



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 21, 2017 – 04:46 PM EDT

PDB ID : 4BZI
EMDB ID: : EMD-2428
Title : The structure of the COPII coat assembled on membranes
Authors : Zanetti, G.; Prinz, S.; Daum, S.; Meister, A.; Schekman, R.; Bacia, K.; Briggs, J.A.G.
Deposited on : unknown
Resolution : 23.00 Å(reported)
Based on PDB ID : 1M2O

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

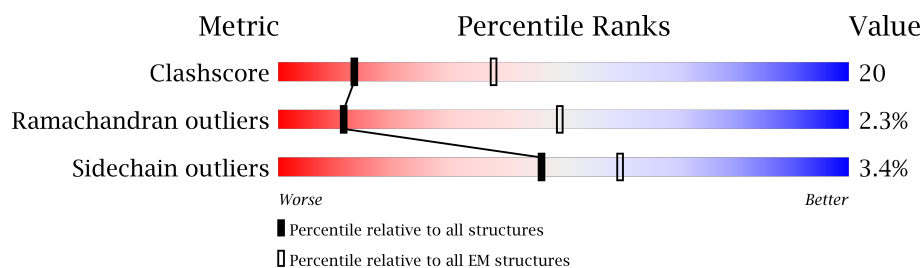
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	768	68% 25% • 5%
1	D	768	68% 25% • 5%
1	G	768	69% 25% • 5%
2	B	190	52% 31% • 14%
2	J	190	53% 31% • 14%
2	K	190	52% 32% • 14%
3	E	926	45% 31% • 21%
3	L	926	45% 31% • 21%
3	M	926	45% 32% • 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	926	99%
4	N	926	98%
4	O	926	98%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SEC23P.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		
1	D	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		
1	G	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		

- Molecule 2 is a protein called SAR1P.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		
2	J	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		
2	K	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	ALA	GLY	conflict	UNP C8ZIG2
J	139	ALA	GLY	conflict	UNP C8ZIG2
K	139	ALA	GLY	conflict	UNP C8ZIG2

- Molecule 3 is a protein called SEC24P.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		
3	L	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		
3	M	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	408	THR	ALA	conflict	UNP C8ZAD6
E	865	VAL	ALA	conflict	UNP C8ZAD6
L	408	THR	ALA	conflict	UNP C8ZAD6
L	865	VAL	ALA	conflict	UNP C8ZAD6
M	408	THR	ALA	conflict	UNP C8ZAD6
M	865	VAL	ALA	conflict	UNP C8ZAD6

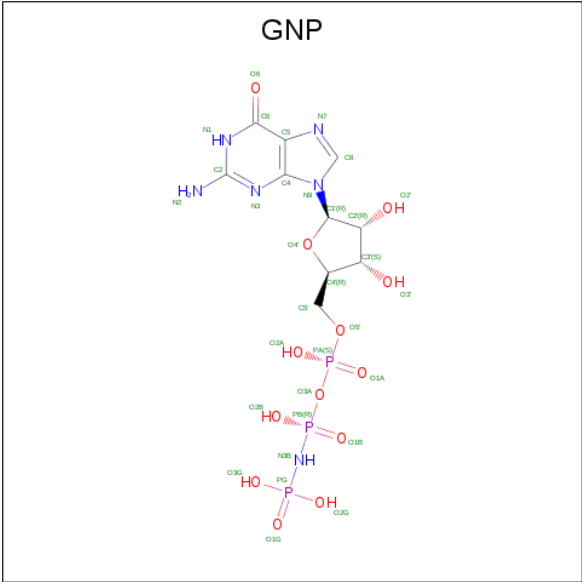
- Molecule 4 is a protein called SEC24P.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	13	Total	C	N	O	0	0
			109	70	19	20		
4	N	14	Total	C	N	O	0	0
			117	74	21	22		
4	O	14	Total	C	N	O	0	0
			117	74	21	22		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	A	1	Total	Zn	0
			1	1	
5	L	1	Total	Zn	0
			1	1	
5	M	1	Total	Zn	0
			1	1	

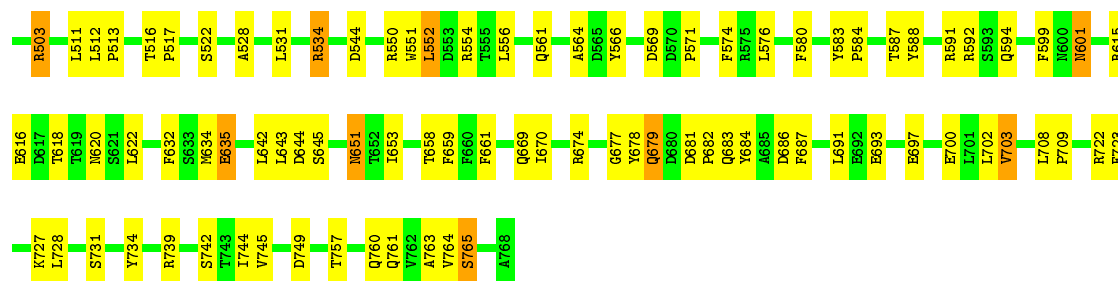
- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			32	10	6	13	3	
6	J	1	Total	C	N	O	P	0
			32	10	6	13	3	
6	K	1	Total	C	N	O	P	0
			32	10	6	13	3	

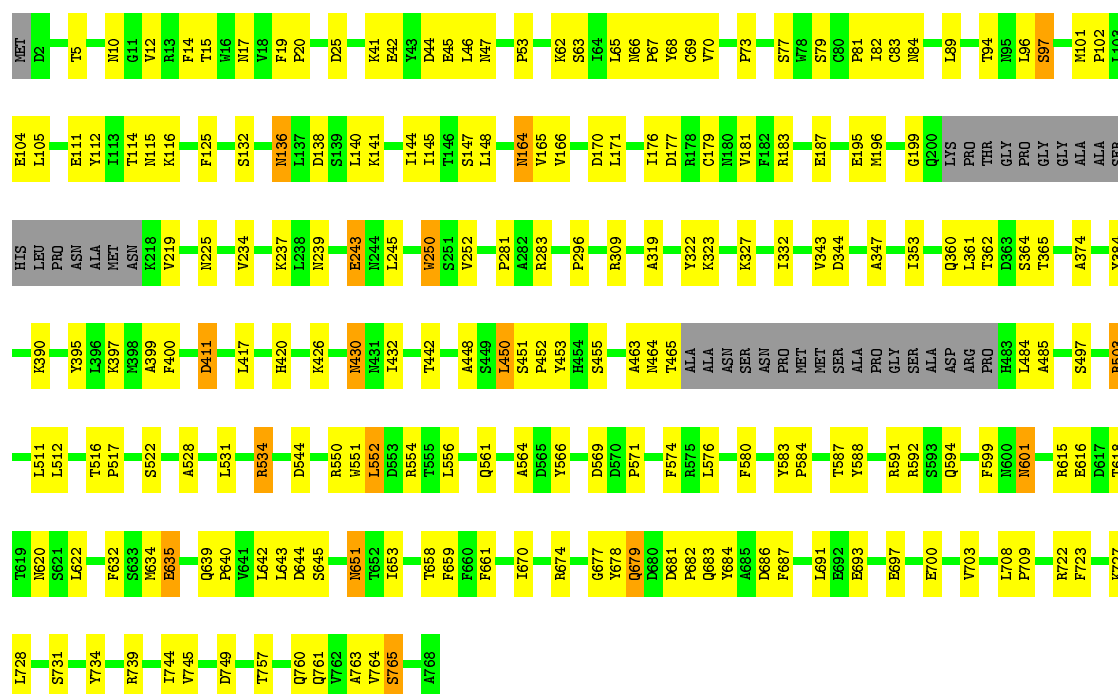
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Mg	0
			1	1	
7	J	1	Total	Mg	0
			1	1	
7	K	1	Total	Mg	0
			1	1	



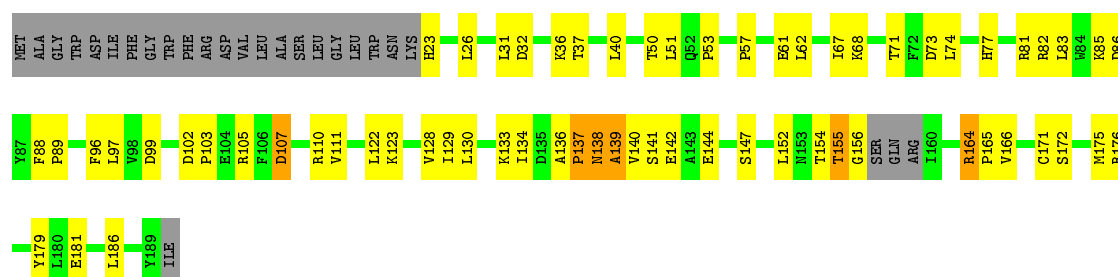
• Molecule 1: SEC23P

Chain G: 69% 25% 5%



• Molecule 2: SAR1P

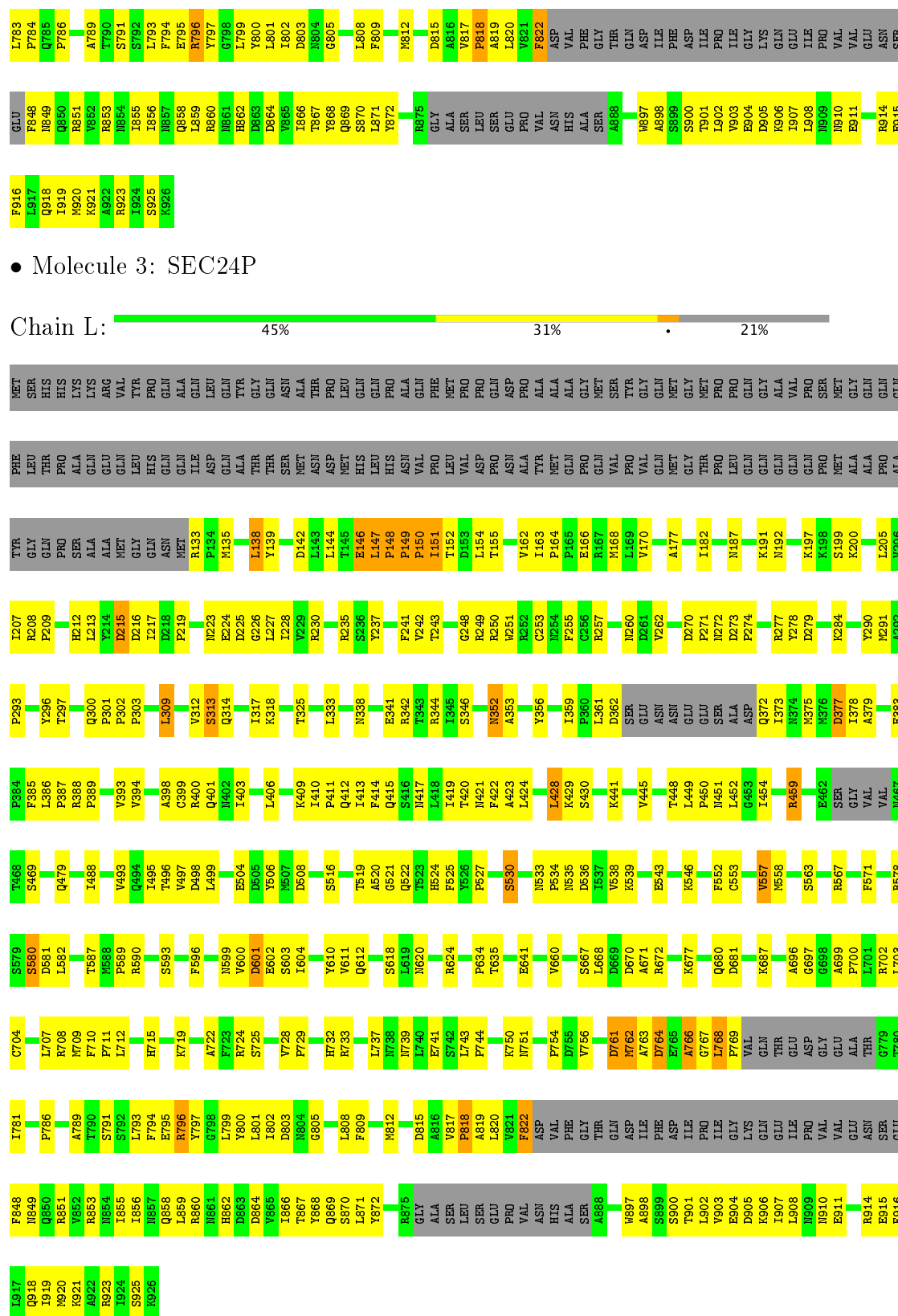
Chain B: 52% 31% 14%



• Molecule 2: SAR1P

Chain J: 53% 31% 14%





• Molecule 3: SEC24P



MET	THR	GLN	THR	GLY	TYR	P209	Y296	E383	SER	S563	A696	GLN	GLN	K906
SER	LEU	THR	LEU	PRO	GLY	Y297	E384	R587	GLY	A697	G697	THR	SER	I907
HIS	THR	PRO	GLN	PRO	GLY	E1213	F385	F571	VAL	G698	G699	GLU	HIS	I908
LYS	ALA	ALA	GLN	SER	ALA	Y214	L386	R578	VAL	A699	A699	ASP	HIS	N909
ARG	GLU	GLU	GLN	ALA	ALA	D216	R387	R579	VAL	L701	L701	GLY	LYS	N910
VAL	GLN	GLN	GLN	MET	ALA	I217	R388	S580	ALA	R702	R702	ALA	ARG	E911
THR	LEU	GLY	HIS	GLY	GLY	D218	R389	S589	THR	L703	L703	THR	VAL	R914
PRO	HIS	GLN	GLN	ASN	ASN	P220	C307	D581	SER	C704	C704	ASN	GLU	E915
ALA	GLN	ASN	GLN	MET	MET	P220	F308	L582	THR	L707	L707	GLN	GLU	F916
GLN	ILE	ASP	ASP	B133	B133	N223	L309	T587	THR	R708	R708	ALA	ASN	L917
LEU	ASP	GLN	GLN	P394	P394	E224	V312	R586	THR	M709	M709	GLN	GLN	Q918
GLN	GLN	ALA	THR	M135	M135	D225	S313	R589	THR	F710	F710	GLN	ALA	N919
TYR	THR	ALA	THR	Y138	Y138	G226	Q314	R590	THR	L711	L711	GLN	GLN	N920
GLY	THR	THR	THR	Y139	Y139	L227	R400	L593	THR	L712	L712	GLN	GLN	A921
ASN	SER	SER	SER	D142	D142	L228	Q401	S593	THR	H715	H715	GLN	GLN	R923
ALA	MET	ASN	ASN	Y143	Y143	Y229	M402	L403	THR	S716	S716	GLN	GLN	N924
ALA	ASN	ASN	ASN	L144	L144	R230	L406	F596	THR	L717	L717	GLN	GLN	S925
PRO	ASP	ASP	ASP	L145	L145	R235	L406	M599	THR	L718	L718	GLN	GLN	R926
LEU	MET	ASP	ASP	T146	T146	Y237	Y506	R601	THR	K719	K719	GLN	GLN	
GLN	HIS	HIS	HIS	E146	E146	Y237	Y507	D602	THR	A722	A722	GLN	GLN	
PRO	HIS	HIS	HIS	L147	L147	F241	D508	S603	THR	R723	R723	GLN	GLN	
ALA	ASN	ASN	ASN	P149	P149	T242	S516	L604	THR	R724	R724	GLN	GLN	
GLN	VAL	VAL	VAL	T150	T150	T243	Y610	V600	THR	S725	S725	GLN	GLN	
PHE	PRO	PRO	PRO	I151	I151	R343	A520	D601	THR	V728	V728	GLN	GLN	
MET	LEU	LEU	LEU	T152	T152	T343	G521	S603	THR	M729	M729	GLN	GLN	
PRO	VAL	VAL	VAL	D153	D153	T344	G522	L612	THR	H732	H732	GLN	GLN	
PRO	ASP	ASP	ASP	L154	L154	S346	T523	S618	THR	R733	R733	GLN	GLN	
GLN	PRO	PRO	PRO	T155	T155	R352	H524	L619	THR	L737	L737	GLN	GLN	
ASP	ASN	ASN	ASN	Y162	Y162	C253	Y526	M620	THR	N738	N738	GLN	GLN	
ALA	TYR	TYR	TYR	I163	I163	N254	P527	R624	THR	M739	M739	GLN	GLN	
ALA	MET	MET	MET	E166	E166	C256	Y556	L424	THR	L740	L740	GLN	GLN	
GLY	PRO	PRO	PRO	R167	R167	R257	F357	L428	THR	S741	S741	GLN	GLN	
MET	GLN	GLN	GLN	M168	M168	N260	T359	K429	THR	E742	E742	GLN	GLN	
MET	VAL	VAL	VAL	L169	L169	N261	P360	P534	THR	L743	L743	GLN	GLN	
TYR	PRO	PRO	PRO	V170	V170	D261	L361	S430	THR	P744	P744	GLN	GLN	
GLY	VAL	VAL	VAL	V262	V262	SER	D362	L435	THR	K750	K750	GLN	GLN	
GLN	MET	MET	MET	A177	A177	GLU	SER	L435	THR	N751	N751	GLN	GLN	
MET	GLY	GLY	GLY	I182	I182	ASN	ASN	K441	THR	P754	P754	GLN	GLN	
MET	THR	THR	THR	N187	N187	GLU	GLU	V445	THR	D755	D755	GLN	GLN	
PRO	LEU	LEU	LEU	N191	N191	SER	SER	E543	THR	V756	V756	GLN	GLN	
GLY	GLN	GLN	GLN	N192	N192	ALA	ALA	K546	THR	D761	D761	GLN	GLN	
ALA	GLN	GLN	GLN	K197	K197	ASP	ASP	R672	THR	M762	M762	GLN	GLN	
VAL	GLN	GLN	GLN	D279	D279	GLU	GLU	N451	THR	A763	A763	GLN	GLN	
PRO	GLN	GLN	GLN	K198	K198	T372	T372	L452	THR	D764	D764	GLN	GLN	
SER	PRO	PRO	PRO	S199	S199	K254	N374	L453	THR	E765	E765	GLN	GLN	
MET	MET	MET	MET	K200	K200	X375	X375	L454	THR	A766	A766	GLN	GLN	
GLY	ALA	ALA	ALA	L205	L205	X376	X376	R459	THR	G767	G767	GLN	GLN	
GLN	PRO	PRO	PRO	D292	D292	T378	T378	A560	THR	L768	L768	GLN	GLN	
GLN	ALA	ALA	ALA	R208	R208	P293	P293	E462	THR	P769	P769	GLN	GLN	

● Molecule 4: SEC24P

Chain F: :: 99%

MET	SER	THR	GLN	THR	GLY	TYR	P61	F61	GLN	GLN	K906	GLN	GLN	K906
SER	LEU	THR	GLN	THR	GLY	TYR	L62	L62	GLY	THR	G697	THR	SER	I907
HIS	HIS	THR	GLN	THR	GLY	TYR	Q66	Q66	GLY	THR	G698	THR	SER	I908
LYS	ALA	ALA	GLN	THR	GLY	TYR	E67	E67	GLY	THR	A699	THR	SER	N909
ARG	GLU	GLU	GLN	THR	GLY	TYR	Q68	Q68	GLY	THR	L701	GLY	LYS	N910
VAL	GLN	GLN	GLN	THR	GLY	TYR	L69	L69	GLY	THR	R702	ALA	ARG	E911
THR	LEU	GLY	HIS	THR	GLY	TYR	Q72	Q72	GLY	THR	L703	THR	VAL	R914
PRO	HIS	GLN	GLN	THR	GLY	TYR	I73	I73	GLY	THR	C704	ASN	GLU	E915
ALA	GLN	ASN	GLN	THR	GLY	TYR	ASP	ASP	GLY	THR	L707	GLN	GLN	F916
GLN	ILE	ASP	ASP	THR	GLY	TYR	GLN	GLN	GLY	THR	R708	GLN	GLN	L917
LEU	ASP	GLN	GLN	THR	GLY	TYR	ALA	ALA	GLY	THR	M709	GLN	GLN	Q918
LYS	GLN	GLN	GLN	THR	GLY	TYR	THR	THR	GLY	THR	F710	GLN	GLN	N919
LYS	GLN	GLN	GLN	THR	GLY	TYR	SER	SER	GLY	THR	L711	GLN	GLN	N920
LYS	GLN	GLN	GLN	THR	GLY	TYR	MET	MET	GLY	THR	L712	GLN	GLN	A921
GLY	ASN	ASN	ASN	THR	GLY	TYR	N854	N854	GLY	THR	H715	GLN	GLN	R923
ASP	ASP	ASN	ASN	THR	GLY	TYR	I855	I855	GLY	THR	S716	GLN	GLN	N924
PHE	THR	ASN	ASN	THR	GLY	TYR	I856	I856	GLY	THR	L717	GLN	GLN	S925
LEU	THR	ASN	ASN	THR	GLY	TYR	M857	M857	GLY	THR	L718	GLN	GLN	R926
LEU	THR	ASN	ASN	THR	GLY	TYR	Q858	Q858	GLY	THR	K719	GLN	GLN	
GLY	THR	ASN	ASN	THR	GLY	TYR	L859	L859	GLY	THR	A722	GLN	GLN	
VAL	THR	ASN	ASN	THR	GLY	TYR	R860	R860	GLY	THR	R723	GLN	GLN	
ILE	THR	ASN	ASN	THR	GLY	TYR	N861	N861	GLY	THR	S725	GLN	GLN	
ARG	THR	ASN	ASN	THR	GLY	TYR	R862	R862	GLY	THR	V728	GLN	GLN	
PRO	THR	ASN	ASN	THR	GLY	TYR	D863	D863	GLY	THR	M729	GLN	GLN	
PRO	THR	ASN	ASN	THR	GLY	TYR	L864	L864	GLY	THR	H732	GLN	GLN	
THR	THR	ASN	ASN	THR	GLY	TYR	V865	V865	GLY	THR	R733	GLN	GLN	
ASP	THR	ASN	ASN	THR	GLY	TYR	T867	T867	GLY	THR	L737	GLN	GLN	
ASP	THR	ASN	ASN	THR	GLY	TYR	R868	R868	GLY	THR	N738	GLN	GLN	
ASP	THR	ASN	ASN	THR	GLY	TYR	Q869	Q869	GLY	THR	M739	GLN	GLN	
ASP	THR	ASN	ASN	THR	GLY	TYR	S870	S870	GLY	THR	L740	GLN	GLN	
ILE	THR	ASN	ASN	THR	GLY	TYR	L871	L871	GLY	THR	E741	GLN	GLN	
PRO	THR	ASN	ASN	THR	GLY	TYR	Y872	Y872	GLY	THR	S742	GLN	GLN	
PRO	THR	ASN	ASN	THR	GLY	TYR	R875	R875	GLY	THR	L743	GLN	GLN	
PRO	THR	ASN	ASN	THR	GLY	TYR	ALA	ALA	GLY	THR	P744	GLN	GLN	
PRO	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	K750	GLN	GLN	
LEU	THR	ASN	ASN	THR	GLY	TYR	PRO	PRO	GLY	THR	N751	GLN	GLN	
VAL	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	P754	GLN	GLN	
ASN	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	D755	GLN	GLN	
GLY	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	V756	GLN	GLN	
ASP	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	D761	GLN	GLN	
GLY	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	M762	GLN	GLN	
ILE	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	A763	GLN	GLN	
VAL	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	D764	GLN	GLN	
ARG	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	E765	GLN	GLN	
ARG	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	A766	GLN	GLN	
VAL	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	G767	GLN	GLN	
VAL	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	L768	GLN	GLN	
THR	THR	ASN	ASN	THR	GLY	TYR	VAL	VAL	GLY	THR	P769	GLN	GLN	

