	0
5	AGS	B	1	31/31	0.12	0.15	31,37,48,50	0
5	AGS	F	1	31/31	0.14	0.15	34,37,44,45	0
3	MG	F	550	1/1	0.13	0.07	30,30,30,30	0
3	MG	I	550	1/1	0.16	0.05	34,34,34,34	0
5	AGS	A	1	31/31	0.12	0.03	35,38,42,44	0
4	K	K	549	1/1	0.13	-0.07	46,46,46,46	0
4	K	F	549	1/1	0.12	-0.10	41,41,41,41	0
3	MG	E	550	1/1	0.10	-0.11	24,24,24,24	0
5	AGS	I	1	31/31	0.14	-0.25	37,41,48,51	0
4	K	L	549	1/1	0.14	-0.53	39,39,39,39	0
4	K	C	549	1/1	0.12	-0.61	45,45,45,45	0
4	K	A	549	1/1	0.12	-0.67	40,40,40,40	0
4	K	B	549	1/1	0.11	-1.31	38,38,38,38	0
4	K	E	4007	1/1	0.11	-1.42	36,36,36,36	0
4	K	D	1	1/1	0.11	-1.90	30,30,30,30	0
4	K	E	549	1/1	0.07	-2.78	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.