Chain N: 98%




GLU	ASN	GLY	ASN	THR	ALA
ASN	LYS	THR	ASN	TYR	THR
ILE	GLU	ILE	GLU	CYS	THR
LEU	LEU	PHE	GLU	GLY	ILE
ASN	ASN	ASN	SER	LEU	LEU
ASN	ARG	GLN	ALA	ILE	ILE
GLU	ARG	GLY	ASN	GLN	SER
LEU	ASN	ILE	ASN	GLN	SER
PHE	PHE	GLY	MET	MET	SER
GLN	GLN	VAL	GLY	ASP	ILE
ASN	GLN	VAL	VAL	GLY	LYS
ILE	ILE	ILE	HIS	GLN	SER
ASN	ASN	GLN	LEU	ASN	VAL
GLU	GLU	ILE	ILE	MET	SER
LEU	ASN	THR	GLY	MET	SER
GLN	ASN	VAL	GLY	ASP	ILE
GLN	GLN	VAL	VAL	ASP	LYS
ILE	ILE	GLY	GLY	GLY	GLY
LEU	ASN	ALA	ILE	ALA	LEU
ASN	ASN	SER	THR	THR	LEU
HIS	ASN	THR	THR	THR	THR
ALA	ASN	VAL	VAL	VAL	THR
ARG	ASN	GLY	GLY	GLY	THR
ASP	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY	GLY	GLY	THR
SER	ASN	GLY	GLY	GLY	THR
LEU	ASN	GLY	GLY	GLY	THR
ILE	ASN	GLY	GLY	GLY	THR
THR	ASN	GLY	GLY	GLY	THR
TYR	ASN	GLY	GLY	GLY	THR
GLN	ASN	GLY			

- Molecule 4: SEC24P

Chain 0: 98%

[illegible]




4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	15000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH TILTED IMAGE WITHIN TOMOGRAM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	19500	Depositor
Image detector	GATAN MULTISCAN	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GNP

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 >2	RMSZ	# Z >2
1	A	0.38	0/5915	0.62	0/8052
1	D	0.38	0/5915	0.62	0/8052
1	G	0.38	0/5915	0.62	0/8052
2	B	0.34	0/1327	0.61	0/1800
2	J	0.34	0/1327	0.61	0/1800
2	K	0.34	0/1327	0.61	0/1800
3	E	0.39	0/5943	0.68	1/8064 (0.0%)
3	L	0.39	0/5943	0.68	1/8064 (0.0%)
3	M	0.39	0/5943	0.68	1/8064 (0.0%)
4	F	0.35	0/111	0.47	0/150
4	N	0.35	0/118	0.47	0/158
4	O	0.35	0/118	0.48	0/158
All	All	0.38	0/39902	0.64	3/54214 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	768	LEU	CA-CB-CG	5.33	127.56	115.30
3	M	768	LEU	CA-CB-CG	5.33	127.56	115.30
3	L	768	LEU	CA-CB-CG	5.32	127.55	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5780	0	5663	201	0
1	D	5780	0	5663	205	0
1	G	5780	0	5663	193	0
2	B	1299	0	1288	65	0
2	J	1299	0	1288	59	0
2	K	1299	0	1288	61	0
3	E	5823	0	5853	291	0
3	L	5823	0	5853	293	0
3	M	5823	0	5853	301	0
4	F	109	0	105	14	0
4	N	117	0	110	14	0
4	O	117	0	110	12	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
6	B	32	0	13	5	0
6	J	32	0	13	4	0
6	K	32	0	13	5	0
7	B	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
All	All	39154	0	38776	1589	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1589) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HB3	1:D:669:GLN:NE2	1.18	1.43
1:A:91:PRO:CB	1:D:669:GLN:HE21	1.35	1.38
1:D:183:ARG:NH1	3:L:383:GLU:HB2	1.53	1.22
1:G:183:ARG:NH1	3:M:383:GLU:HB2	1.53	1.22
1:A:183:ARG:NH1	3:E:383:GLU:HB2	1.53	1.21
3:E:272:ASN:OD1	3:M:906:LYS:HD3	1.41	1.19
1:A:176:ILE:CD1	3:E:413:ILE:HG12	1.73	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:ILE:CD1	3:M:413:ILE:HG12	1.73	1.17
1:D:176:ILE:CD1	3:L:413:ILE:HG12	1.73	1.17
3:L:147:LEU:HB3	3:L:148:PRO:HD2	1.16	1.16
1:A:101:MET:CE	4:F:61:PHE:HZ	1.63	1.12
1:D:101:MET:CE	4:N:61:PHE:HZ	1.63	1.11
1:G:101:MET:CE	4:O:61:PHE:HZ	1.63	1.11
3:M:147:LEU:HB3	3:M:148:PRO:HD2	1.16	1.10
3:E:907:ILE:HG22	3:E:908:LEU:HG	1.35	1.08
3:E:147:LEU:HB3	3:E:148:PRO:HD2	1.16	1.08
3:M:907:ILE:HG22	3:M:908:LEU:HG	1.35	1.07
1:A:91:PRO:CB	1:D:669:GLN:NE2	2.05	1.05
3:L:907:ILE:HG22	3:L:908:LEU:HG	1.35	1.05
1:A:101:MET:HE2	4:F:61:PHE:CZ	1.93	1.03
1:G:101:MET:HE2	4:O:61:PHE:CZ	1.93	1.03
1:D:651:ASN:HD22	1:D:651:ASN:H	1.05	1.01
1:G:101:MET:HE2	4:O:61:PHE:HZ	1.22	0.99
1:D:183:ARG:HH12	3:L:383:GLU:HB2	1.23	0.99
1:A:651:ASN:HD22	1:A:651:ASN:H	1.05	0.98
1:D:176:ILE:HD11	3:L:413:ILE:HG12	1.44	0.98
1:D:101:MET:CE	4:N:61:PHE:CZ	2.45	0.98
1:A:101:MET:HE2	4:F:61:PHE:HZ	1.22	0.98
1:G:176:ILE:HD11	3:M:413:ILE:HG12	1.44	0.98
1:G:101:MET:CE	4:O:61:PHE:CZ	2.45	0.98
1:A:101:MET:CE	4:F:61:PHE:CZ	2.46	0.98
1:D:101:MET:HE2	4:N:61:PHE:CZ	1.99	0.97
1:A:176:ILE:HD11	3:E:413:ILE:HG12	1.44	0.96
3:E:147:LEU:CB	3:E:148:PRO:HD2	1.97	0.95
3:M:147:LEU:CB	3:M:148:PRO:HD2	1.97	0.94
1:D:101:MET:HE2	4:N:61:PHE:HZ	1.27	0.94
1:A:183:ARG:HH12	3:E:383:GLU:CB	1.81	0.94
3:L:147:LEU:CB	3:L:148:PRO:HD2	1.97	0.93
1:D:183:ARG:HH12	3:L:383:GLU:CB	1.81	0.93
1:A:183:ARG:HH12	3:E:383:GLU:HB2	1.23	0.93
1:G:183:ARG:HH12	3:M:383:GLU:CB	1.81	0.92
1:G:651:ASN:HD22	1:G:651:ASN:H	1.05	0.92
1:G:183:ARG:HH12	3:M:383:GLU:HB2	1.23	0.91
3:L:375:MET:HE1	3:L:413:ILE:HG21	1.53	0.90
3:L:441:LYS:HE2	3:L:498:ASP:OD2	1.72	0.90
3:M:441:LYS:HE2	3:M:498:ASP:OD2	1.72	0.90
3:M:147:LEU:HB3	3:M:148:PRO:CD	2.02	0.89
2:B:137:PRO:O	1:G:62:LYS:HE3	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:147:LEU:HB3	3:L:148:PRO:CD	2.02	0.88
1:D:176:ILE:HD11	3:L:413:ILE:CG1	2.03	0.88
3:L:459:ARG:HH11	3:L:459:ARG:HG2	1.38	0.88
1:A:176:ILE:HD11	3:E:413:ILE:CG1	2.03	0.87
3:E:441:LYS:HE2	3:E:498:ASP:OD2	1.72	0.87
1:G:176:ILE:HD11	3:M:413:ILE:CG1	2.03	0.87
3:E:459:ARG:HG2	3:E:459:ARG:HH11	1.39	0.87
3:M:459:ARG:HG2	3:M:459:ARG:HH11	1.39	0.85
1:A:722:ARG:HD3	6:B:1190:GNP:H5'1	1.57	0.85
3:E:352:ASN:HD22	3:E:353:ALA:N	1.75	0.85
3:L:352:ASN:HD22	3:L:353:ALA:N	1.75	0.84
3:E:147:LEU:HB3	3:E:148:PRO:CD	2.02	0.84
1:G:96:LEU:HG	1:G:97:SER:H	1.43	0.84
1:D:722:ARG:HD3	6:J:1190:GNP:H5'1	1.57	0.84
1:G:722:ARG:HD3	6:K:1190:GNP:H5'1	1.57	0.84
3:E:272:ASN:OD1	3:M:906:LYS:CD	2.25	0.83
3:M:333:LEU:HB2	3:M:400:ARG:NH2	1.93	0.83
3:M:352:ASN:HD22	3:M:353:ALA:N	1.75	0.83
1:A:96:LEU:HG	1:A:97:SER:H	1.43	0.82
3:E:333:LEU:HB2	3:E:400:ARG:NH2	1.93	0.82
3:L:333:LEU:HB2	3:L:400:ARG:NH2	1.93	0.82
1:A:176:ILE:HD12	3:E:413:ILE:HG12	1.62	0.81
3:M:375:MET:HE1	3:M:413:ILE:HG21	1.63	0.81
1:G:616:GLU:HG3	1:G:620:ASN:HB2	1.63	0.81
1:D:176:ILE:CD1	3:L:413:ILE:CG1	2.56	0.81
1:G:176:ILE:CD1	3:M:413:ILE:CG1	2.56	0.81
1:D:96:LEU:HG	1:D:97:SER:H	1.43	0.80
1:D:616:GLU:HG3	1:D:620:ASN:HB2	1.63	0.80
1:A:176:ILE:CD1	3:E:413:ILE:CG1	2.56	0.80
1:D:176:ILE:HD12	3:L:413:ILE:HG12	1.62	0.80
3:E:375:MET:HE1	3:E:413:ILE:HG21	1.62	0.79
3:M:147:LEU:HD13	3:M:914:ARG:NH1	1.97	0.79
3:L:147:LEU:HD13	3:L:914:ARG:NH1	1.97	0.79
1:G:176:ILE:HD12	3:M:413:ILE:HG12	1.62	0.79
3:E:147:LEU:HD13	3:E:914:ARG:NH1	1.97	0.79
3:M:709:MET:HE1	3:M:712:LEU:HD23	1.65	0.79
3:L:919:ILE:O	3:L:923:ARG:HG3	1.83	0.79
1:A:616:GLU:HG3	1:A:620:ASN:HB2	1.63	0.79
3:E:919:ILE:O	3:E:923:ARG:HG3	1.83	0.79
3:E:680:GLN:HG3	3:E:920:MET:HE1	1.65	0.79
3:M:919:ILE:O	3:M:923:ARG:HG3	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HH11	3:E:383:GLU:HB2	1.46	0.79
2:K:140:VAL:HG12	2:K:141:SER:N	1.99	0.78
3:M:680:GLN:HG3	3:M:920:MET:HE1	1.64	0.77
1:G:164:ASN:HD22	1:G:164:ASN:N	1.81	0.77
2:J:140:VAL:HG12	2:J:141:SER:N	1.99	0.77
1:A:164:ASN:HD22	1:A:164:ASN:N	1.81	0.77
2:B:140:VAL:HG12	2:B:141:SER:N	1.99	0.77
3:L:680:GLN:HG3	3:L:920:MET:HE1	1.65	0.77
3:M:147:LEU:O	3:M:148:PRO:C	2.22	0.77
1:D:114:THR:HG22	1:D:115:ASN:H	1.50	0.76
1:D:164:ASN:HD22	1:D:164:ASN:H	1.33	0.76
3:M:296:TYR:O	3:M:624:ARG:NH1	2.19	0.76
3:L:296:TYR:O	3:L:624:ARG:NH1	2.19	0.76
3:E:147:LEU:O	3:E:148:PRO:C	2.22	0.76
1:G:114:THR:HG22	1:G:115:ASN:H	1.51	0.76
1:A:183:ARG:NH1	3:E:383:GLU:CB	2.39	0.76
3:E:660:VAL:HG11	3:E:741:GLU:HB3	1.68	0.76
3:E:296:TYR:O	3:E:624:ARG:NH1	2.19	0.76
1:G:164:ASN:HD22	1:G:164:ASN:H	1.33	0.75
1:A:164:ASN:HD22	1:A:164:ASN:H	1.33	0.75
2:B:140:VAL:HG12	2:B:141:SER:H	1.52	0.75
3:L:660:VAL:HG11	3:L:741:GLU:HB3	1.68	0.75
1:G:183:ARG:HH11	3:M:383:GLU:HB2	1.46	0.74
2:K:140:VAL:HG12	2:K:141:SER:H	1.52	0.74
3:L:147:LEU:O	3:L:148:PRO:C	2.21	0.74
1:D:512:LEU:HD13	1:D:516:THR:HG21	1.70	0.74
1:G:651:ASN:H	1:G:651:ASN:ND2	1.85	0.74
3:L:567:ARG:HH21	3:L:599:ASN:HD22	1.36	0.74
1:A:512:LEU:HD13	1:A:516:THR:HG21	1.70	0.74
3:L:142:ASP:CG	3:L:700:PRO:HB3	2.08	0.74
1:D:164:ASN:N	1:D:164:ASN:HD22	1.81	0.74
3:L:154:LEU:HG	3:L:709:MET:HE2	1.70	0.74
3:M:660:VAL:HG11	3:M:741:GLU:HB3	1.68	0.74
3:M:567:ARG:HH21	3:M:599:ASN:HD22	1.36	0.73
3:E:142:ASP:CG	3:E:700:PRO:HB3	2.08	0.73
3:E:567:ARG:HH21	3:E:599:ASN:HD22	1.36	0.73
1:D:183:ARG:HH11	3:L:383:GLU:HB2	1.46	0.73
1:A:114:THR:HG22	1:A:115:ASN:H	1.50	0.73
1:A:101:MET:SD	4:F:61:PHE:HZ	2.12	0.73
3:M:557:VAL:HG13	3:M:582:LEU:HD11	1.70	0.73
1:G:512:LEU:HD13	1:G:516:THR:HG21	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:674:ARG:HA	1:G:679:GLN:NE2	2.04	0.72
3:L:557:VAL:HG13	3:L:582:LEU:HD11	1.70	0.72
1:D:101:MET:SD	4:N:61:PHE:HZ	2.12	0.72
3:M:142:ASP:CG	3:M:700:PRO:HB3	2.08	0.72
1:G:101:MET:SD	4:O:61:PHE:HZ	2.12	0.72
1:D:674:ARG:HA	1:D:679:GLN:NE2	2.04	0.72
3:E:709:MET:HE1	3:E:712:LEU:HD23	1.70	0.72
3:E:557:VAL:HG13	3:E:582:LEU:HD11	1.70	0.72
2:J:140:VAL:HG12	2:J:141:SER:H	1.52	0.72
3:E:225:ASP:OD2	3:E:227:LEU:HB3	1.90	0.72
3:L:225:ASP:OD2	3:L:227:LEU:HB3	1.90	0.72
3:L:226:GLY:O	3:L:293:PRO:HG3	1.90	0.71
3:L:142:ASP:O	3:L:146:GLU:HG2	1.91	0.71
1:A:674:ARG:HA	1:A:679:GLN:NE2	2.04	0.71
3:M:142:ASP:O	3:M:146:GLU:HG2	1.91	0.71
1:A:88:HIS:CE1	1:D:742:SER:HB2	2.25	0.71
3:E:154:LEU:HG	3:E:709:MET:HE2	1.73	0.71
3:E:493:VAL:HG23	3:E:495:ILE:HG13	1.73	0.71
3:E:142:ASP:O	3:E:146:GLU:HG2	1.91	0.71
3:E:226:GLY:O	3:E:293:PRO:HG3	1.90	0.71
3:M:225:ASP:OD2	3:M:227:LEU:HB3	1.90	0.71
1:G:616:GLU:CG	1:G:620:ASN:HB2	2.21	0.71
1:A:347:ALA:HB2	1:A:353:ILE:HD13	1.73	0.71
1:G:430:ASN:HD22	1:G:430:ASN:H	1.39	0.70
1:D:616:GLU:CG	1:D:620:ASN:HB2	2.21	0.70
1:G:183:ARG:NH1	3:M:383:GLU:CB	2.39	0.70
1:A:651:ASN:ND2	1:A:651:ASN:H	1.85	0.70
3:L:279:ASP:HA	3:L:284:LYS:HE3	1.74	0.70
1:D:651:ASN:ND2	1:D:651:ASN:H	1.85	0.70
3:M:226:GLY:O	3:M:293:PRO:HG3	1.90	0.70
3:L:696:ALA:HB2	3:L:702:ARG:HH21	1.57	0.70
1:A:616:GLU:CG	1:A:620:ASN:HB2	2.21	0.70
3:L:493:VAL:HG23	3:L:495:ILE:HG13	1.73	0.70
3:M:696:ALA:HB2	3:M:702:ARG:HH21	1.57	0.70
1:D:347:ALA:HB2	1:D:353:ILE:HD13	1.73	0.70
3:M:459:ARG:HG2	3:M:459:ARG:NH1	2.07	0.70
1:G:399:ALA:HB3	1:G:450:LEU:HD13	1.74	0.69
1:A:114:THR:HG22	1:A:115:ASN:N	2.07	0.69
1:D:399:ALA:HB3	1:D:450:LEU:HD13	1.74	0.69
3:E:279:ASP:HA	3:E:284:LYS:HE3	1.74	0.69
3:L:801:LEU:HD11	3:L:808:LEU:HD22	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:801:LEU:HD11	3:M:808:LEU:HD22	1.74	0.69
1:D:430:ASN:H	1:D:430:ASN:HD22	1.39	0.69
2:J:36:LYS:HG2	2:J:97:LEU:HD13	1.75	0.69
3:E:801:LEU:HD11	3:E:808:LEU:HD22	1.74	0.69
1:D:181:VAL:HB	3:L:378:ILE:HG12	1.75	0.69
1:G:114:THR:HG22	1:G:115:ASN:N	2.07	0.69
1:G:181:VAL:HB	3:M:378:ILE:HG12	1.75	0.69
3:L:709:MET:HE1	3:L:712:LEU:HD23	1.73	0.69
3:M:493:VAL:HG23	3:M:495:ILE:HG13	1.73	0.69
1:A:179:CYS:O	3:E:377:ASP:HB2	1.93	0.68
1:D:114:THR:HG22	1:D:115:ASN:N	2.07	0.68
3:E:696:ALA:HB2	3:E:702:ARG:HH21	1.57	0.68
3:E:699:ALA:HB1	3:E:921:LYS:NZ	2.08	0.68
3:E:768:LEU:HG	3:E:769:PRO:HD2	1.74	0.68
3:M:768:LEU:HG	3:M:769:PRO:HD2	1.74	0.68
3:E:766:ALA:O	3:E:768:LEU:N	2.26	0.68
3:L:768:LEU:HG	3:L:769:PRO:HD2	1.74	0.68
2:B:137:PRO:O	1:G:62:LYS:CE	2.42	0.68
2:K:36:LYS:HG2	2:K:97:LEU:HD13	1.75	0.68
1:G:179:CYS:O	3:M:377:ASP:HB2	1.94	0.68
1:G:347:ALA:HB2	1:G:353:ILE:HD13	1.73	0.68
1:G:96:LEU:CG	1:G:97:SER:H	2.07	0.68
3:L:766:ALA:O	3:L:768:LEU:N	2.26	0.68
3:M:279:ASP:HA	3:M:284:LYS:HE3	1.74	0.68
1:A:181:VAL:HB	3:E:378:ILE:HG12	1.75	0.67
3:M:766:ALA:O	3:M:768:LEU:N	2.26	0.67
2:B:130:LEU:HD22	2:B:171:CYS:SG	2.35	0.67
2:B:36:LYS:HG2	2:B:97:LEU:HD13	1.75	0.67
1:G:634:MET:HE1	1:G:686:ASP:O	1.94	0.67
2:K:130:LEU:HD22	2:K:171:CYS:SG	2.35	0.67
3:L:699:ALA:HB1	3:L:921:LYS:NZ	2.08	0.67
3:M:699:ALA:HB1	3:M:921:LYS:NZ	2.08	0.67
1:A:430:ASN:HD22	1:A:430:ASN:H	1.39	0.67
2:J:130:LEU:HD22	2:J:171:CYS:SG	2.35	0.67
1:D:179:CYS:O	3:L:377:ASP:HB2	1.94	0.67
3:M:303:PRO:HG3	3:M:342:ARG:CZ	2.25	0.67
1:A:96:LEU:CG	1:A:97:SER:H	2.07	0.67
1:A:399:ALA:HB3	1:A:450:LEU:HD13	1.74	0.67
1:D:634:MET:HE1	1:D:686:ASP:O	1.95	0.67
1:D:745:VAL:CG1	2:J:50:THR:HG21	2.25	0.67
1:A:634:MET:HE1	1:A:686:ASP:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:VAL:CG1	2:B:50:THR:HG21	2.25	0.67
2:K:61:GLU:OE1	2:K:68:LYS:HE2	1.95	0.67
2:B:61:GLU:OE1	2:B:68:LYS:HE2	1.95	0.66
3:E:750:LYS:HE3	3:E:805:GLY:HA2	1.77	0.66
1:G:745:VAL:CG1	2:K:50:THR:HG21	2.25	0.66
3:L:312:VAL:HG11	3:L:414:PHE:CD1	2.30	0.66
3:L:812:MET:SD	3:L:820:LEU:HD22	2.36	0.66
3:E:312:VAL:HG11	3:E:414:PHE:CD1	2.30	0.66
3:E:764:ASP:HA	3:E:851:ARG:HH22	1.60	0.66
3:L:750:LYS:HE3	3:L:805:GLY:HA2	1.77	0.66
3:M:312:VAL:HG11	3:M:414:PHE:CD1	2.30	0.66
3:M:750:LYS:HE3	3:M:805:GLY:HA2	1.77	0.66
3:E:271:PRO:O	3:M:906:LYS:NZ	2.25	0.66
3:E:303:PRO:HG3	3:E:342:ARG:CZ	2.25	0.66
3:L:764:ASP:HA	3:L:851:ARG:HH22	1.60	0.66
3:M:362:ASP:OD1	3:M:401:GLN:HB2	1.95	0.66
3:L:312:VAL:HG11	3:L:414:PHE:CG	2.31	0.66
3:M:147:LEU:HD13	3:M:914:ARG:HH12	1.61	0.66
3:L:422:PHE:H	3:L:451:ASN:HB3	1.61	0.66
3:E:362:ASP:OD1	3:E:401:GLN:HB2	1.95	0.66
3:L:818:PRO:C	3:L:820:LEU:H	2.00	0.66
1:A:432:ILE:HD13	1:A:442:THR:HA	1.78	0.65
3:L:149:PRO:O	3:L:151:ILE:HG12	1.97	0.65
3:L:303:PRO:HG3	3:L:342:ARG:CZ	2.25	0.65
3:M:312:VAL:HG11	3:M:414:PHE:CG	2.31	0.65
3:M:422:PHE:H	3:M:451:ASN:HB3	1.61	0.65
3:M:764:ASP:HA	3:M:851:ARG:HH22	1.60	0.65
1:D:323:LYS:O	1:D:327:LYS:HG2	1.97	0.65
3:E:399:CYS:O	3:E:403:ILE:HG13	1.97	0.65
3:E:812:MET:SD	3:E:820:LEU:HD22	2.36	0.65
1:G:432:ILE:HD13	1:G:442:THR:HA	1.78	0.65
1:G:757:THR:O	1:G:761:GLN:HG3	1.97	0.65
3:L:672:ARG:HH11	3:L:725:SER:HB3	1.62	0.65
3:M:149:PRO:O	3:M:151:ILE:HG12	1.97	0.65
3:M:812:MET:SD	3:M:820:LEU:HD22	2.36	0.65
1:G:177:ASP:OD1	1:G:237:LYS:HE3	1.96	0.65
3:L:297:THR:HG22	3:L:624:ARG:HD3	1.79	0.65
1:D:432:ILE:HD13	1:D:442:THR:HA	1.78	0.65
3:L:362:ASP:OD1	3:L:401:GLN:HB2	1.95	0.65
3:M:920:MET:HA	3:M:920:MET:HE3	1.79	0.65
1:A:177:ASP:OD1	1:A:237:LYS:HE3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:399:CYS:O	3:M:403:ILE:HG13	1.97	0.65
1:D:164:ASN:ND2	1:D:164:ASN:H	1.94	0.65
2:J:61:GLU:OE1	2:J:68:LYS:HE2	1.95	0.65
1:A:164:ASN:ND2	1:A:164:ASN:H	1.94	0.65
3:E:422:PHE:H	3:E:451:ASN:HB3	1.61	0.65
1:G:164:ASN:H	1:G:164:ASN:ND2	1.94	0.65
1:A:757:THR:O	1:A:761:GLN:HG3	1.97	0.64
1:D:96:LEU:CG	1:D:97:SER:H	2.07	0.64
1:D:757:THR:O	1:D:761:GLN:HG3	1.97	0.64
3:L:147:LEU:HD13	3:L:914:ARG:HH12	1.61	0.64
1:D:177:ASP:OD1	1:D:237:LYS:HE3	1.96	0.64
3:M:297:THR:HG22	3:M:624:ARG:HD3	1.79	0.64
1:A:651:ASN:N	1:A:651:ASN:HD22	1.81	0.64
3:E:297:THR:HG22	3:E:624:ARG:HD3	1.79	0.64
3:E:149:PRO:O	3:E:151:ILE:HG12	1.97	0.64
3:E:312:VAL:HG11	3:E:414:PHE:CG	2.31	0.64
1:A:323:LYS:O	1:A:327:LYS:HG2	1.97	0.64
3:L:525:PHE:CE2	3:L:527:PRO:HG3	2.33	0.64
3:E:789:ALA:O	3:E:904:GLU:HB2	1.98	0.64
3:M:672:ARG:HH11	3:M:725:SER:HB3	1.62	0.64
3:E:680:GLN:CG	3:E:920:MET:HE1	2.28	0.64
3:E:672:ARG:HH11	3:E:725:SER:HB3	1.62	0.64
3:E:147:LEU:HD13	3:E:914:ARG:HH12	1.61	0.64
2:K:164:ARG:HG2	2:K:166:VAL:HG23	1.80	0.64
3:L:255:PHE:CZ	3:L:612:GLN:HB2	2.33	0.64
3:M:255:PHE:CZ	3:M:612:GLN:HB2	2.33	0.64
1:D:19:PHE:HB2	1:D:511:LEU:HD23	1.80	0.63
1:G:323:LYS:O	1:G:327:LYS:HG2	1.97	0.63
3:M:817:VAL:C	3:M:819:ALA:H	2.01	0.63
3:M:856:ILE:HD13	3:M:871:LEU:HD22	1.79	0.63
1:G:19:PHE:HB2	1:G:511:LEU:HD23	1.80	0.63
3:L:399:CYS:O	3:L:403:ILE:HG13	1.97	0.63
1:A:19:PHE:HB2	1:A:511:LEU:HD23	1.80	0.63
3:E:818:PRO:C	3:E:820:LEU:H	2.00	0.63
3:L:539:LYS:HA	3:L:868:TYR:CD2	2.34	0.63
3:L:808:LEU:O	3:L:871:LEU:HD12	1.98	0.63
3:L:789:ALA:O	3:L:904:GLU:HB2	1.98	0.63
3:M:525:PHE:CE2	3:M:527:PRO:HG3	2.33	0.63
3:M:818:PRO:C	3:M:820:LEU:H	2.00	0.63
3:M:808:LEU:O	3:M:871:LEU:HD12	1.99	0.63
2:J:164:ARG:HG2	2:J:166:VAL:HG23	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:789:ALA:O	3:M:904:GLU:HB2	1.98	0.63
1:D:484:LEU:CD1	4:N:69:LEU:HD21	2.29	0.63
3:L:856:ILE:HD13	3:L:871:LEU:HD22	1.79	0.63
3:M:154:LEU:HG	3:M:709:MET:HE2	1.80	0.63
3:E:750:LYS:HD2	3:E:803:ASP:OD2	1.98	0.63
3:L:750:LYS:HD2	3:L:803:ASP:OD2	1.98	0.63
3:L:817:VAL:C	3:L:819:ALA:H	2.01	0.63
2:B:164:ARG:HG2	2:B:166:VAL:HG23	1.80	0.63
1:D:183:ARG:NH1	3:L:383:GLU:CB	2.39	0.63
3:E:312:VAL:HG12	3:E:312:VAL:O	1.99	0.63
3:E:525:PHE:CE2	3:E:527:PRO:HG3	2.33	0.63
1:D:722:ARG:HH12	6:J:1190:GNP:HNB3	1.46	0.63
2:J:140:VAL:CG1	2:J:141:SER:H	2.12	0.63
2:K:140:VAL:CG1	2:K:141:SER:H	2.12	0.63
3:E:914:ARG:O	3:E:918:GLN:HG2	1.98	0.63
3:L:449:LEU:HD12	3:L:450:PRO:HD2	1.81	0.63
3:L:914:ARG:O	3:L:918:GLN:HG2	1.98	0.63
3:M:539:LYS:HA	3:M:868:TYR:CD2	2.34	0.63
1:A:96:LEU:HD21	1:A:101:MET:SD	2.39	0.62
3:E:255:PHE:CZ	3:E:612:GLN:HB2	2.33	0.62
1:G:170:ASP:C	1:G:171:LEU:HD12	2.20	0.62
3:M:914:ARG:O	3:M:918:GLN:HG2	1.98	0.62
3:M:680:GLN:CG	3:M:920:MET:HE1	2.28	0.62
1:D:170:ASP:C	1:D:171:LEU:HD12	2.20	0.62
1:D:96:LEU:HD21	1:D:101:MET:SD	2.39	0.62
3:E:539:LYS:HA	3:E:868:TYR:CD2	2.34	0.62
3:L:312:VAL:HG12	3:L:312:VAL:O	1.99	0.62
3:E:808:LEU:O	3:E:871:LEU:HD12	1.99	0.62
3:E:856:ILE:HD13	3:E:871:LEU:HD22	1.79	0.62
3:L:424:LEU:HG	3:L:428:LEU:HD22	1.81	0.62
1:G:484:LEU:CD1	4:O:69:LEU:HD21	2.29	0.62
1:D:136:ASN:HD21	1:D:374:ALA:HB1	1.65	0.62
1:G:96:LEU:HD21	1:G:101:MET:SD	2.39	0.62
1:G:136:ASN:HD21	1:G:374:ALA:HB1	1.65	0.62
1:A:484:LEU:CD1	4:F:69:LEU:HD21	2.29	0.62
3:E:817:VAL:C	3:E:819:ALA:H	2.01	0.62
1:A:219:VAL:HG22	1:A:225:ASN:ND2	2.14	0.62
2:B:140:VAL:CG1	2:B:141:SER:H	2.12	0.62
3:L:680:GLN:CG	3:L:920:MET:HE1	2.28	0.62
1:A:170:ASP:C	1:A:171:LEU:HD12	2.20	0.62
3:E:449:LEU:HD12	3:E:450:PRO:HD2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:722:ARG:HH12	6:K:1190:GNP:HNB3	1.46	0.62
2:B:154:THR:HB	2:B:166:VAL:O	2.00	0.62
3:E:920:MET:HE3	3:E:920:MET:HA	1.81	0.62
3:M:750:LYS:HD2	3:M:803:ASP:OD2	1.98	0.62
1:A:136:ASN:HD21	1:A:374:ALA:HB1	1.65	0.62
3:E:424:LEU:HG	3:E:428:LEU:HD22	1.81	0.62
3:M:449:LEU:HD12	3:M:450:PRO:HD2	1.81	0.62
1:G:219:VAL:HG22	1:G:225:ASN:ND2	2.14	0.61
3:M:312:VAL:HG12	3:M:312:VAL:O	1.99	0.61
3:M:687:LYS:NZ	3:M:925:SER:HA	2.15	0.61
3:E:687:LYS:NZ	3:E:925:SER:HA	2.15	0.61
2:K:154:THR:HB	2:K:166:VAL:O	2.00	0.61
3:E:135:MET:HE2	3:E:641:GLU:OE1	2.01	0.61
3:L:920:MET:HE3	3:L:920:MET:HA	1.82	0.61
1:A:722:ARG:HH12	6:B:1190:GNP:HNB3	1.46	0.61
2:J:154:THR:HB	2:J:166:VAL:O	2.00	0.61
1:D:219:VAL:HG22	1:D:225:ASN:ND2	2.14	0.61
3:M:352:ASN:ND2	3:M:353:ALA:N	2.49	0.61
3:M:424:LEU:HG	3:M:428:LEU:HD22	1.81	0.61
3:E:272:ASN:HA	3:M:906:LYS:NZ	2.15	0.61
3:M:270:ASP:HB2	3:M:273:ASP:HB3	1.83	0.61
3:L:205:LEU:HD13	3:L:611:VAL:HG11	1.83	0.60
1:G:176:ILE:CG1	3:M:413:ILE:HG12	2.31	0.60
1:A:411:ASP:N	1:A:411:ASP:OD1	2.33	0.60
3:E:205:LEU:HD13	3:E:611:VAL:HG11	1.83	0.60
3:E:524:HIS:CE1	3:E:866:ILE:HD11	2.36	0.60
3:L:270:ASP:HB2	3:L:273:ASP:HB3	1.83	0.60
3:L:352:ASN:HD22	3:L:353:ALA:H	1.47	0.60
3:L:352:ASN:ND2	3:L:353:ALA:N	2.49	0.60
1:D:176:ILE:CG1	3:L:413:ILE:HG12	2.31	0.60
1:A:101:MET:SD	4:F:61:PHE:CZ	2.95	0.60
2:K:23:HIS:CD2	2:K:67:ILE:HA	2.36	0.60
1:D:618:THR:O	1:D:622:LEU:HG	2.01	0.60
3:L:687:LYS:NZ	3:L:925:SER:HA	2.15	0.60
3:M:539:LYS:HE3	3:M:543:GLU:OE2	2.02	0.60
3:E:459:ARG:HG2	3:E:459:ARG:NH1	2.07	0.60
3:L:459:ARG:HG2	3:L:459:ARG:NH1	2.07	0.60
1:A:618:THR:O	1:A:622:LEU:HG	2.01	0.60
3:E:375:MET:CE	3:E:413:ILE:HG21	2.31	0.60
2:J:23:HIS:CD2	2:J:67:ILE:HA	2.36	0.60
3:L:539:LYS:HE3	3:L:543:GLU:OE2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:MET:HA	1:D:634:MET:HE3	1.83	0.60
1:G:651:ASN:HD22	1:G:651:ASN:N	1.81	0.60
3:L:333:LEU:HB2	3:L:400:ARG:CZ	2.32	0.60
3:L:764:ASP:HA	3:L:851:ARG:NH2	2.16	0.60
1:A:634:MET:HA	1:A:634:MET:HE3	1.84	0.60
1:D:681:ASP:HB2	1:D:682:PRO:HD2	1.84	0.60
1:A:176:ILE:CG1	3:E:413:ILE:HG12	2.31	0.60
1:G:618:THR:O	1:G:622:LEU:HG	2.01	0.60
3:M:205:LEU:HD13	3:M:611:VAL:HG11	1.83	0.60
2:B:23:HIS:CD2	2:B:67:ILE:HA	2.36	0.59
3:E:668:LEU:HG	3:E:672:ARG:HH21	1.67	0.59
3:E:915:GLU:O	3:E:919:ILE:HG13	2.02	0.59
2:B:142:GLU:HB3	1:G:426:LYS:HZ3	1.67	0.59
3:L:524:HIS:CE1	3:L:866:ILE:HD11	2.37	0.59
3:M:375:MET:CE	3:M:413:ILE:HG21	2.31	0.59
3:L:209:PRO:HG3	3:L:558:MET:CE	2.32	0.59
3:M:209:PRO:HG3	3:M:558:MET:CE	2.32	0.59
3:M:668:LEU:HG	3:M:672:ARG:HH21	1.66	0.59
3:E:539:LYS:HE3	3:E:543:GLU:OE2	2.02	0.59
3:L:729:PRO:HB2	3:L:732:HIS:HD2	1.68	0.59
3:M:524:HIS:CE1	3:M:866:ILE:HD11	2.37	0.59
3:E:270:ASP:HB2	3:E:273:ASP:HB3	1.83	0.59
2:K:140:VAL:CG1	2:K:141:SER:N	2.65	0.59
2:K:141:SER:OG	2:K:144:GLU:HG3	2.03	0.59
3:M:915:GLU:O	3:M:919:ILE:HG13	2.02	0.59
1:G:101:MET:SD	4:O:61:PHE:CZ	2.95	0.59
1:D:484:LEU:HD11	4:N:69:LEU:HD21	1.85	0.59
3:E:209:PRO:HG3	3:E:558:MET:CE	2.32	0.59
3:L:668:LEU:HG	3:L:672:ARG:HH21	1.66	0.59
1:D:511:LEU:O	1:D:512:LEU:HD23	2.03	0.59
2:J:140:VAL:CG1	2:J:141:SER:N	2.65	0.59
3:L:133:ARG:NH2	3:L:635:THR:O	2.36	0.59
3:M:333:LEU:HB2	3:M:400:ARG:CZ	2.32	0.59
1:A:68:TYR:HE1	4:F:69:LEU:HD22	1.68	0.59
3:E:764:ASP:HA	3:E:851:ARG:NH2	2.17	0.59
2:B:140:VAL:CG1	2:B:141:SER:N	2.65	0.59
3:E:333:LEU:HB2	3:E:400:ARG:CZ	2.32	0.59
3:E:667:SER:HB3	3:E:670:ASP:HB2	1.85	0.59
1:A:681:ASP:HB2	1:A:682:PRO:HD2	1.84	0.59
3:E:133:ARG:NH2	3:E:635:THR:O	2.36	0.59
3:E:352:ASN:ND2	3:E:353:ALA:N	2.49	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:141:SER:OG	2:J:144:GLU:HG3	2.03	0.59
3:M:352:ASN:HD22	3:M:353:ALA:H	1.47	0.58
3:M:728:VAL:HG21	3:M:733:ARG:NH2	2.18	0.58
3:E:209:PRO:HG3	3:E:558:MET:HE1	1.85	0.58
3:E:849:ASN:OD1	3:E:853:ARG:HD3	2.04	0.58
3:L:667:SER:HB3	3:L:670:ASP:HB2	1.85	0.58
3:M:563:SER:HB3	3:M:610:TYR:H	1.68	0.58
3:M:764:ASP:HA	3:M:851:ARG:NH2	2.17	0.58
1:G:511:LEU:O	1:G:512:LEU:HD23	2.03	0.58
3:M:667:SER:HB3	3:M:670:ASP:HB2	1.85	0.58
1:A:722:ARG:NH1	6:B:1190:GNP:HNB3	2.01	0.58
1:G:10:ASN:O	1:G:12:VAL:HG23	2.03	0.58
2:B:83:LEU:O	2:B:86:ASP:HB2	2.04	0.58
1:A:250:TRP:CD1	3:E:389:PRO:HB3	2.38	0.58
1:G:234:VAL:O	1:G:234:VAL:HG12	2.04	0.58
3:L:147:LEU:CB	3:L:148:PRO:CD	2.74	0.58
3:L:228:ILE:HD13	3:L:290:TYR:CD2	2.39	0.58
3:L:915:GLU:O	3:L:919:ILE:HG13	2.02	0.58
1:A:44:ASP:O	1:A:45:GLU:HG3	2.04	0.58
1:A:511:LEU:O	1:A:512:LEU:HD23	2.03	0.58
1:D:96:LEU:HG	1:D:97:SER:N	2.18	0.58
1:D:722:ARG:NH1	6:J:1190:GNP:HNB3	2.01	0.58
2:J:83:LEU:O	2:J:86:ASP:HB2	2.04	0.58
3:L:672:ARG:NH1	3:L:725:SER:HB3	2.19	0.58
3:M:699:ALA:HB1	3:M:921:LYS:HZ1	1.68	0.58
1:A:10:ASN:O	1:A:12:VAL:HG23	2.03	0.58
3:E:272:ASN:HA	3:M:906:LYS:HZ2	1.67	0.58
3:E:352:ASN:HD22	3:E:353:ALA:H	1.47	0.58
2:J:140:VAL:CG1	2:J:144:GLU:HB2	2.34	0.58
3:L:138:LEU:HD22	3:L:704:CYS:HB3	1.85	0.58
3:M:272:ASN:O	3:M:274:PRO:HD3	2.03	0.58
1:G:250:TRP:CD1	3:M:389:PRO:HB3	2.38	0.58
3:E:672:ARG:NH1	3:E:725:SER:HB3	2.19	0.58
1:G:681:ASP:HB2	1:G:682:PRO:HD2	1.84	0.58
1:D:10:ASN:O	1:D:12:VAL:HG23	2.03	0.58
1:D:250:TRP:CD1	3:L:389:PRO:HB3	2.38	0.58
1:D:44:ASP:O	1:D:45:GLU:HG3	2.04	0.58
1:A:88:HIS:HE1	1:D:742:SER:HB2	1.66	0.58
3:E:729:PRO:HB2	3:E:732:HIS:HD2	1.68	0.58
3:L:728:VAL:HG21	3:L:733:ARG:NH2	2.18	0.58
3:M:133:ARG:NH2	3:M:635:THR:O	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:729:PRO:HB2	3:M:732:HIS:HD2	1.68	0.58
1:G:68:TYR:HE1	4:O:69:LEU:HD22	1.68	0.58
3:E:138:LEU:HD22	3:E:704:CYS:HB3	1.85	0.58
1:G:44:ASP:O	1:G:45:GLU:HG3	2.04	0.58
3:M:228:ILE:HD13	3:M:290:TYR:CD2	2.39	0.58
3:M:138:LEU:HD22	3:M:704:CYS:HB3	1.85	0.58
3:M:849:ASN:OD1	3:M:853:ARG:HD3	2.04	0.58
1:A:484:LEU:HD11	4:F:69:LEU:HD21	1.85	0.57
1:G:484:LEU:HD11	4:O:69:LEU:HD21	1.85	0.57
2:K:83:LEU:O	2:K:86:ASP:HB2	2.04	0.57
3:E:303:PRO:HG3	3:E:342:ARG:NH1	2.19	0.57
3:E:563:SER:HB3	3:E:610:TYR:H	1.68	0.57
1:G:722:ARG:NH1	6:K:1190:GNP:HNB3	2.01	0.57
2:K:140:VAL:CG1	2:K:144:GLU:HB2	2.34	0.57
3:L:209:PRO:HG3	3:L:558:MET:HE1	1.84	0.57
3:M:672:ARG:NH1	3:M:725:SER:HB3	2.19	0.57
3:L:593:SER:HB2	3:L:744:PRO:HA	1.86	0.57
3:L:563:SER:HB3	3:L:610:TYR:H	1.68	0.57
3:L:872:TYR:CE2	3:L:897:TRP:HZ3	2.23	0.57
2:B:141:SER:OG	2:B:144:GLU:HG3	2.03	0.57
1:D:234:VAL:O	1:D:234:VAL:HG12	2.04	0.57
3:L:272:ASN:O	3:L:274:PRO:HD3	2.03	0.57
3:M:378:ILE:HD11	3:M:387:PRO:HG3	1.86	0.57
1:A:450:LEU:N	1:A:450:LEU:HD12	2.19	0.57
2:B:140:VAL:CG1	2:B:144:GLU:HB2	2.34	0.57
1:D:102:PRO:HD2	1:D:105:LEU:HD12	1.87	0.57
1:D:179:CYS:O	3:L:377:ASP:N	2.29	0.57
3:E:272:ASN:O	3:E:274:PRO:HD3	2.03	0.57
3:E:728:VAL:HG21	3:E:733:ARG:NH2	2.18	0.57
1:G:450:LEU:HD12	1:G:450:LEU:N	2.19	0.57
1:D:651:ASN:HD22	1:D:651:ASN:N	1.81	0.57
3:E:228:ILE:HD13	3:E:290:TYR:CD2	2.39	0.57
1:D:450:LEU:HD12	1:D:450:LEU:N	2.19	0.57
1:D:68:TYR:HE1	4:N:69:LEU:HD22	1.68	0.57
1:G:635:GLU:H	1:G:635:GLU:CD	2.08	0.57
3:L:802:ILE:O	3:L:808:LEU:HD23	2.05	0.57
1:G:196:MET:HE3	3:M:379:ALA:HB3	1.87	0.57
1:G:96:LEU:HG	1:G:97:SER:N	2.18	0.57
3:L:147:LEU:HD13	3:L:914:ARG:CZ	2.34	0.57
3:L:849:ASN:OD1	3:L:853:ARG:HD3	2.04	0.57
2:B:142:GLU:HB3	1:G:426:LYS:NZ	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:872:TYR:CE2	3:M:897:TRP:HZ3	2.22	0.57
1:D:101:MET:SD	4:N:61:PHE:CZ	2.95	0.57
3:E:593:SER:HB2	3:E:744:PRO:HA	1.86	0.56
1:D:196:MET:HE3	3:L:379:ALA:HB3	1.87	0.56
3:L:696:ALA:CB	3:L:702:ARG:HH21	2.18	0.56
3:E:378:ILE:HD11	3:E:387:PRO:HG3	1.86	0.56
3:E:872:TYR:CE2	3:E:897:TRP:HZ3	2.23	0.56
3:L:303:PRO:HG3	3:L:342:ARG:NH1	2.19	0.56
3:M:147:LEU:HD13	3:M:914:ARG:CZ	2.34	0.56
3:M:303:PRO:HG3	3:M:342:ARG:NH1	2.19	0.56
1:A:234:VAL:HG12	1:A:234:VAL:O	2.04	0.56
2:K:122:LEU:O	2:K:164:ARG:NH2	2.38	0.56
3:L:378:ILE:HD11	3:L:387:PRO:HG3	1.86	0.56
1:A:102:PRO:HD2	1:A:105:LEU:HD12	1.87	0.56
3:L:135:MET:HE2	3:L:641:GLU:OE1	2.04	0.56
1:G:179:CYS:O	3:M:377:ASP:N	2.29	0.56
3:M:696:ALA:CB	3:M:702:ARG:HH21	2.18	0.56
1:G:145:ILE:HA	1:G:148:LEU:HD12	1.88	0.56
1:G:65:LEU:HD11	1:G:105:LEU:HD21	1.88	0.56
3:M:802:ILE:O	3:M:808:LEU:HD23	2.05	0.56
1:A:145:ILE:HA	1:A:148:LEU:HD12	1.88	0.56
1:A:635:GLU:CD	1:A:635:GLU:H	2.08	0.56
2:B:122:LEU:O	2:B:164:ARG:NH2	2.38	0.56
1:D:145:ILE:HA	1:D:148:LEU:HD12	1.88	0.56
2:J:23:HIS:HD2	2:J:67:ILE:HA	1.70	0.56
3:E:699:ALA:HB1	3:E:921:LYS:HZ1	1.68	0.56
1:G:102:PRO:HD2	1:G:105:LEU:HD12	1.87	0.56
1:G:77:SER:HA	1:G:89:LEU:HB2	1.88	0.56
3:M:593:SER:HB2	3:M:744:PRO:HA	1.86	0.56
1:A:219:VAL:HG22	1:A:225:ASN:HD22	1.71	0.56
1:A:96:LEU:HG	1:A:97:SER:N	2.18	0.56
1:D:634:MET:HA	1:D:634:MET:CE	2.36	0.56
1:D:679:GLN:HG3	1:D:687:PHE:CE2	2.41	0.56
1:D:77:SER:HA	1:D:89:LEU:HB2	1.88	0.56
1:D:635:GLU:H	1:D:635:GLU:CD	2.08	0.56
3:L:375:MET:CE	3:L:413:ILE:HG21	2.31	0.56
1:A:68:TYR:O	1:A:81:PRO:HG3	2.07	0.56
1:A:196:MET:HE3	3:E:379:ALA:HB3	1.87	0.56
1:G:679:GLN:HG3	1:G:687:PHE:CE2	2.41	0.56
3:L:680:GLN:CB	3:L:920:MET:HE1	2.36	0.56
2:B:23:HIS:HD2	2:B:67:ILE:HA	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:PRO:HB3	2:B:74:LEU:HD13	1.89	0.55
3:E:147:LEU:HD13	3:E:914:ARG:CZ	2.34	0.55
3:E:802:ILE:O	3:E:808:LEU:HD23	2.05	0.55
1:G:68:TYR:O	1:G:81:PRO:HG3	2.06	0.55
2:J:122:LEU:O	2:J:164:ARG:NH2	2.38	0.55
2:K:23:HIS:HD2	2:K:67:ILE:HA	1.70	0.55
3:L:677:LYS:HG2	3:L:681:ASP:OD2	2.06	0.55
3:E:677:LYS:HG2	3:E:681:ASP:OD2	2.07	0.55
1:G:219:VAL:HG22	1:G:225:ASN:HD22	1.71	0.55
1:G:583:TYR:HB3	1:G:584:PRO:HD3	1.88	0.55
1:G:634:MET:CE	1:G:634:MET:HA	2.36	0.55
1:A:114:THR:HG22	1:A:116:LYS:H	1.72	0.55
1:A:46:LEU:HD12	1:A:47:ASN:H	1.71	0.55
1:D:46:LEU:HD12	1:D:47:ASN:H	1.71	0.55
2:K:57:PRO:HB3	2:K:74:LEU:HD13	1.89	0.55
1:A:679:GLN:HG3	1:A:687:PHE:CE2	2.41	0.55
1:G:455:SER:O	1:G:534:ARG:NH2	2.40	0.55
3:L:699:ALA:HB1	3:L:921:LYS:HZ1	1.70	0.55
1:A:65:LEU:HD11	1:A:105:LEU:HD21	1.88	0.55
3:E:696:ALA:CB	3:E:702:ARG:HH21	2.18	0.55
3:M:209:PRO:HG3	3:M:558:MET:HE1	1.88	0.55
1:A:583:TYR:HB3	1:A:584:PRO:HD3	1.88	0.55
3:E:410:ILE:HB	3:E:411:PRO:HD3	1.89	0.55
3:L:216:ASP:O	3:L:219:PRO:HD3	2.07	0.55
3:L:488:ILE:HD11	3:L:578:ARG:HH22	1.71	0.55
3:L:822:PHE:N	3:L:822:PHE:CD1	2.74	0.55
2:J:57:PRO:HB3	2:J:74:LEU:HD13	1.89	0.55
2:K:50:THR:O	2:K:50:THR:HG23	2.07	0.55
3:M:822:PHE:CD1	3:M:822:PHE:N	2.74	0.55
1:A:564:ALA:HB2	1:A:576:LEU:HD13	1.89	0.55
1:D:219:VAL:HG22	1:D:225:ASN:HD22	1.71	0.55
1:D:68:TYR:O	1:D:81:PRO:HG3	2.07	0.55
1:A:566:TYR:CG	1:A:764:VAL:HG12	2.42	0.54
1:A:761:GLN:O	1:A:765:SER:HB2	2.07	0.54
1:D:564:ALA:HB2	1:D:576:LEU:HD13	1.89	0.54
2:K:137:PRO:HG2	2:K:138:ASN:H	1.71	0.54
3:M:216:ASP:O	3:M:219:PRO:HD3	2.07	0.54
3:M:677:LYS:HG2	3:M:681:ASP:OD2	2.07	0.54
1:D:583:TYR:HB3	1:D:584:PRO:HD3	1.88	0.54
3:E:822:PHE:N	3:E:822:PHE:CD1	2.74	0.54
3:E:809:PHE:CD2	3:E:898:ALA:HB2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:102:ASP:N	2:K:103:PRO:HD3	2.23	0.54
3:M:488:ILE:HD11	3:M:578:ARG:HH22	1.71	0.54
2:B:102:ASP:N	2:B:103:PRO:HD3	2.22	0.54
1:D:411:ASP:OD1	1:D:411:ASP:N	2.33	0.54
1:D:566:TYR:CG	1:D:764:VAL:HG12	2.42	0.54
3:M:277:ARG:O	3:M:279:ASP:N	2.41	0.54
1:A:455:SER:O	1:A:534:ARG:NH2	2.40	0.54
1:A:634:MET:HA	1:A:634:MET:CE	2.36	0.54
1:D:114:THR:HG22	1:D:116:LYS:H	1.72	0.54
3:E:162:VAL:O	3:E:634:PRO:HG3	2.08	0.54
3:E:216:ASP:O	3:E:219:PRO:HD3	2.07	0.54
3:E:680:GLN:CB	3:E:920:MET:HE1	2.38	0.54
1:G:96:LEU:HD11	1:G:102:PRO:HD3	1.90	0.54
1:G:46:LEU:HD12	1:G:47:ASN:H	1.71	0.54
3:L:146:GLU:O	3:L:147:LEU:O	2.26	0.54
3:L:496:THR:HA	3:L:519:THR:HB	1.89	0.54
2:B:50:THR:HG23	2:B:50:THR:O	2.07	0.54
1:D:430:ASN:ND2	1:D:430:ASN:H	2.06	0.54
1:D:644:ASP:OD1	1:D:645:SER:N	2.41	0.54
1:G:566:TYR:CG	1:G:764:VAL:HG12	2.42	0.54
1:G:644:ASP:OD1	1:G:645:SER:N	2.41	0.54
3:M:801:LEU:HD12	3:M:809:PHE:O	2.07	0.54
2:B:137:PRO:HG2	2:B:138:ASN:H	1.71	0.54
1:D:679:GLN:HG2	1:D:691:LEU:CD1	2.37	0.54
1:A:96:LEU:HD11	1:A:102:PRO:HD3	1.90	0.54
1:A:179:CYS:O	3:E:377:ASP:N	2.28	0.54
1:D:455:SER:O	1:D:534:ARG:NH2	2.40	0.54
3:E:488:ILE:HD11	3:E:578:ARG:HH22	1.71	0.54
3:L:801:LEU:HD12	3:L:809:PHE:O	2.07	0.54
3:M:135:MET:HE2	3:M:641:GLU:OE1	2.07	0.54
1:A:679:GLN:HG2	1:A:691:LEU:CD1	2.38	0.54
1:A:77:SER:HA	1:A:89:LEU:HB2	1.88	0.54
3:E:277:ARG:O	3:E:279:ASP:N	2.41	0.54
1:G:679:GLN:HG2	1:G:691:LEU:CD1	2.37	0.54
1:G:761:GLN:O	1:G:765:SER:HB2	2.07	0.54
2:J:137:PRO:HG2	2:J:138:ASN:H	1.71	0.54
3:L:162:VAL:O	3:L:634:PRO:HG3	2.08	0.54
3:L:809:PHE:CD2	3:L:898:ALA:HB2	2.42	0.54
3:M:809:PHE:CD2	3:M:898:ALA:HB2	2.42	0.54
3:E:191:LYS:HE3	3:E:604:ILE:O	2.08	0.54
3:E:801:LEU:HD12	3:E:809:PHE:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:277:ARG:O	3:L:279:ASP:N	2.41	0.54
3:M:142:ASP:OD2	3:M:700:PRO:HB3	2.08	0.54
3:M:601:ASP:OD1	3:M:602:GLU:N	2.41	0.54
3:M:162:VAL:O	3:M:634:PRO:HG3	2.08	0.54
3:E:146:GLU:O	3:E:147:LEU:O	2.26	0.54
3:E:429:LYS:HD2	3:E:454:ILE:CD1	2.38	0.54
3:L:601:ASP:OD1	3:L:602:GLU:N	2.41	0.54
3:M:146:GLU:O	3:M:147:LEU:O	2.26	0.54
3:M:352:ASN:HA	3:M:452:LEU:HD23	1.90	0.54
1:D:65:LEU:HD11	1:D:105:LEU:HD21	1.88	0.53
3:E:361:LEU:HD22	3:E:398:ALA:HB1	1.90	0.53
3:E:496:THR:HA	3:E:519:THR:HB	1.89	0.53
3:E:601:ASP:OD1	3:E:602:GLU:N	2.41	0.53
3:L:361:LEU:HD22	3:L:398:ALA:HB1	1.90	0.53
3:L:410:ILE:HB	3:L:411:PRO:HD3	1.89	0.53
3:M:191:LYS:HE3	3:M:604:ILE:O	2.08	0.53
1:G:114:THR:HG22	1:G:116:LYS:H	1.72	0.53
2:J:102:ASP:N	2:J:103:PRO:HD3	2.22	0.53
1:D:96:LEU:HD11	1:D:102:PRO:HD3	1.90	0.53
1:G:564:ALA:HB2	1:G:576:LEU:HD13	1.89	0.53
2:J:50:THR:HG23	2:J:50:THR:O	2.07	0.53
3:M:361:LEU:HD22	3:M:398:ALA:HB1	1.90	0.53
1:A:644:ASP:OD1	1:A:645:SER:N	2.41	0.53
1:D:171:LEU:HD22	1:D:234:VAL:HG11	1.91	0.53
1:D:761:GLN:O	1:D:765:SER:HB2	2.07	0.53
3:E:819:ALA:HA	3:E:822:PHE:CE1	2.44	0.53
2:K:155:THR:CG2	2:K:166:VAL:H	2.21	0.53
3:E:142:ASP:OD2	3:E:700:PRO:HB3	2.08	0.53
3:L:819:ALA:HA	3:L:822:PHE:CE1	2.44	0.53
3:E:699:ALA:N	3:E:700:PRO:HD3	2.24	0.53
1:D:723:PHE:O	1:D:727:LYS:HG2	2.09	0.53
3:E:147:LEU:CB	3:E:148:PRO:CD	2.74	0.53
3:E:346:SER:OG	3:E:393:VAL:HG22	2.09	0.53
3:L:191:LYS:HE3	3:L:604:ILE:O	2.08	0.53
3:M:410:ILE:HB	3:M:411:PRO:HD3	1.89	0.53
3:M:817:VAL:O	3:M:819:ALA:N	2.42	0.53
3:M:819:ALA:HA	3:M:822:PHE:CE1	2.44	0.53
3:E:754:PRO:HG3	3:E:901:THR:O	2.09	0.53
3:L:429:LYS:HD2	3:L:454:ILE:CD1	2.38	0.53
3:M:496:THR:HA	3:M:519:THR:HB	1.89	0.53
1:A:430:ASN:ND2	1:A:430:ASN:H	2.06	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:352:ASN:HA	3:E:452:LEU:HD23	1.90	0.52
1:G:723:PHE:O	1:G:727:LYS:HG2	2.09	0.52
3:L:498:ASP:C	3:L:499:LEU:HD12	2.30	0.52
3:M:498:ASP:C	3:M:499:LEU:HD12	2.30	0.52
3:L:352:ASN:HA	3:L:452:LEU:HD23	1.90	0.52
3:L:817:VAL:O	3:L:819:ALA:N	2.42	0.52
3:E:250:ARG:HB3	3:E:260:ASN:O	2.09	0.52
3:L:142:ASP:OD2	3:L:700:PRO:HB3	2.08	0.52
3:M:346:SER:OG	3:M:393:VAL:HG22	2.09	0.52
3:M:429:LYS:HD2	3:M:454:ILE:CD1	2.38	0.52
3:M:822:PHE:HD1	3:M:822:PHE:N	2.08	0.52
3:M:754:PRO:HG3	3:M:901:THR:O	2.09	0.52
1:D:682:PRO:O	1:D:683:GLN:HB3	2.10	0.52
3:E:817:VAL:O	3:E:819:ALA:N	2.42	0.52
3:M:699:ALA:N	3:M:700:PRO:HD3	2.24	0.52
1:A:682:PRO:C	1:A:684:TYR:H	2.13	0.52
1:A:723:PHE:O	1:A:727:LYS:HG2	2.09	0.52
2:B:32:ASP:OD1	2:B:77:HIS:HA	2.10	0.52
2:J:155:THR:CG2	2:J:166:VAL:H	2.21	0.52
2:J:82:ARG:O	2:J:85:LYS:HE2	2.09	0.52
3:L:303:PRO:HG3	3:L:342:ARG:NH2	2.24	0.52
3:L:822:PHE:N	3:L:822:PHE:HD1	2.08	0.52
3:M:250:ARG:HB3	3:M:260:ASN:O	2.09	0.52
3:E:303:PRO:HG3	3:E:342:ARG:NH2	2.24	0.52
1:G:682:PRO:C	1:G:684:TYR:H	2.13	0.52
2:K:128:VAL:HG23	2:K:186:LEU:HD13	1.91	0.52
2:K:32:ASP:OD1	2:K:77:HIS:HA	2.10	0.52
3:M:303:PRO:HG3	3:M:342:ARG:NH2	2.24	0.52
3:M:519:THR:O	3:M:520:ALA:HB3	2.10	0.52
1:A:171:LEU:HD22	1:A:234:VAL:HG11	1.91	0.52
2:K:82:ARG:O	2:K:85:LYS:HE2	2.09	0.52
3:L:352:ASN:C	3:L:352:ASN:HD22	2.12	0.52
3:L:699:ALA:N	3:L:700:PRO:HD3	2.24	0.52
3:E:498:ASP:C	3:E:499:LEU:HD12	2.30	0.52
3:E:533:ASN:HB3	3:E:536:ASP:OD2	2.10	0.52
3:L:722:ALA:HB1	3:L:737:LEU:HD23	1.92	0.52
3:L:754:PRO:HG3	3:L:901:THR:O	2.09	0.52
3:E:704:CYS:SG	3:E:707:LEU:HD12	2.50	0.52
1:G:430:ASN:ND2	1:G:430:ASN:H	2.06	0.52
2:J:128:VAL:HG23	2:J:186:LEU:HD13	1.91	0.52
3:L:250:ARG:HB3	3:L:260:ASN:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ARG:O	2:B:85:LYS:HE2	2.09	0.52
3:E:822:PHE:N	3:E:822:PHE:HD1	2.08	0.52
1:G:682:PRO:O	1:G:683:GLN:HB3	2.10	0.52
3:L:346:SER:OG	3:L:393:VAL:HG22	2.09	0.52
3:L:519:THR:O	3:L:520:ALA:HB3	2.10	0.52
3:M:162:VAL:O	3:M:163:ILE:HD13	2.10	0.52
3:M:533:ASN:HB3	3:M:536:ASP:OD2	2.10	0.52
1:D:114:THR:CG2	1:D:115:ASN:H	2.22	0.51
3:E:715:HIS:HB2	3:E:916:PHE:CE2	2.45	0.51
1:G:114:THR:CG2	1:G:115:ASN:H	2.23	0.51
1:A:682:PRO:O	1:A:683:GLN:HB3	2.10	0.51
2:K:136:ALA:HB1	2:K:137:PRO:HD2	1.92	0.51
3:L:764:ASP:CA	3:L:851:ARG:HH22	2.24	0.51
3:M:420:THR:O	3:M:420:THR:HG22	2.10	0.51
2:B:155:THR:CG2	2:B:166:VAL:H	2.21	0.51
3:E:420:THR:HG22	3:E:420:THR:O	2.10	0.51
3:L:420:THR:HG22	3:L:420:THR:O	2.10	0.51
3:L:533:ASN:HB3	3:L:536:ASP:OD2	2.10	0.51
3:M:406:LEU:O	3:M:410:ILE:HG13	2.10	0.51
3:M:516:SER:HB2	3:M:522:GLN:N	2.26	0.51
3:M:704:CYS:SG	3:M:707:LEU:HD12	2.50	0.51
1:A:365:THR:HB	1:A:448:ALA:HB3	1.92	0.51
1:D:682:PRO:C	1:D:684:TYR:H	2.13	0.51
1:G:171:LEU:HD22	1:G:234:VAL:HG11	1.91	0.51
3:L:406:LEU:O	3:L:410:ILE:HG13	2.10	0.51
3:E:406:LEU:O	3:E:410:ILE:HG13	2.10	0.51
1:G:171:LEU:HD12	1:G:171:LEU:N	2.26	0.51
1:G:739:ARG:HH11	1:G:739:ARG:HG3	1.76	0.51
1:G:745:VAL:HG13	2:K:50:THR:HG21	1.92	0.51
2:J:155:THR:HG22	2:J:166:VAL:H	1.75	0.51
3:M:715:HIS:HB2	3:M:916:PHE:CE2	2.45	0.51
2:B:107:ASP:O	2:B:111:VAL:HG23	2.11	0.51
1:D:171:LEU:HD12	1:D:171:LEU:N	2.25	0.51
3:L:704:CYS:SG	3:L:707:LEU:HD12	2.50	0.51
2:B:155:THR:HG23	2:B:156:GLY:N	2.26	0.51
3:L:162:VAL:O	3:L:163:ILE:HD13	2.10	0.51
3:L:906:LYS:O	3:L:907:ILE:HD13	2.11	0.51
3:M:722:ALA:HB1	3:M:737:LEU:HD23	1.92	0.51
3:E:516:SER:HB2	3:E:522:GLN:N	2.26	0.51
2:J:107:ASP:O	2:J:111:VAL:HG23	2.11	0.51
2:K:172:SER:OG	2:K:175:MET:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:817:VAL:C	3:L:819:ALA:N	2.64	0.51
2:B:136:ALA:HB1	2:B:137:PRO:HD2	1.92	0.51
2:B:155:THR:HG22	2:B:166:VAL:H	1.75	0.51
3:E:279:ASP:CA	3:E:284:LYS:HE3	2.40	0.51
3:E:722:ALA:HB1	3:E:737:LEU:HD23	1.92	0.51
3:L:715:HIS:CE1	3:L:719:LYS:HE3	2.46	0.51
1:A:171:LEU:HD12	1:A:171:LEU:N	2.26	0.51
3:E:764:ASP:CA	3:E:851:ARG:HH22	2.23	0.51
1:A:144:ILE:O	1:A:148:LEU:HG	2.11	0.50
1:A:739:ARG:HG3	1:A:739:ARG:HH11	1.76	0.50
2:B:128:VAL:HG23	2:B:186:LEU:HD13	1.91	0.50
1:D:745:VAL:HG13	2:J:50:THR:HG21	1.92	0.50
3:E:448:THR:HG22	3:E:449:LEU:O	2.11	0.50
3:E:516:SER:HB2	3:E:521:GLY:C	2.31	0.50
3:L:372:GLN:HG2	3:L:373:ILE:N	2.26	0.50
3:L:516:SER:HB2	3:L:522:GLN:N	2.26	0.50
3:M:372:GLN:HG2	3:M:373:ILE:N	2.27	0.50
2:B:172:SER:OG	2:B:175:MET:HG2	2.11	0.50
1:D:144:ILE:O	1:D:148:LEU:HG	2.12	0.50
1:D:430:ASN:N	1:D:430:ASN:HD22	2.03	0.50
3:E:906:LYS:O	3:E:907:ILE:HD13	2.11	0.50
3:M:710:PHE:HB3	3:M:711:PRO:HD3	1.93	0.50
1:D:365:THR:HB	1:D:448:ALA:HB3	1.92	0.50
3:E:162:VAL:O	3:E:163:ILE:HD13	2.10	0.50
2:K:107:ASP:O	2:K:111:VAL:HG23	2.11	0.50
1:G:722:ARG:NH1	6:K:1190:GNP:N3B	2.57	0.50
3:L:715:HIS:HB2	3:L:916:PHE:CE2	2.45	0.50
3:M:516:SER:HB2	3:M:521:GLY:C	2.31	0.50
1:A:66:ASN:HD22	1:A:68:TYR:H	1.60	0.50
3:E:519:THR:O	3:E:520:ALA:HB3	2.10	0.50
3:E:715:HIS:CE1	3:E:719:LYS:HE3	2.46	0.50
3:E:860:ARG:HG2	3:E:869:GLN:HB2	1.93	0.50
2:J:155:THR:HG23	2:J:156:GLY:N	2.26	0.50
2:J:32:ASP:OD1	2:J:77:HIS:HA	2.10	0.50
3:M:855:ILE:O	3:M:858:GLN:HB3	2.12	0.50
3:M:906:LYS:O	3:M:907:ILE:HD13	2.11	0.50
3:M:680:GLN:CB	3:M:920:MET:HE1	2.41	0.50
1:D:66:ASN:HD22	1:D:68:TYR:H	1.60	0.50
3:E:855:ILE:O	3:E:858:GLN:HB3	2.12	0.50
2:J:136:ALA:HB1	2:J:137:PRO:HD2	1.92	0.50
3:L:250:ARG:HA	3:L:262:VAL:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:722:ALA:HB1	3:E:737:LEU:CD2	2.41	0.50
2:K:155:THR:HG22	2:K:166:VAL:H	1.75	0.50
3:L:499:LEU:HD12	3:L:499:LEU:N	2.27	0.50
3:L:504:GLU:OE2	3:L:530:SER:HB3	2.12	0.50
3:M:715:HIS:CE1	3:M:719:LYS:HE3	2.46	0.50
1:D:101:MET:HE1	4:N:61:PHE:CZ	2.42	0.50
1:A:745:VAL:HG13	2:B:50:THR:HG21	1.92	0.50
3:L:710:PHE:HB3	3:L:711:PRO:HD3	1.93	0.50
3:M:250:ARG:HA	3:M:262:VAL:HG23	1.94	0.50
1:G:144:ILE:O	1:G:148:LEU:HG	2.11	0.50
1:G:365:THR:HB	1:G:448:ALA:HB3	1.92	0.50
2:J:140:VAL:HG13	2:J:144:GLU:CD	2.32	0.50
3:L:516:SER:HB2	3:L:521:GLY:C	2.31	0.50
3:M:499:LEU:N	3:M:499:LEU:HD12	2.27	0.50
2:K:176:ARG:HA	2:K:179:TYR:HE2	1.77	0.50
3:M:504:GLU:OE2	3:M:530:SER:HB3	2.12	0.50
1:D:739:ARG:HH11	1:D:739:ARG:HG3	1.76	0.49
1:G:645:SER:HA	1:G:728:LEU:HD13	1.94	0.49
2:K:140:VAL:HG13	2:K:144:GLU:CD	2.33	0.49
2:K:155:THR:HG23	2:K:156:GLY:N	2.26	0.49
3:L:448:THR:HG22	3:L:449:LEU:O	2.11	0.49
3:L:907:ILE:HG22	3:L:908:LEU:N	2.27	0.49
3:M:279:ASP:CA	3:M:284:LYS:HE3	2.39	0.49
3:M:448:THR:HG22	3:M:449:LEU:O	2.11	0.49
3:M:818:PRO:C	3:M:820:LEU:N	2.66	0.49
3:M:860:ARG:HG2	3:M:869:GLN:HB2	1.93	0.49
1:G:644:ASP:OD2	1:G:731:SER:HB3	2.13	0.49
3:L:150:PRO:HG2	3:L:708:ARG:HH11	1.78	0.49
3:M:817:VAL:C	3:M:819:ALA:N	2.64	0.49
3:E:768:LEU:CG	3:E:769:PRO:HD2	2.40	0.49
3:E:907:ILE:HG22	3:E:908:LEU:N	2.27	0.49
3:L:722:ALA:HB1	3:L:737:LEU:CD2	2.41	0.49
3:E:423:ALA:HA	3:E:452:LEU:O	2.13	0.49
1:G:390:LYS:HD2	1:G:390:LYS:N	2.28	0.49
3:L:911:GLU:HG3	3:L:919:ILE:HD11	1.94	0.49
3:M:907:ILE:HG22	3:M:908:LEU:N	2.27	0.49
1:D:645:SER:HA	1:D:728:LEU:HD13	1.94	0.49
3:E:504:GLU:OE2	3:E:530:SER:HB3	2.12	0.49
3:M:722:ALA:HB1	3:M:737:LEU:CD2	2.41	0.49
1:A:171:LEU:CD2	1:A:234:VAL:HG11	2.43	0.49
1:D:395:TYR:CD1	1:D:497:SER:HA	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:372:GLN:HG2	3:E:373:ILE:N	2.26	0.49
3:E:589:PRO:O	3:E:590:ARG:HD3	2.13	0.49
3:E:687:LYS:HZ2	3:E:925:SER:HA	1.77	0.49
3:M:794:PHE:HA	3:M:800:TYR:CZ	2.48	0.49
3:M:911:GLU:HG3	3:M:919:ILE:HD11	1.94	0.49
1:G:171:LEU:CD2	1:G:234:VAL:HG11	2.43	0.49
2:K:176:ARG:HA	2:K:179:TYR:CE2	2.48	0.49
3:L:423:ALA:HA	3:L:452:LEU:O	2.13	0.49
3:L:818:PRO:C	3:L:820:LEU:N	2.66	0.49
3:M:150:PRO:HG2	3:M:708:ARG:HH11	1.78	0.49
2:B:140:VAL:HG13	2:B:144:GLU:CD	2.33	0.49
1:D:644:ASP:OD2	1:D:731:SER:HB3	2.13	0.49
3:E:499:LEU:HD12	3:E:499:LEU:N	2.27	0.49
1:G:430:ASN:HD22	1:G:430:ASN:N	2.03	0.49
3:M:764:ASP:CA	3:M:851:ARG:HH22	2.24	0.49
1:A:390:LYS:HD2	1:A:390:LYS:N	2.28	0.49
1:A:395:TYR:CD1	1:A:497:SER:HA	2.48	0.49
1:A:645:SER:HA	1:A:728:LEU:HD13	1.94	0.49
2:B:176:ARG:HA	2:B:179:TYR:CE2	2.48	0.49
1:D:147:SER:HB3	1:D:384:TYR:CE2	2.48	0.49
1:D:390:LYS:HD2	1:D:390:LYS:N	2.28	0.49
3:E:911:GLU:HG3	3:E:919:ILE:HD11	1.94	0.49
2:J:172:SER:OG	2:J:175:MET:HG2	2.11	0.49
3:L:794:PHE:HA	3:L:800:TYR:CZ	2.48	0.49
3:M:703:LEU:HG	3:M:704:CYS:H	1.77	0.49
2:B:85:LYS:HA	2:B:88:PHE:CD2	2.48	0.49
1:A:91:PRO:CA	1:D:669:GLN:NE2	2.73	0.49
3:E:710:PHE:HB3	3:E:711:PRO:HD3	1.93	0.49
1:G:176:ILE:HD12	3:M:413:ILE:CG1	2.38	0.49
2:J:176:ARG:HA	2:J:179:TYR:CE2	2.48	0.49
3:L:279:ASP:CA	3:L:284:LYS:HE3	2.39	0.49
3:L:860:ARG:HG2	3:L:869:GLN:HB2	1.93	0.49
3:M:795:GLU:C	3:M:797:TYR:H	2.17	0.49
3:E:352:ASN:C	3:E:352:ASN:ND2	2.67	0.48
3:E:356:TYR:OH	3:E:430:SER:HB3	2.13	0.48
1:G:147:SER:HB3	1:G:384:TYR:CE2	2.48	0.48
1:G:616:GLU:CG	1:G:620:ASN:CB	2.91	0.48
2:J:88:PHE:N	2:J:89:PRO:CD	2.76	0.48
3:L:312:VAL:O	3:L:312:VAL:CG1	2.61	0.48
3:L:703:LEU:HG	3:L:704:CYS:H	1.77	0.48
3:M:135:MET:HE1	3:M:634:PRO:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:215:ASP:O	3:M:219:PRO:HG3	2.13	0.48
3:E:818:PRO:C	3:E:820:LEU:N	2.66	0.48
1:G:451:SER:C	1:G:453:TYR:H	2.17	0.48
3:M:589:PRO:O	3:M:590:ARG:HD3	2.13	0.48
3:E:338:ASN:OD1	3:E:341:GLU:HA	2.13	0.48
2:J:176:ARG:HA	2:J:179:TYR:HE2	1.77	0.48
2:K:88:PHE:N	2:K:89:PRO:CD	2.76	0.48
1:A:644:ASP:OD2	1:A:731:SER:HB3	2.12	0.48
2:B:134:ILE:HG12	2:B:172:SER:HB2	1.96	0.48
2:B:88:PHE:N	2:B:89:PRO:CD	2.76	0.48
1:D:171:LEU:CD2	1:D:234:VAL:HG11	2.43	0.48
3:E:215:ASP:O	3:E:219:PRO:HG3	2.13	0.48
3:E:794:PHE:HA	3:E:800:TYR:CZ	2.48	0.48
3:E:817:VAL:C	3:E:819:ALA:N	2.64	0.48
1:G:66:ASN:HD22	1:G:68:TYR:H	1.60	0.48
2:J:103:PRO:HG3	2:J:140:VAL:HG21	1.96	0.48
3:L:248:GLY:O	3:L:277:ARG:NH2	2.33	0.48
3:L:534:PRO:O	3:L:538:VAL:HG23	2.13	0.48
3:L:192:ASN:HA	3:L:603:SER:HA	1.96	0.48
3:L:855:ILE:O	3:L:858:GLN:HB3	2.12	0.48
3:M:534:PRO:O	3:M:538:VAL:HG23	2.13	0.48
1:D:616:GLU:CG	1:D:620:ASN:CB	2.91	0.48
3:E:230:ARG:HD3	3:E:237:TYR:CD2	2.49	0.48
3:E:192:ASN:HA	3:E:603:SER:HA	1.96	0.48
2:J:32:ASP:HB3	2:J:77:HIS:N	2.29	0.48
2:K:32:ASP:HB3	2:K:77:HIS:N	2.29	0.48
2:K:99:ASP:OD1	2:K:133:LYS:HD2	2.14	0.48
3:L:230:ARG:HD3	3:L:237:TYR:CD2	2.49	0.48
3:M:423:ALA:HA	3:M:452:LEU:O	2.13	0.48
1:A:147:SER:HB3	1:A:384:TYR:CE2	2.48	0.48
1:D:739:ARG:HG2	1:D:744:ILE:HD11	1.96	0.48
3:E:703:LEU:HG	3:E:704:CYS:H	1.77	0.48
2:J:134:ILE:HG12	2:J:172:SER:HB2	1.96	0.48
2:J:99:ASP:OD1	2:J:133:LYS:HD2	2.14	0.48
3:L:224:GLU:HA	3:L:291:MET:HG3	1.96	0.48
3:L:488:ILE:HD11	3:L:578:ARG:NH2	2.28	0.48
3:M:230:ARG:HD3	3:M:237:TYR:CD2	2.49	0.48
3:M:312:VAL:CG1	3:M:312:VAL:O	2.61	0.48
1:D:68:TYR:CE1	4:N:69:LEU:HD22	2.49	0.48
1:A:114:THR:CG2	1:A:115:ASN:H	2.23	0.48
1:A:17:ASN:HB2	1:A:522:SER:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ARG:HA	2:B:179:TYR:HE2	1.77	0.48
2:B:32:ASP:HB3	2:B:77:HIS:N	2.29	0.48
1:D:96:LEU:CG	1:D:97:SER:N	2.76	0.48
3:E:250:ARG:HA	3:E:262:VAL:HG23	1.94	0.48
3:E:312:VAL:CG1	3:E:312:VAL:O	2.61	0.48
2:J:85:LYS:HA	2:J:88:PHE:CD2	2.48	0.48
2:K:134:ILE:HG12	2:K:172:SER:HB2	1.96	0.48
3:L:352:ASN:C	3:L:352:ASN:ND2	2.67	0.48
3:M:192:ASN:HA	3:M:603:SER:HA	1.96	0.48
1:A:739:ARG:HG2	1:A:744:ILE:HD11	1.96	0.48
2:B:103:PRO:HG3	2:B:140:VAL:HG21	1.96	0.48
3:E:534:PRO:O	3:E:538:VAL:HG23	2.13	0.48
3:E:795:GLU:C	3:E:797:TYR:H	2.16	0.48
1:G:395:TYR:CD1	1:G:497:SER:HA	2.48	0.48
3:L:215:ASP:O	3:L:219:PRO:HG3	2.13	0.48
3:L:338:ASN:OD1	3:L:341:GLU:HA	2.13	0.48
3:M:352:ASN:N	3:M:352:ASN:HD22	2.11	0.48
3:M:488:ILE:HD11	3:M:578:ARG:NH2	2.28	0.48
3:M:768:LEU:CG	3:M:769:PRO:HD2	2.40	0.48
1:A:96:LEU:CG	1:A:97:SER:N	2.76	0.48
3:E:150:PRO:HG2	3:E:708:ARG:HH11	1.78	0.48
2:K:85:LYS:HA	2:K:88:PHE:CD2	2.48	0.48
3:L:795:GLU:HB3	3:L:797:TYR:CE2	2.49	0.48
3:M:356:TYR:OH	3:M:430:SER:HB3	2.13	0.48
1:D:42:GLU:OE2	1:D:397:LYS:HE2	2.14	0.48
2:K:137:PRO:C	2:K:139:ALA:H	2.18	0.48
3:L:589:PRO:O	3:L:590:ARG:HD3	2.13	0.48
3:L:796:ARG:NH1	3:L:815:ASP:OD2	2.47	0.48
3:M:338:ASN:OD1	3:M:341:GLU:HA	2.13	0.48
3:E:133:ARG:NE	3:E:135:MET:SD	2.87	0.47
1:G:679:GLN:HG3	1:G:687:PHE:HE2	1.79	0.47
1:G:96:LEU:CG	1:G:97:SER:N	2.76	0.47
2:J:137:PRO:C	2:J:139:ALA:H	2.18	0.47
3:L:230:ARG:HD2	3:L:235:ARG:O	2.14	0.47
3:L:667:SER:HB3	3:L:670:ASP:CB	2.44	0.47
3:L:795:GLU:C	3:L:797:TYR:H	2.17	0.47
3:M:224:GLU:HA	3:M:291:MET:HG3	1.96	0.47
3:M:352:ASN:ND2	3:M:352:ASN:C	2.67	0.47
3:M:580:SER:O	3:M:581:ASP:HB2	2.14	0.47
1:A:616:GLU:CG	1:A:620:ASN:CB	2.91	0.47
1:D:19:PHE:HB2	1:D:511:LEU:CD2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ASN:HB2	1:D:522:SER:HB2	1.96	0.47
3:E:580:SER:O	3:E:581:ASP:HB2	2.14	0.47
3:E:796:ARG:NH1	3:E:815:ASP:OD2	2.47	0.47
1:A:68:TYR:CE1	4:F:69:LEU:HD22	2.49	0.47
1:G:195:GLU:O	1:G:199:GLY:N	2.41	0.47
3:L:277:ARG:C	3:L:279:ASP:H	2.17	0.47
3:L:356:TYR:OH	3:L:430:SER:HB3	2.13	0.47
3:L:715:HIS:NE2	3:L:719:LYS:HE3	2.30	0.47
3:M:177:ALA:HB1	3:M:182:ILE:HG22	1.96	0.47
3:M:277:ARG:C	3:M:279:ASP:H	2.18	0.47
3:M:796:ARG:NH1	3:M:815:ASP:OD2	2.47	0.47
3:E:488:ILE:HD11	3:E:578:ARG:NH2	2.28	0.47
3:E:795:GLU:HB3	3:E:797:TYR:CE2	2.49	0.47
1:G:634:MET:HA	1:G:634:MET:HE3	1.94	0.47
2:K:103:PRO:HG3	2:K:140:VAL:HG21	1.96	0.47
2:B:137:PRO:C	2:B:139:ALA:H	2.18	0.47
3:E:352:ASN:N	3:E:352:ASN:HD22	2.11	0.47
3:L:580:SER:O	3:L:581:ASP:HB2	2.14	0.47
3:M:761:ASP:O	3:M:762:MET:O	2.33	0.47
1:A:42:GLU:OE2	1:A:397:LYS:HE2	2.14	0.47
1:A:451:SER:C	1:A:453:TYR:H	2.17	0.47
1:A:679:GLN:HG3	1:A:687:PHE:HE2	1.79	0.47
2:B:99:ASP:OD1	2:B:133:LYS:HD2	2.14	0.47
3:E:149:PRO:O	3:E:150:PRO:C	2.53	0.47
1:G:561:GLN:HG2	1:G:763:ALA:HA	1.96	0.47
3:L:135:MET:HE1	3:L:634:PRO:HB2	1.96	0.47
3:M:795:GLU:HB3	3:M:797:TYR:CE2	2.49	0.47
3:E:248:GLY:O	3:E:277:ARG:NH2	2.33	0.47
2:K:23:HIS:HD2	2:K:68:LYS:H	1.62	0.47
3:M:325:THR:OG1	3:M:445:VAL:HG11	2.15	0.47
3:M:667:SER:HB3	3:M:670:ASP:CB	2.44	0.47
3:E:378:ILE:CD1	3:E:387:PRO:HG3	2.45	0.47
3:E:388:ARG:HB2	3:E:389:PRO:HD2	1.97	0.47
3:L:352:ASN:HD22	3:L:352:ASN:N	2.11	0.47
3:L:205:LEU:CD1	3:L:611:VAL:HG11	2.44	0.47
3:M:352:ASN:C	3:M:352:ASN:HD22	2.12	0.47
1:A:561:GLN:HG2	1:A:763:ALA:HA	1.96	0.47
1:D:96:LEU:HD11	1:D:101:MET:HA	1.97	0.47
3:E:230:ARG:HD2	3:E:235:ARG:O	2.15	0.47
3:E:761:ASP:O	3:E:762:MET:O	2.33	0.47
3:L:133:ARG:HG3	3:L:135:MET:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:ILE:HD13	3:L:709:MET:HE1	1.96	0.47
3:M:149:PRO:O	3:M:150:PRO:C	2.53	0.47
1:A:66:ASN:HD21	1:A:68:TYR:HB2	1.80	0.47
1:D:164:ASN:HD22	1:D:165:VAL:H	1.63	0.47
3:E:848:PHE:O	3:E:851:ARG:HB2	2.15	0.47
1:G:594:GLN:HE21	1:G:601:ASN:HD21	1.63	0.47
3:M:249:ARG:O	3:M:250:ARG:HG2	2.15	0.47
3:E:177:ALA:HB1	3:E:182:ILE:HG22	1.96	0.47
3:E:224:GLU:HA	3:E:291:MET:HG3	1.96	0.47
3:E:325:THR:OG1	3:E:445:VAL:HG11	2.15	0.47
1:G:651:ASN:ND2	1:G:651:ASN:N	2.53	0.47
1:G:739:ARG:HG2	1:G:744:ILE:HD11	1.96	0.47
3:M:133:ARG:HG3	3:M:135:MET:HG2	1.97	0.47
3:M:248:GLY:O	3:M:277:ARG:NH2	2.33	0.47
1:A:430:ASN:HD22	1:A:430:ASN:N	2.03	0.47
2:B:62:LEU:HD12	2:B:71:THR:HG21	1.97	0.47
1:D:551:TRP:CE3	1:D:552:LEU:HD13	2.50	0.47
1:G:551:TRP:CE3	1:G:552:LEU:HD13	2.50	0.47
2:J:62:LEU:HD12	2:J:71:THR:HG21	1.97	0.47
3:M:133:ARG:HH21	3:M:135:MET:HE2	1.79	0.47
1:D:661:PHE:HA	1:D:709:PRO:HB2	1.97	0.46
3:E:133:ARG:HG3	3:E:135:MET:HG2	1.97	0.46
1:G:17:ASN:HB2	1:G:522:SER:HB2	1.96	0.46
1:G:485:ALA:HB2	1:G:511:LEU:HD11	1.97	0.46
3:L:177:ALA:HB1	3:L:182:ILE:HG22	1.96	0.46
3:L:388:ARG:HB2	3:L:389:PRO:HD2	1.97	0.46
3:L:325:THR:OG1	3:L:445:VAL:HG11	2.15	0.46
3:M:301:PRO:HA	3:M:302:PRO:HD3	1.68	0.46
3:M:600:VAL:HG13	3:M:604:ILE:HD11	1.96	0.46
2:K:62:LEU:HD12	2:K:71:THR:HG21	1.96	0.46
3:L:133:ARG:NE	3:L:135:MET:SD	2.87	0.46
3:M:150:PRO:HG2	3:M:708:ARG:HD3	1.97	0.46
3:M:230:ARG:HD2	3:M:235:ARG:O	2.15	0.46
1:A:485:ALA:HB2	1:A:511:LEU:HD11	1.97	0.46
1:A:556:LEU:HD22	1:A:587:THR:HG21	1.98	0.46
1:D:343:VAL:O	1:D:362:THR:HG22	2.16	0.46
1:D:451:SER:C	1:D:453:TYR:H	2.17	0.46
1:D:594:GLN:HE21	1:D:601:ASN:HD21	1.63	0.46
1:D:66:ASN:HD21	1:D:68:TYR:HB2	1.80	0.46
3:E:168:MET:SD	3:E:175:SER:OG	2.69	0.46
3:E:314:GLN:CG	3:E:318:LYS:HE3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:600:VAL:HG13	3:E:604:ILE:HD11	1.96	0.46
1:G:42:GLU:OE2	1:G:397:LYS:HE2	2.14	0.46
1:G:661:PHE:HA	1:G:709:PRO:HB2	1.97	0.46
3:L:378:ILE:CD1	3:L:387:PRO:HG3	2.45	0.46
3:M:212:HIS:O	3:M:590:ARG:HB3	2.16	0.46
3:M:715:HIS:NE2	3:M:719:LYS:HE3	2.30	0.46
1:D:679:GLN:HG3	1:D:687:PHE:HE2	1.79	0.46
3:E:277:ARG:C	3:E:279:ASP:H	2.18	0.46
1:G:687:PHE:CE2	1:G:691:LEU:HD11	2.51	0.46
3:L:768:LEU:CG	3:L:769:PRO:HD2	2.40	0.46
3:M:822:PHE:H	3:M:822:PHE:HD1	1.63	0.46
3:M:900:SER:HA	3:M:907:ILE:HG21	1.97	0.46
3:E:715:HIS:NE2	3:E:719:LYS:HE3	2.29	0.46
3:E:822:PHE:H	3:E:822:PHE:HD1	1.63	0.46
1:G:96:LEU:HD11	1:G:101:MET:HA	1.97	0.46
2:J:23:HIS:HD2	2:J:68:LYS:H	1.62	0.46
3:L:314:GLN:CG	3:L:318:LYS:HE3	2.46	0.46
3:L:144:LEU:HD22	3:L:918:GLN:NE2	2.31	0.46
3:L:687:LYS:HZ1	3:L:925:SER:HA	1.80	0.46
3:M:133:ARG:NE	3:M:135:MET:SD	2.88	0.46
3:E:170:VAL:HG12	3:E:170:VAL:O	2.16	0.46
1:G:19:PHE:HB2	1:G:511:LEU:CD2	2.44	0.46
1:G:432:ILE:CD1	1:G:442:THR:HA	2.44	0.46
3:L:149:PRO:O	3:L:150:PRO:C	2.53	0.46
3:L:212:HIS:O	3:L:590:ARG:HB3	2.16	0.46
3:L:600:VAL:HG13	3:L:604:ILE:HD11	1.96	0.46
3:L:761:ASP:O	3:L:762:MET:O	2.33	0.46
3:E:667:SER:HB3	3:E:670:ASP:CB	2.44	0.46
3:L:249:ARG:O	3:L:250:ARG:HG2	2.15	0.46
3:L:279:ASP:C	3:L:284:LYS:HE3	2.36	0.46
3:M:378:ILE:HD13	3:M:385:PHE:CZ	2.51	0.46
3:M:378:ILE:CD1	3:M:387:PRO:HG3	2.45	0.46
3:M:388:ARG:HB2	3:M:389:PRO:HD2	1.97	0.46
1:A:432:ILE:CD1	1:A:442:THR:HA	2.44	0.46
1:D:485:ALA:HB2	1:D:511:LEU:HD11	1.97	0.46
3:E:205:LEU:CD1	3:E:611:VAL:HG11	2.44	0.46
1:G:343:VAL:O	1:G:362:THR:HG22	2.16	0.46
2:K:31:LEU:HD22	2:K:81:ARG:NH2	2.31	0.46
3:L:848:PHE:O	3:L:851:ARG:HB2	2.15	0.46
3:M:314:GLN:CG	3:M:318:LYS:HE3	2.46	0.46
1:D:561:GLN:HG2	1:D:763:ALA:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:LEU:HD22	2:J:81:ARG:NH2	2.31	0.46
3:M:795:GLU:O	3:M:797:TYR:N	2.49	0.46
3:M:848:PHE:O	3:M:851:ARG:HB2	2.15	0.46
1:A:164:ASN:HD22	1:A:165:VAL:H	1.63	0.46
2:B:31:LEU:HD22	2:B:81:ARG:NH2	2.31	0.46
1:D:556:LEU:HD22	1:D:587:THR:HG21	1.98	0.46
3:E:249:ARG:O	3:E:250:ARG:HG2	2.15	0.46
3:E:900:SER:HA	3:E:907:ILE:HG21	1.97	0.46
3:M:147:LEU:CB	3:M:148:PRO:CD	2.74	0.46
3:M:197:LYS:HA	3:M:197:LYS:HD2	1.72	0.46
3:M:417:ASN:OD1	3:M:419:ILE:N	2.41	0.46
1:D:734:TYR:HA	1:D:744:ILE:HG21	1.98	0.45
3:E:144:LEU:HD22	3:E:918:GLN:NE2	2.31	0.45
3:E:150:PRO:HG2	3:E:708:ARG:HD3	1.97	0.45
3:L:313:SER:O	3:L:317:ILE:HG12	2.16	0.45
3:L:378:ILE:HD13	3:L:385:PHE:CZ	2.51	0.45
3:L:454:ILE:HG13	3:L:454:ILE:H	1.49	0.45
3:L:795:GLU:O	3:L:797:TYR:N	2.49	0.45
3:M:205:LEU:CD1	3:M:611:VAL:HG11	2.44	0.45
3:M:417:ASN:HD21	3:M:419:ILE:HD12	1.81	0.45
3:M:920:MET:CA	3:M:920:MET:HE3	2.45	0.45
1:A:96:LEU:HD11	1:A:101:MET:HA	1.97	0.45
1:A:687:PHE:CE2	1:A:691:LEU:HD11	2.51	0.45
1:D:687:PHE:CE2	1:D:691:LEU:HD11	2.51	0.45
3:E:417:ASN:HD21	3:E:419:ILE:HD12	1.81	0.45
2:K:110:ARG:HH11	2:K:110:ARG:HG3	1.82	0.45
2:K:32:ASP:O	2:K:105:ARG:NH2	2.49	0.45
3:L:822:PHE:H	3:L:822:PHE:HD1	1.63	0.45
1:A:464:ASN:ND2	1:A:465:THR:H	2.15	0.45
1:A:551:TRP:CE3	1:A:552:LEU:HD13	2.50	0.45
1:A:594:GLN:HE21	1:A:601:ASN:HD21	1.63	0.45
2:B:32:ASP:O	2:B:105:ARG:NH2	2.49	0.45
2:B:97:LEU:HD12	2:B:97:LEU:N	2.31	0.45
1:D:432:ILE:CD1	1:D:442:THR:HA	2.43	0.45
3:E:795:GLU:O	3:E:797:TYR:N	2.49	0.45
3:L:417:ASN:HD21	3:L:419:ILE:HD12	1.81	0.45
3:L:668:LEU:HD21	3:L:733:ARG:NH1	2.31	0.45
1:A:176:ILE:HD12	3:E:413:ILE:CG1	2.38	0.45
1:A:661:PHE:HA	1:A:709:PRO:HB2	1.97	0.45
3:E:135:MET:HE1	3:E:634:PRO:HB2	1.99	0.45
1:G:44:ASP:C	1:G:45:GLU:HG3	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:32:ASP:O	2:J:105:ARG:NH2	2.49	0.45
3:M:170:VAL:O	3:M:170:VAL:HG12	2.16	0.45
3:M:144:LEU:HD22	3:M:918:GLN:NE2	2.31	0.45
1:A:734:TYR:HA	1:A:744:ILE:HG21	1.98	0.45
2:B:23:HIS:HD2	2:B:68:LYS:H	1.62	0.45
1:G:164:ASN:HD22	1:G:165:VAL:H	1.63	0.45
3:L:147:LEU:O	3:L:149:PRO:N	2.50	0.45
1:D:101:MET:HE1	4:N:61:PHE:CE2	2.51	0.45
2:K:97:LEU:N	2:K:97:LEU:HD12	2.31	0.45
3:L:900:SER:HA	3:L:907:ILE:HG21	1.98	0.45
3:M:672:ARG:NH1	3:M:725:SER:HA	2.32	0.45
1:A:19:PHE:HB2	1:A:511:LEU:CD2	2.44	0.45
1:A:44:ASP:C	1:A:45:GLU:HG3	2.37	0.45
2:B:40:LEU:HD22	2:B:73:ASP:HB2	1.99	0.45
3:E:424:LEU:O	3:E:428:LEU:HB2	2.17	0.45
3:E:506:TYR:CE2	3:E:508:ASP:HB2	2.52	0.45
3:E:212:HIS:O	3:E:590:ARG:HB3	2.16	0.45
3:E:756:VAL:O	3:E:786:PRO:HA	2.17	0.45
2:B:142:GLU:CB	1:G:426:LYS:HZ3	2.30	0.45
3:L:791:SER:H	3:L:905:ASP:CG	2.20	0.45
3:M:279:ASP:C	3:M:284:LYS:HE3	2.36	0.45
3:E:313:SER:O	3:E:317:ILE:HG12	2.16	0.45
4:F:62:LEU:HA	4:F:66:GLN:OE1	2.17	0.45
1:G:66:ASN:HD21	1:G:68:TYR:HB2	1.80	0.45
2:J:85:LYS:HA	2:J:88:PHE:CE2	2.52	0.45
2:K:155:THR:OG1	2:K:156:GLY:N	2.50	0.45
3:M:908:LEU:C	3:M:910:ASN:H	2.21	0.45
1:A:343:VAL:O	1:A:362:THR:HG22	2.16	0.45
1:D:464:ASN:ND2	1:D:465:THR:H	2.15	0.45
3:E:279:ASP:C	3:E:284:LYS:HE3	2.36	0.45
3:E:672:ARG:NH1	3:E:725:SER:HA	2.32	0.45
1:G:46:LEU:HG	1:G:47:ASN:N	2.32	0.45
1:G:68:TYR:CE1	4:O:69:LEU:HD22	2.49	0.45
1:G:734:TYR:HA	1:G:744:ILE:HG21	1.98	0.45
2:K:125:VAL:HA	2:K:126:PRO:HD3	1.87	0.45
2:K:37:THR:HG22	2:K:51:LEU:HD13	1.99	0.45
3:M:791:SER:H	3:M:905:ASP:CG	2.21	0.45
4:O:62:LEU:HA	4:O:66:GLN:OE1	2.17	0.45
1:A:187:GLU:HB2	1:A:296:PRO:HG3	1.99	0.45
2:B:110:ARG:HG3	2:B:110:ARG:HH11	1.82	0.45
1:D:187:GLU:HB2	1:D:296:PRO:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASP:C	1:D:45:GLU:HG3	2.37	0.45
1:G:411:ASP:N	1:G:411:ASP:OD1	2.33	0.45
1:G:556:LEU:HD22	1:G:587:THR:HG21	1.98	0.45
3:L:150:PRO:HG2	3:L:708:ARG:HD3	1.97	0.45
3:M:756:VAL:O	3:M:786:PRO:HA	2.17	0.45
1:D:588:TYR:O	1:D:591:ARG:HG2	2.18	0.44
3:E:417:ASN:OD1	3:E:419:ILE:N	2.42	0.44
3:E:571:PHE:HD2	3:E:596:PHE:CE1	2.36	0.44
3:L:309:LEU:C	3:L:309:LEU:HD12	2.38	0.44
3:L:506:TYR:CE2	3:L:508:ASP:HB2	2.52	0.44
3:L:154:LEU:CG	3:L:709:MET:HE2	2.45	0.44
3:M:424:LEU:O	3:M:428:LEU:HB2	2.17	0.44
1:A:138:ASP:HA	1:A:141:LYS:HD2	1.99	0.44
1:D:430:ASN:N	1:D:430:ASN:ND2	2.65	0.44
3:L:417:ASN:OD1	3:L:419:ILE:N	2.41	0.44
3:L:672:ARG:NH1	3:L:725:SER:HA	2.32	0.44
3:M:300:GLN:O	3:M:301:PRO:C	2.56	0.44
3:M:313:SER:O	3:M:317:ILE:HG12	2.16	0.44
3:M:668:LEU:HD21	3:M:733:ARG:NH1	2.31	0.44
3:M:919:ILE:HG22	3:M:923:ARG:HD2	1.99	0.44
1:D:561:GLN:CG	1:D:763:ALA:HA	2.48	0.44
3:E:223:ASN:O	3:E:291:MET:HG2	2.17	0.44
3:E:378:ILE:HD13	3:E:385:PHE:CZ	2.51	0.44
3:E:557:VAL:CG1	3:E:582:LEU:HD11	2.44	0.44
3:E:908:LEU:C	3:E:910:ASN:H	2.21	0.44
1:G:599:PHE:HD2	2:K:51:LEU:HD22	1.82	0.44
2:J:40:LEU:HD22	2:J:73:ASP:HB2	1.99	0.44
2:K:85:LYS:HA	2:K:88:PHE:CE2	2.52	0.44
3:L:223:ASN:O	3:L:291:MET:HG2	2.17	0.44
3:L:756:VAL:O	3:L:786:PRO:HA	2.17	0.44
3:L:147:LEU:CD1	3:L:914:ARG:NH1	2.77	0.44
3:M:163:ILE:HD13	3:M:634:PRO:HG3	1.99	0.44
1:A:722:ARG:NH1	6:B:1190:GNP:N3B	2.57	0.44
2:B:134:ILE:CG1	2:B:172:SER:HB2	2.47	0.44
1:D:46:LEU:HG	1:D:47:ASN:N	2.33	0.44
1:D:599:PHE:HD2	2:J:51:LEU:HD22	1.82	0.44
3:E:668:LEU:HD21	3:E:733:ARG:NH1	2.31	0.44
1:G:138:ASP:HA	1:G:141:LYS:HD2	1.99	0.44
1:G:653:ILE:HG13	1:G:670:ILE:HD13	2.00	0.44
2:J:97:LEU:HD12	2:J:97:LEU:N	2.31	0.44
3:L:163:ILE:HD13	3:L:634:PRO:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:170:VAL:O	3:L:170:VAL:HG12	2.16	0.44
3:M:750:LYS:HE3	3:M:805:GLY:CA	2.46	0.44
1:A:15:THR:HG22	1:A:528:ALA:HA	1.99	0.44
1:A:653:ILE:HG13	1:A:670:ILE:HD13	1.99	0.44
2:B:155:THR:OG1	2:B:156:GLY:N	2.50	0.44
1:D:15:THR:HG22	1:D:528:ALA:HA	1.99	0.44
1:D:69:CYS:SG	1:D:81:PRO:HD3	2.58	0.44
3:E:147:LEU:O	3:E:149:PRO:N	2.50	0.44
3:E:309:LEU:HD12	3:E:309:LEU:C	2.38	0.44
3:E:419:ILE:HG22	3:E:421:ASN:H	1.82	0.44
2:K:40:LEU:HD22	2:K:73:ASP:HB2	1.99	0.44
3:L:133:ARG:HH21	3:L:135:MET:HE2	1.81	0.44
3:L:242:VAL:CG1	3:L:251:TRP:HB2	2.48	0.44
3:M:223:ASN:O	3:M:291:MET:HG2	2.17	0.44
3:M:419:ILE:HG22	3:M:421:ASN:H	1.82	0.44
4:O:68:GLN:O	4:O:72:GLN:HG3	2.18	0.44
1:A:111:GLU:HB2	1:A:503:ARG:HD3	1.99	0.44
1:A:550:ARG:O	1:A:554:ARG:HG3	2.18	0.44
1:A:588:TYR:O	1:A:591:ARG:HG2	2.18	0.44
3:E:242:VAL:CG1	3:E:251:TRP:HB2	2.48	0.44
1:G:550:ARG:O	1:G:554:ARG:HG3	2.18	0.44
1:G:69:CYS:SG	1:G:81:PRO:HD3	2.57	0.44
3:L:424:LEU:O	3:L:428:LEU:HB2	2.17	0.44
3:M:167:ARG:HD3	3:M:167:ARG:HA	1.81	0.44
1:A:66:ASN:ND2	1:A:68:TYR:H	2.16	0.44
2:B:85:LYS:HA	2:B:88:PHE:CE2	2.52	0.44
1:D:550:ARG:O	1:D:554:ARG:HG3	2.18	0.44
4:F:68:GLN:O	4:F:72:GLN:HG3	2.17	0.44
1:G:66:ASN:ND2	1:G:68:TYR:H	2.16	0.44
2:J:125:VAL:HA	2:J:126:PRO:HD3	1.87	0.44
2:J:155:THR:HG21	2:J:165:PRO:HA	2.00	0.44
3:M:242:VAL:CG1	3:M:251:TRP:HB2	2.48	0.44
3:M:309:LEU:HD12	3:M:309:LEU:C	2.38	0.44
1:A:69:CYS:SG	1:A:81:PRO:HD3	2.57	0.44
1:D:138:ASP:HA	1:D:141:LYS:HD2	1.99	0.44
3:E:292:ALA:HA	3:E:293:PRO:HD3	1.83	0.44
1:G:464:ASN:ND2	1:G:465:THR:H	2.15	0.44
1:G:561:GLN:CG	1:G:763:ALA:HA	2.48	0.44
2:J:110:ARG:HG3	2:J:110:ARG:HH11	1.82	0.44
2:J:134:ILE:CG1	2:J:172:SER:HB2	2.47	0.44
2:K:134:ILE:CG1	2:K:172:SER:HB2	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:506:TYR:CE2	3:M:508:ASP:HB2	2.52	0.44
3:M:668:LEU:O	3:M:671:ALA:HB3	2.18	0.44
1:A:561:GLN:CG	1:A:763:ALA:HA	2.48	0.44
1:D:66:ASN:ND2	1:D:68:TYR:H	2.16	0.44
3:E:764:ASP:O	3:E:851:ARG:NH2	2.51	0.44
3:E:783:LEU:HA	3:E:784:PRO:HD3	1.81	0.44
1:G:588:TYR:O	1:G:591:ARG:HG2	2.18	0.44
3:L:168:MET:HG2	3:L:241:PHE:CE1	2.53	0.44
1:G:187:GLU:HB2	1:G:296:PRO:HG3	1.99	0.43
2:J:155:THR:OG1	2:J:156:GLY:N	2.50	0.43
2:J:37:THR:HG22	2:J:51:LEU:HD13	1.99	0.43
3:L:253:CYS:SG	3:L:255:PHE:HB2	2.58	0.43
3:L:300:GLN:O	3:L:301:PRO:C	2.56	0.43
3:L:361:LEU:HD23	3:L:399:CYS:SG	2.58	0.43
3:L:668:LEU:O	3:L:671:ALA:HB3	2.18	0.43
3:M:344:ARG:HA	3:M:394:VAL:O	2.18	0.43
3:M:571:PHE:HD2	3:M:596:PHE:CE1	2.36	0.43
3:M:717:LEU:HA	3:M:717:LEU:HD12	1.83	0.43
4:N:62:LEU:HA	4:N:66:GLN:OE1	2.17	0.43
1:A:46:LEU:HG	1:A:47:ASN:N	2.32	0.43
1:D:653:ILE:HG13	1:D:670:ILE:HD13	2.00	0.43
3:E:250:ARG:HD2	3:E:260:ASN:O	2.18	0.43
3:L:764:ASP:O	3:L:851:ARG:NH2	2.51	0.43
3:L:808:LEU:O	3:L:872:TYR:N	2.48	0.43
3:M:147:LEU:O	3:M:149:PRO:N	2.50	0.43
3:M:808:LEU:O	3:M:872:TYR:N	2.48	0.43
3:M:872:TYR:CE2	3:M:897:TRP:CZ3	3.06	0.43
2:B:32:ASP:HA	6:B:1190:GNP:O3G	2.18	0.43
1:D:281:PRO:HB3	1:D:400:PHE:HB3	2.00	0.43
3:E:150:PRO:O	3:E:151:ILE:HB	2.18	0.43
3:E:163:ILE:HD13	3:E:634:PRO:HG3	2.00	0.43
3:E:919:ILE:HG22	3:E:923:ARG:HD2	1.99	0.43
3:L:302:PRO:HA	3:L:303:PRO:HD3	1.73	0.43
3:L:872:TYR:CE2	3:L:897:TRP:CZ3	3.06	0.43
1:A:114:THR:CG2	1:A:115:ASN:N	2.76	0.43
1:A:599:PHE:HD2	2:B:51:LEU:HD22	1.82	0.43
3:E:253:CYS:SG	3:E:255:PHE:HB2	2.58	0.43
3:L:147:LEU:HD23	3:L:147:LEU:HA	1.74	0.43
3:L:419:ILE:HG22	3:L:421:ASN:H	1.82	0.43
3:M:253:CYS:SG	3:M:255:PHE:HB2	2.58	0.43
1:A:281:PRO:HB3	1:A:400:PHE:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.79	0.43
2:B:37:THR:HG22	2:B:51:LEU:HD13	1.99	0.43
1:D:90:PRO:HA	1:D:91:PRO:HD3	1.86	0.43
3:E:668:LEU:O	3:E:671:ALA:HB3	2.18	0.43
1:G:15:THR:HG23	1:G:531:LEU:HD12	2.00	0.43
2:K:155:THR:HG21	2:K:165:PRO:HA	2.00	0.43
3:L:571:PHE:HD2	3:L:596:PHE:CE1	2.36	0.43
1:D:283:ARG:NE	1:D:344:ASP:OD2	2.51	0.43
3:E:301:PRO:HA	3:E:302:PRO:HD3	1.68	0.43
3:E:791:SER:H	3:E:905:ASP:CG	2.20	0.43
1:A:101:MET:HE1	4:F:61:PHE:CZ	2.49	0.43
3:L:359:ILE:HD11	3:L:406:LEU:HD23	2.01	0.43
3:L:919:ILE:HG22	3:L:923:ARG:HD2	1.99	0.43
3:M:147:LEU:HA	3:M:147:LEU:HD23	1.74	0.43
1:A:15:THR:HG23	1:A:531:LEU:HD12	2.01	0.43
1:A:417:LEU:C	1:A:417:LEU:HD23	2.39	0.43
1:D:417:LEU:HD23	1:D:417:LEU:C	2.39	0.43
1:D:642:LEU:O	1:D:644:ASP:N	2.48	0.43
3:E:409:LYS:O	3:E:412:GLN:N	2.48	0.43
3:E:750:LYS:HE3	3:E:805:GLY:CA	2.46	0.43
1:G:111:GLU:HB2	1:G:503:ARG:HD3	1.99	0.43
3:M:217:ILE:HG13	3:M:217:ILE:H	1.64	0.43
3:M:557:VAL:CG1	3:M:582:LEU:HD11	2.44	0.43
1:A:677:GLY:O	1:A:679:GLN:N	2.52	0.43
2:B:181:GLU:CD	2:B:181:GLU:H	2.22	0.43
1:D:111:GLU:HB2	1:D:503:ARG:HD3	1.99	0.43
3:E:168:MET:HG2	3:E:241:PHE:CE1	2.53	0.43
3:E:253:CYS:O	3:E:257:ARG:HA	2.19	0.43
3:E:361:LEU:HD23	3:E:399:CYS:SG	2.58	0.43
1:G:283:ARG:NE	1:G:344:ASP:OD2	2.51	0.43
3:L:344:ARG:HA	3:L:394:VAL:O	2.18	0.43
3:M:154:LEU:HD21	3:M:709:MET:HE3	2.01	0.43
3:M:546:LYS:NZ	3:M:862:HIS:O	2.52	0.43
1:D:152:PRO:HA	1:D:153:PRO:HD3	1.93	0.43
1:D:677:GLY:O	1:D:679:GLN:N	2.52	0.43
1:G:360:GLN:HG2	1:G:364:SER:OG	2.19	0.43
1:G:15:THR:HG22	1:G:528:ALA:HA	1.99	0.43
1:G:642:LEU:O	1:G:644:ASP:N	2.48	0.43
1:G:677:GLY:O	1:G:679:GLN:N	2.52	0.43
3:L:250:ARG:HD2	3:L:260:ASN:O	2.18	0.43
3:L:908:LEU:C	3:L:910:ASN:H	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:168:MET:HG2	3:M:241:PHE:CE1	2.53	0.43
3:M:687:LYS:HZ1	3:M:925:SER:HA	1.84	0.43
3:E:144:LEU:HD22	3:E:918:GLN:HE22	1.84	0.43
3:E:344:ARG:HA	3:E:394:VAL:O	2.18	0.43
1:G:516:THR:HA	1:G:517:PRO:HD3	1.88	0.43
2:J:32:ASP:HA	6:J:1190:GNP:O3G	2.18	0.43
2:K:181:GLU:CD	2:K:181:GLU:H	2.22	0.43
3:M:361:LEU:HD23	3:M:399:CYS:SG	2.58	0.43
4:N:68:GLN:O	4:N:72:GLN:HG3	2.18	0.43
2:B:155:THR:HG21	2:B:165:PRO:HA	2.00	0.42
3:E:428:LEU:HA	3:E:428:LEU:HD12	1.89	0.42
3:E:546:LYS:NZ	3:E:862:HIS:O	2.52	0.42
1:G:281:PRO:HB3	1:G:400:PHE:HB3	2.00	0.42
2:K:32:ASP:HA	6:K:1190:GNP:O3G	2.18	0.42
3:L:144:LEU:HD22	3:L:918:GLN:HE22	1.84	0.42
3:M:250:ARG:HD2	3:M:260:ASN:O	2.18	0.42
3:M:209:PRO:CG	3:M:558:MET:CE	2.97	0.42
3:M:802:ILE:HB	3:M:809:PHE:HB2	2.01	0.42
3:M:764:ASP:O	3:M:851:ARG:NH2	2.51	0.42
1:A:20:PRO:HB3	1:A:25:ASP:HB2	2.02	0.42
1:D:15:THR:HG23	1:D:531:LEU:HD12	2.00	0.42
1:D:632:PHE:CE2	1:D:693:GLU:HG3	2.55	0.42
1:D:74:ARG:HG3	1:D:74:ARG:H	1.66	0.42
3:E:151:ILE:HD13	3:E:709:MET:HE1	2.01	0.42
2:B:142:GLU:CD	1:G:426:LYS:HZ3	2.22	0.42
2:K:147:SER:OG	2:K:152:LEU:HD21	2.19	0.42
3:L:224:GLU:HA	3:L:291:MET:CG	2.49	0.42
3:M:150:PRO:O	3:M:151:ILE:HB	2.18	0.42
3:M:553:CYS:O	3:M:587:THR:HA	2.19	0.42
1:A:63:SER:OG	1:A:82:ILE:HG13	2.20	0.42
1:D:360:GLN:HG2	1:D:364:SER:OG	2.19	0.42
1:D:66:ASN:HB2	1:D:67:PRO:CD	2.49	0.42
3:E:300:GLN:O	3:E:301:PRO:C	2.56	0.42
2:J:181:GLU:H	2:J:181:GLU:CD	2.22	0.42
3:M:224:GLU:HA	3:M:291:MET:CG	2.49	0.42
1:G:417:LEU:C	1:G:417:LEU:HD23	2.39	0.42
1:G:66:ASN:HB2	1:G:67:PRO:CD	2.49	0.42
3:L:209:PRO:CG	3:L:558:MET:CE	2.97	0.42
3:L:546:LYS:NZ	3:L:862:HIS:O	2.52	0.42
3:L:553:CYS:O	3:L:587:THR:HA	2.19	0.42
3:L:750:LYS:HE3	3:L:805:GLY:CA	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:NE	1:A:344:ASP:OD2	2.51	0.42
2:B:26:LEU:HB2	2:B:71:THR:HG22	2.02	0.42
1:D:512:LEU:HA	1:D:513:PRO:HD3	1.79	0.42
1:D:66:ASN:ND2	1:D:68:TYR:HB2	2.35	0.42
3:E:224:GLU:HA	3:E:291:MET:CG	2.49	0.42
1:G:632:PHE:CE2	1:G:693:GLU:HG3	2.55	0.42
1:G:661:PHE:C	1:G:661:PHE:CD1	2.93	0.42
3:L:150:PRO:O	3:L:151:ILE:HB	2.18	0.42
3:L:864:ASP:N	3:L:864:ASP:OD1	2.53	0.42
3:M:789:ALA:HB1	3:M:902:LEU:HA	2.01	0.42
1:A:360:GLN:HG2	1:A:364:SER:OG	2.19	0.42
1:D:53:PRO:HG3	1:D:112:TYR:CG	2.55	0.42
1:D:574:PHE:CD2	1:D:760:GLN:HG2	2.55	0.42
3:E:151:ILE:HD13	3:E:709:MET:CE	2.50	0.42
3:E:359:ILE:HD11	3:E:406:LEU:HD23	2.01	0.42
3:M:799:LEU:HD13	3:M:812:MET:CE	2.50	0.42
1:A:561:GLN:HG2	1:A:763:ALA:O	2.20	0.42
1:D:516:THR:HA	1:D:517:PRO:HD3	1.88	0.42
1:D:552:LEU:HD12	1:D:552:LEU:HA	1.91	0.42
1:D:63:SER:OG	1:D:82:ILE:HG13	2.20	0.42
3:E:219:PRO:HA	3:E:220:PRO:HD3	1.95	0.42
1:G:243:GLU:OE1	1:G:243:GLU:HA	2.20	0.42
3:L:386:LEU:HA	3:L:387:PRO:HD3	1.81	0.42
3:L:151:ILE:HD13	3:L:709:MET:CE	2.50	0.42
3:L:799:LEU:HD13	3:L:812:MET:CE	2.50	0.42
3:M:212:HIS:CD2	3:M:217:ILE:HB	2.55	0.42
2:B:147:SER:OG	2:B:152:LEU:HD21	2.19	0.42
1:D:411:ASP:HA	1:D:463:ALA:HB3	2.02	0.42
3:E:212:HIS:CD2	3:E:217:ILE:HB	2.55	0.42
3:E:789:ALA:HB1	3:E:902:LEU:HA	2.01	0.42
3:E:799:LEU:HD13	3:E:812:MET:CE	2.50	0.42
1:G:658:THR:O	1:G:659:PHE:HB3	2.20	0.42
3:L:212:HIS:CD2	3:L:217:ILE:HB	2.55	0.42
3:L:253:CYS:O	3:L:257:ARG:HA	2.19	0.42
1:D:181:VAL:N	3:L:377:ASP:O	2.40	0.42
3:M:302:PRO:HA	3:M:303:PRO:HD3	1.73	0.42
3:M:497:VAL:HG12	3:M:499:LEU:HD11	2.01	0.42
1:A:430:ASN:ND2	1:A:430:ASN:N	2.65	0.42
1:D:243:GLU:OE1	1:D:243:GLU:HA	2.20	0.42
1:D:561:GLN:HG2	1:D:763:ALA:O	2.20	0.42
1:D:80:CYS:HA	1:D:81:PRO:HD3	1.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:497:VAL:HG12	3:E:499:LEU:HD11	2.01	0.42
3:E:553:CYS:O	3:E:587:THR:HA	2.19	0.42
1:G:411:ASP:HA	1:G:463:ALA:HB3	2.02	0.42
1:G:53:PRO:HG3	1:G:112:TYR:CG	2.55	0.42
1:G:576:LEU:HG	1:G:580:PHE:HB3	2.02	0.42
1:G:574:PHE:CD2	1:G:760:GLN:HG2	2.55	0.42
3:L:242:VAL:CG1	3:L:243:THR:N	2.83	0.42
1:A:66:ASN:HB2	1:A:67:PRO:CD	2.49	0.42
3:E:333:LEU:HD12	3:E:400:ARG:NE	2.35	0.42
1:G:420:HIS:CE1	1:G:615:ARG:HB2	2.55	0.42
3:L:333:LEU:HD12	3:L:400:ARG:NE	2.35	0.42
3:L:789:ALA:HB1	3:L:902:LEU:HA	2.01	0.42
1:A:574:PHE:CD2	1:A:760:GLN:HG2	2.55	0.41
1:D:114:THR:CG2	1:D:115:ASN:N	2.76	0.41
1:D:176:ILE:HD12	3:L:413:ILE:CG1	2.38	0.41
1:D:332:ILE:HG22	1:D:361:LEU:HD21	2.02	0.41
1:D:52:ASN:HA	1:D:53:PRO:HD3	1.87	0.41
1:A:91:PRO:HB3	1:D:669:GLN:HE21	0.43	0.41
3:L:409:LYS:O	3:L:412:GLN:N	2.48	0.41
3:M:144:LEU:HD22	3:M:918:GLN:HE22	1.84	0.41
3:M:496:THR:OG1	3:M:587:THR:HG23	2.20	0.41
1:A:195:GLU:O	1:A:199:GLY:N	2.41	0.41
1:A:41:LYS:O	1:A:503:ARG:NH2	2.54	0.41
1:D:658:THR:O	1:D:659:PHE:HB3	2.20	0.41
1:G:63:SER:OG	1:G:82:ILE:HG13	2.20	0.41
1:G:83:CYS:O	1:G:84:ASN:HB2	2.20	0.41
2:K:26:LEU:HB2	2:K:71:THR:HG22	2.02	0.41
3:L:808:LEU:HA	3:L:808:LEU:HD23	1.88	0.41
3:M:242:VAL:CG1	3:M:243:THR:N	2.83	0.41
3:M:253:CYS:O	3:M:257:ARG:HA	2.19	0.41
3:M:362:ASP:CG	3:M:401:GLN:HB2	2.41	0.41
1:D:420:HIS:CE1	1:D:615:ARG:HB2	2.55	0.41
1:D:569:ASP:O	1:D:571:PRO:HD3	2.20	0.41
1:D:632:PHE:CD1	1:D:632:PHE:N	2.88	0.41
1:D:96:LEU:O	1:D:97:SER:HB3	2.21	0.41
3:E:362:ASP:CG	3:E:401:GLN:HB2	2.40	0.41
3:E:802:ILE:HB	3:E:809:PHE:HB2	2.01	0.41
1:G:42:GLU:HG3	1:G:452:PRO:HB3	2.02	0.41
1:G:96:LEU:O	1:G:97:SER:HB3	2.20	0.41
2:J:147:SER:OG	2:J:152:LEU:HD21	2.19	0.41
2:J:26:LEU:HB2	2:J:71:THR:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:163:ILE:HA	3:L:164:PRO:HD3	1.90	0.41
3:L:187:ASN:O	3:L:634:PRO:HD2	2.20	0.41
3:L:802:ILE:HB	3:L:809:PHE:HB2	2.01	0.41
1:A:101:MET:CE	4:F:61:PHE:CE2	3.00	0.41
1:A:411:ASP:HA	1:A:463:ALA:HB3	2.02	0.41
1:A:420:HIS:CE1	1:A:615:ARG:HB2	2.55	0.41
1:A:632:PHE:CD1	1:A:632:PHE:N	2.88	0.41
1:A:632:PHE:CE2	1:A:693:GLU:HG3	2.55	0.41
1:A:70:VAL:HB	1:A:79:SER:OG	2.21	0.41
1:A:88:HIS:HE1	1:D:742:SER:CB	2.32	0.41
1:D:83:CYS:O	1:D:84:ASN:HB2	2.20	0.41
3:E:209:PRO:CG	3:E:558:MET:CE	2.97	0.41
1:G:569:ASP:O	1:G:571:PRO:HD3	2.20	0.41
1:G:722:ARG:CZ	2:K:53:PRO:HG3	2.51	0.41
2:K:164:ARG:O	2:K:164:ARG:HG2	2.21	0.41
3:L:242:VAL:HG12	3:L:243:THR:N	2.34	0.41
3:L:535:ASN:O	3:L:536:ASP:C	2.59	0.41
3:L:209:PRO:CG	3:L:558:MET:HE1	2.51	0.41
3:M:729:PRO:HB2	3:M:732:HIS:CD2	2.52	0.41
1:A:164:ASN:HD22	1:A:165:VAL:N	2.19	0.41
1:A:658:THR:O	1:A:659:PHE:HB3	2.20	0.41
1:A:67:PRO:HD3	1:A:104:GLU:O	2.21	0.41
3:E:242:VAL:HG12	3:E:243:THR:N	2.34	0.41
3:E:496:THR:OG1	3:E:587:THR:HG23	2.20	0.41
3:L:277:ARG:C	3:L:279:ASP:N	2.74	0.41
3:M:187:ASN:O	3:M:634:PRO:HD2	2.20	0.41
3:M:781:ILE:HB	3:M:858:GLN:OE1	2.21	0.41
1:A:332:ILE:HG22	1:A:361:LEU:HD21	2.02	0.41
1:A:569:ASP:O	1:A:571:PRO:HD3	2.20	0.41
3:E:242:VAL:CG1	3:E:243:THR:N	2.83	0.41
3:E:920:MET:CA	3:E:920:MET:HE3	2.48	0.41
1:G:140:LEU:O	1:G:144:ILE:HG13	2.21	0.41
1:G:332:ILE:HG22	1:G:361:LEU:HD21	2.02	0.41
3:L:155:THR:O	3:L:155:THR:HG22	2.21	0.41
3:L:496:THR:OG1	3:L:587:THR:HG23	2.20	0.41
3:L:497:VAL:HG12	3:L:499:LEU:HD11	2.01	0.41
3:M:359:ILE:HD11	3:M:406:LEU:HD23	2.01	0.41
3:M:633:MET:HA	3:M:634:PRO:HD3	1.89	0.41
1:A:239:ASN:O	1:A:243:GLU:HB2	2.20	0.41
1:A:243:GLU:HA	1:A:243:GLU:OE1	2.20	0.41
1:A:569:ASP:C	1:A:571:PRO:HD3	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ASN:HD22	1:D:165:VAL:N	2.19	0.41
1:D:20:PRO:HB3	1:D:25:ASP:HB2	2.02	0.41
1:D:42:GLU:HG3	1:D:452:PRO:HB3	2.02	0.41
1:D:661:PHE:C	1:D:661:PHE:CD1	2.93	0.41
1:D:643:LEU:HD12	1:D:728:LEU:HD23	2.03	0.41
3:E:151:ILE:HA	3:E:151:ILE:HD13	1.82	0.41
1:G:239:ASN:O	1:G:243:GLU:HB2	2.20	0.41
1:G:569:ASP:C	1:G:571:PRO:HD3	2.41	0.41
3:L:352:ASN:ND2	3:L:352:ASN:N	2.69	0.41
3:M:151:ILE:HD13	3:M:709:MET:CE	2.50	0.41
3:M:270:ASP:CB	3:M:273:ASP:HB3	2.50	0.41
1:D:41:LYS:O	1:D:503:ARG:NH2	2.54	0.41
1:D:702:LEU:O	1:D:703:VAL:C	2.59	0.41
3:E:133:ARG:HH21	3:E:135:MET:HE2	1.86	0.41
1:G:561:GLN:HG2	1:G:763:ALA:O	2.20	0.41
1:D:176:ILE:HG13	3:L:413:ILE:HG12	2.02	0.41
3:M:242:VAL:HG12	3:M:243:THR:N	2.34	0.41
3:M:820:LEU:C	3:M:822:PHE:N	2.74	0.41
1:A:53:PRO:HG3	1:A:112:TYR:CG	2.55	0.41
1:A:576:LEU:HG	1:A:580:PHE:HB3	2.02	0.41
1:A:66:ASN:ND2	1:A:68:TYR:HB2	2.35	0.41
1:D:239:ASN:O	1:D:243:GLU:HB2	2.20	0.41
1:D:319:ALA:HB1	1:D:322:TYR:HB2	2.03	0.41
3:E:207:ILE:HG22	3:E:209:PRO:HD3	2.03	0.41
3:E:187:ASN:O	3:E:634:PRO:HD2	2.20	0.41
1:G:632:PHE:CD1	1:G:632:PHE:N	2.88	0.41
1:G:66:ASN:ND2	1:G:68:TYR:HB2	2.35	0.41
1:G:70:VAL:HB	1:G:79:SER:OG	2.21	0.41
3:L:557:VAL:CG1	3:L:582:LEU:HD11	2.44	0.41
3:M:217:ILE:C	3:M:219:PRO:HD3	2.41	0.41
3:M:219:PRO:HA	3:M:220:PRO:HD3	1.95	0.41
3:M:560:ALA:HA	3:M:612:GLN:O	2.21	0.41
3:M:864:ASP:N	3:M:864:ASP:OD1	2.53	0.41
3:M:809:PHE:HD2	3:M:898:ALA:HB2	1.86	0.41
1:D:140:LEU:O	1:D:144:ILE:HG13	2.21	0.41
1:D:451:SER:C	1:D:453:TYR:N	2.75	0.41
1:D:569:ASP:C	1:D:571:PRO:HD3	2.41	0.41
1:D:70:VAL:HB	1:D:79:SER:OG	2.21	0.41
3:E:277:ARG:C	3:E:279:ASP:N	2.74	0.41
1:A:181:VAL:N	3:E:377:ASP:O	2.40	0.41
3:E:820:LEU:C	3:E:822:PHE:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:96:PHE:HB3	2:K:129:ILE:HD13	2.03	0.41
3:L:808:LEU:O	3:L:871:LEU:HA	2.21	0.41
1:A:661:PHE:C	1:A:661:PHE:CD1	2.93	0.41
1:A:80:CYS:HA	1:A:81:PRO:HD3	1.86	0.41
1:D:67:PRO:HD3	1:D:104:GLU:O	2.21	0.41
1:A:176:ILE:HG13	3:E:413:ILE:HG12	2.02	0.41
3:E:864:ASP:OD1	3:E:864:ASP:N	2.53	0.41
1:G:41:LYS:O	1:G:503:ARG:NH2	2.54	0.41
1:G:639:GLN:HA	1:G:640:PRO:HD3	1.90	0.41
1:G:67:PRO:HD3	1:G:104:GLU:O	2.21	0.41
3:L:197:LYS:HD2	3:L:197:LYS:HA	1.72	0.41
3:L:207:ILE:HG22	3:L:209:PRO:HD3	2.03	0.41
3:M:199:SER:O	3:M:200:LYS:HB2	2.21	0.41
3:M:358:LYS:HA	3:M:391:SER:O	2.21	0.41
3:M:333:LEU:HD12	3:M:400:ARG:NE	2.35	0.41
3:M:307:CYS:HB2	3:M:435:ILE:HG21	2.03	0.41
1:A:140:LEU:O	1:A:144:ILE:HG13	2.21	0.40
1:A:319:ALA:HB1	1:A:322:TYR:HB2	2.03	0.40
1:A:464:ASN:ND2	1:A:465:THR:N	2.69	0.40
1:A:83:CYS:O	1:A:84:ASN:HB2	2.21	0.40
3:E:312:VAL:CG1	3:E:414:PHE:CD1	3.03	0.40
1:G:164:ASN:HD22	1:G:165:VAL:N	2.19	0.40
1:G:171:LEU:HB3	1:G:237:LYS:HD3	2.03	0.40
1:G:20:PRO:HB3	1:G:25:ASP:HB2	2.02	0.40
3:L:270:ASP:CB	3:L:273:ASP:HB3	2.50	0.40
3:M:699:ALA:HB1	3:M:921:LYS:HZ2	1.86	0.40
1:A:639:GLN:HA	1:A:640:PRO:HD3	1.90	0.40
2:B:96:PHE:HB3	2:B:129:ILE:HD13	2.03	0.40
1:D:141:LYS:NZ	1:D:245:LEU:O	2.50	0.40
1:D:252:VAL:HA	1:D:253:PRO:HD2	1.92	0.40
3:E:585:PHE:HB3	3:E:587:THR:O	2.22	0.40
3:E:154:LEU:CG	3:E:709:MET:HE2	2.48	0.40
3:E:716:SER:HB2	3:E:752:ILE:HG22	2.04	0.40
3:L:699:ALA:HB1	3:L:921:LYS:HZ2	1.84	0.40
3:M:552:PHE:CD1	3:M:552:PHE:C	2.95	0.40
1:A:602:SER:OG	1:A:605:GLU:HB2	2.22	0.40
1:A:643:LEU:HD12	1:A:728:LEU:HD23	2.03	0.40
1:A:96:LEU:O	1:A:97:SER:HB3	2.21	0.40
1:A:722:ARG:CZ	2:B:53:PRO:HG3	2.51	0.40
1:D:722:ARG:CZ	2:J:53:PRO:HG3	2.51	0.40
3:E:141:ILE:HD12	3:E:146:GLU:HG3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:352:ASN:N	3:E:352:ASN:ND2	2.69	0.40
1:G:319:ALA:HB1	1:G:322:TYR:HB2	2.03	0.40
3:L:781:ILE:HB	3:L:858:GLN:OE1	2.21	0.40
1:A:19:PHE:HA	1:A:20:PRO:HD3	1.94	0.40
1:A:451:SER:C	1:A:453:TYR:N	2.75	0.40
1:A:642:LEU:O	1:A:644:ASP:N	2.48	0.40
1:D:171:LEU:HB3	1:D:237:LYS:HD3	2.03	0.40
1:G:464:ASN:ND2	1:G:465:THR:N	2.69	0.40
3:L:199:SER:O	3:L:200:LYS:HB2	2.21	0.40
3:L:362:ASP:CG	3:L:401:GLN:HB2	2.41	0.40
3:M:703:LEU:HD12	3:M:703:LEU:HA	1.96	0.40
3:M:808:LEU:O	3:M:871:LEU:HA	2.21	0.40
1:A:702:LEU:O	1:A:703:VAL:C	2.59	0.40
1:D:576:LEU:HG	1:D:580:PHE:HB3	2.02	0.40
3:E:552:PHE:CD1	3:E:552:PHE:C	2.95	0.40
1:G:12:VAL:HG11	1:G:14:PHE:CE1	2.57	0.40
1:G:451:SER:C	1:G:453:TYR:N	2.74	0.40
1:G:643:LEU:HD12	1:G:728:LEU:HD23	2.03	0.40
3:L:139:TYR:CD1	3:L:139:TYR:N	2.90	0.40
3:L:552:PHE:CD1	3:L:552:PHE:C	2.95	0.40
3:M:139:TYR:CD1	3:M:139:TYR:N	2.90	0.40
3:M:155:THR:O	3:M:155:THR:HG22	2.21	0.40
3:M:417:ASN:OD1	3:M:419:ILE:HB	2.22	0.40
3:M:808:LEU:HD23	3:M:808:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	727/768 (95%)	687 (94%)	35 (5%)	5 (1%)	25 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	727/768 (95%)	688 (95%)	34 (5%)	5 (1%)	25	68
1	G	727/768 (95%)	688 (95%)	34 (5%)	5 (1%)	25	68
2	B	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	5	37
2	J	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	5	37
2	K	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	5	37
3	E	723/926 (78%)	640 (88%)	55 (8%)	28 (4%)	3	31
3	L	723/926 (78%)	641 (89%)	54 (8%)	28 (4%)	3	31
3	M	723/926 (78%)	641 (89%)	54 (8%)	28 (4%)	3	31
4	F	11/926 (1%)	10 (91%)	1 (9%)	0	100	100
4	N	11/926 (1%)	10 (91%)	1 (9%)	0	100	100
4	O	11/926 (1%)	10 (91%)	1 (9%)	0	100	100
All	All	4863/8430 (58%)	4441 (91%)	308 (6%)	114 (2%)	11	43

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	VAL
2	B	139	ALA
2	B	155	THR
1	D	703	VAL
3	E	147	LEU
3	E	148	PRO
3	E	151	ILE
3	E	601	ASP
3	E	762	MET
3	E	766	ALA
3	E	767	GLY
3	E	796	ARG
1	G	703	VAL
2	J	139	ALA
2	J	155	THR
2	K	139	ALA
2	K	155	THR
3	L	147	LEU
3	L	148	PRO
3	L	151	ILE
3	L	601	ASP
3	L	762	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	766	ALA
3	L	767	GLY
3	L	796	ARG
3	M	147	LEU
3	M	148	PRO
3	M	151	ILE
3	M	601	ASP
3	M	762	MET
3	M	766	ALA
3	M	767	GLY
3	M	796	ARG
1	A	678	TYR
1	D	678	TYR
3	E	278	TYR
3	E	313	SER
3	E	415	GLN
3	E	469	SER
3	E	580	SER
3	E	697	GLY
3	E	867	THR
3	E	903	VAL
1	G	678	TYR
3	L	278	TYR
3	L	313	SER
3	L	415	GLN
3	L	469	SER
3	L	580	SER
3	L	697	GLY
3	L	867	THR
3	L	903	VAL
3	M	278	TYR
3	M	313	SER
3	M	415	GLN
3	M	469	SER
3	M	580	SER
3	M	697	GLY
3	M	867	THR
3	M	903	VAL
1	A	73	PRO
1	A	97	SER
2	B	123	LYS
1	D	73	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	97	SER
3	E	479	GLN
3	E	530	SER
3	E	620	ASN
3	E	724	ARG
3	E	793	LEU
1	G	73	PRO
1	G	97	SER
2	J	123	LYS
2	K	123	LYS
3	L	479	GLN
3	L	530	SER
3	L	620	ASN
3	L	724	ARG
3	L	793	LEU
3	M	479	GLN
3	M	530	SER
3	M	620	ASN
3	M	724	ARG
3	M	793	LEU
2	B	137	PRO
3	E	149	PRO
2	J	137	PRO
2	K	137	PRO
3	L	149	PRO
3	M	149	PRO
1	A	94	THR
1	D	94	THR
3	E	818	PRO
3	E	859	LEU
1	G	94	THR
3	L	818	PRO
3	L	859	LEU
3	M	818	PRO
3	M	859	LEU
2	B	138	ASN
3	E	146	GLU
3	E	215	ASP
3	E	271	PRO
3	E	763	ALA
2	J	138	ASN
2	K	138	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	146	GLU
3	L	215	ASP
3	L	271	PRO
3	L	763	ALA
3	M	146	GLU
3	M	215	ASP
3	M	271	PRO
3	M	763	ALA

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 PDB entries followed by that with respect to all EM entries.

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	644/668 (96%)	616 (96%)	28 (4%)	33	64
1	D	644/668 (96%)	616 (96%)	28 (4%)	33	64
1	G	644/668 (96%)	616 (96%)	28 (4%)	33	64
2	B	138/159 (87%)	136 (99%)	2 (1%)	71	86
2	J	138/159 (87%)	136 (99%)	2 (1%)	71	86
2	K	138/159 (87%)	136 (99%)	2 (1%)	71	86
3	E	660/819 (81%)	640 (97%)	20 (3%)	46	72
3	L	660/819 (81%)	640 (97%)	20 (3%)	46	72
3	M	660/819 (81%)	640 (97%)	20 (3%)	46	72
4	F	12/817 (2%)	12 (100%)	0	100	100
4	N	13/817 (2%)	13 (100%)	0	100	100
4	O	13/817 (2%)	13 (100%)	0	100	100
All	All	4364/7389 (59%)	4214 (97%)	150 (3%)	46	69

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	125	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	132	SER
1	A	136	ASN
1	A	164	ASN
1	A	166	VAL
1	A	243	GLU
1	A	245	LEU
1	A	250	TRP
1	A	252	VAL
1	A	309	ARG
1	A	411	ASP
1	A	430	ASN
1	A	450	LEU
1	A	503	ARG
1	A	534	ARG
1	A	544	ASP
1	A	552	LEU
1	A	592	ARG
1	A	601	ASN
1	A	635	GLU
1	A	651	ASN
1	A	679	GLN
1	A	697	GLU
1	A	700	GLU
1	A	708	LEU
1	A	749	ASP
1	A	765	SER
2	B	107	ASP
2	B	164	ARG
1	D	5	THR
1	D	125	PHE
1	D	132	SER
1	D	136	ASN
1	D	164	ASN
1	D	166	VAL
1	D	243	GLU
1	D	245	LEU
1	D	250	TRP
1	D	252	VAL
1	D	309	ARG
1	D	411	ASP
1	D	430	ASN
1	D	450	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	503	ARG
1	D	534	ARG
1	D	544	ASP
1	D	552	LEU
1	D	592	ARG
1	D	601	ASN
1	D	635	GLU
1	D	651	ASN
1	D	679	GLN
1	D	697	GLU
1	D	700	GLU
1	D	708	LEU
1	D	749	ASP
1	D	765	SER
3	E	138	LEU
3	E	150	PRO
3	E	152	THR
3	E	166	GLU
3	E	208	ARG
3	E	213	LEU
3	E	309	LEU
3	E	352	ASN
3	E	377	ASP
3	E	428	LEU
3	E	459	ARG
3	E	557	VAL
3	E	618	SER
3	E	739	ASN
3	E	743	LEU
3	E	751	ASN
3	E	761	ASP
3	E	764	ASP
3	E	822	PHE
3	E	870	SER
1	G	5	THR
1	G	125	PHE
1	G	132	SER
1	G	136	ASN
1	G	164	ASN
1	G	166	VAL
1	G	243	GLU
1	G	245	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	250	TRP
1	G	252	VAL
1	G	309	ARG
1	G	411	ASP
1	G	430	ASN
1	G	450	LEU
1	G	503	ARG
1	G	534	ARG
1	G	544	ASP
1	G	552	LEU
1	G	592	ARG
1	G	601	ASN
1	G	635	GLU
1	G	651	ASN
1	G	679	GLN
1	G	697	GLU
1	G	700	GLU
1	G	708	LEU
1	G	749	ASP
1	G	765	SER
2	J	107	ASP
2	J	164	ARG
2	K	107	ASP
2	K	164	ARG
3	L	138	LEU
3	L	150	PRO
3	L	152	THR
3	L	166	GLU
3	L	208	ARG
3	L	213	LEU
3	L	309	LEU
3	L	352	ASN
3	L	377	ASP
3	L	428	LEU
3	L	459	ARG
3	L	557	VAL
3	L	618	SER
3	L	739	ASN
3	L	743	LEU
3	L	751	ASN
3	L	761	ASP
3	L	764	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	822	PHE
3	L	870	SER
3	M	138	LEU
3	M	150	PRO
3	M	152	THR
3	M	166	GLU
3	M	208	ARG
3	M	213	LEU
3	M	309	LEU
3	M	352	ASN
3	M	377	ASP
3	M	428	LEU
3	M	459	ARG
3	M	557	VAL
3	M	618	SER
3	M	739	ASN
3	M	743	LEU
3	M	751	ASN
3	M	761	ASP
3	M	764	ASP
3	M	822	PHE
3	M	870	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	66	ASN
1	A	88	HIS
1	A	136	ASN
1	A	164	ASN
1	A	189	GLN
1	A	233	GLN
1	A	279	ASN
1	A	430	ASN
1	A	464	ASN
1	A	509	ASN
1	A	601	ASN
1	A	651	ASN
1	A	669	GLN
1	A	679	GLN
1	A	735	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	760	GLN
2	B	23	HIS
2	B	66	ASN
1	D	47	ASN
1	D	66	ASN
1	D	136	ASN
1	D	164	ASN
1	D	189	GLN
1	D	233	GLN
1	D	279	ASN
1	D	430	ASN
1	D	464	ASN
1	D	509	ASN
1	D	601	ASN
1	D	651	ASN
1	D	669	GLN
1	D	679	GLN
1	D	735	GLN
1	D	760	GLN
3	E	352	ASN
3	E	372	GLN
3	E	374	ASN
3	E	421	ASN
3	E	479	GLN
3	E	485	ASN
3	E	524	HIS
3	E	533	ASN
3	E	535	ASN
3	E	599	ASN
3	E	732	HIS
3	E	857	ASN
3	E	918	GLN
4	F	72	GLN
1	G	47	ASN
1	G	66	ASN
1	G	136	ASN
1	G	164	ASN
1	G	189	GLN
1	G	233	GLN
1	G	279	ASN
1	G	430	ASN
1	G	464	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	509	ASN
1	G	601	ASN
1	G	651	ASN
1	G	679	GLN
1	G	735	GLN
1	G	760	GLN
2	J	23	HIS
2	J	66	ASN
2	K	23	HIS
2	K	66	ASN
3	L	272	ASN
3	L	352	ASN
3	L	372	GLN
3	L	374	ASN
3	L	421	ASN
3	L	479	GLN
3	L	485	ASN
3	L	524	HIS
3	L	533	ASN
3	L	535	ASN
3	L	599	ASN
3	L	732	HIS
3	L	857	ASN
3	L	918	GLN
3	M	352	ASN
3	M	372	GLN
3	M	374	ASN
3	M	421	ASN
3	M	479	GLN
3	M	485	ASN
3	M	524	HIS
3	M	533	ASN
3	M	535	ASN
3	M	599	ASN
3	M	732	HIS
3	M	857	ASN
3	M	918	GLN
4	N	72	GLN
4	O	72	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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$
6	GNP	B	1190	7	27,34,34	2.26	7 (25%)	26,54,54	1.67	4 (15%)
6	GNP	J	1190	7	27,34,34	2.26	7 (25%)	26,54,54	1.67	4 (15%)
6	GNP	K	1190	7	27,34,34	2.26	7 (25%)	26,54,54	1.66	4 (15%)

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
6	GNP	B	1190	7	-	0/16/38/38	0/3/3/3
6	GNP	J	1190	7	-	0/16/38/38	0/3/3/3
6	GNP	K	1190	7	-	0/16/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1190	GNP	C4-N9	-7.18	1.38	1.47
6	J	1190	GNP	C4-N9	-7.18	1.38	1.47
6	B	1190	GNP	C4-N9	-7.13	1.38	1.47
6	B	1190	GNP	PB-O2B	-4.08	1.45	1.56
6	J	1190	GNP	PB-O2B	-4.06	1.45	1.56
6	K	1190	GNP	PB-O2B	-4.05	1.45	1.56
6	B	1190	GNP	C5-C6	-3.26	1.47	1.53
6	J	1190	GNP	C5-C6	-3.26	1.47	1.53
6	K	1190	GNP	C5-C6	-3.26	1.47	1.53
6	K	1190	GNP	PG-O2G	-3.20	1.48	1.56
6	B	1190	GNP	PG-O2G	-3.19	1.48	1.56
6	J	1190	GNP	PG-O2G	-3.19	1.48	1.56
6	K	1190	GNP	C8-N9	-2.49	1.39	1.46
6	B	1190	GNP	C8-N9	-2.48	1.39	1.46
6	J	1190	GNP	C8-N9	-2.47	1.39	1.46
6	K	1190	GNP	PB-O3A	2.29	1.61	1.59
6	J	1190	GNP	PB-O3A	2.34	1.62	1.59
6	B	1190	GNP	PB-O3A	2.35	1.62	1.59
6	J	1190	GNP	C6-N1	4.65	1.41	1.33
6	K	1190	GNP	C6-N1	4.68	1.41	1.33
6	B	1190	GNP	C6-N1	4.70	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1190	GNP	O3G-PG-O1G	-4.24	102.63	113.41
6	B	1190	GNP	O3G-PG-O1G	-4.23	102.65	113.41
6	J	1190	GNP	O3G-PG-O1G	-4.23	102.66	113.41
6	J	1190	GNP	O6-C6-N1	-2.86	118.89	122.70
6	B	1190	GNP	O6-C6-N1	-2.85	118.90	122.70
6	K	1190	GNP	O6-C6-N1	-2.84	118.92	122.70
6	K	1190	GNP	O1G-PG-N3B	2.54	115.58	111.79
6	B	1190	GNP	O1G-PG-N3B	2.54	115.59	111.79
6	J	1190	GNP	O1G-PG-N3B	2.57	115.64	111.79
6	K	1190	GNP	O6-C6-C5	4.92	129.10	119.69
6	J	1190	GNP	O6-C6-C5	4.93	129.12	119.69
6	B	1190	GNP	O6-C6-C5	4.94	129.15	119.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1190	GNP	5	0
6	J	1190	GNP	4	0
6	K	1190	GNP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.