



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:25 PM GMT

PDB ID : 3WVL
Title : Crystal structure of the football-shaped GroEL-GroES complex (GroEL: GroES2:ATP14) from Escherichia coli
Authors : Koike-Takeshita, A.; Arakawa, T.; Taguchi, H.; Shimamura, T.
Deposited on : 2014-05-23
Resolution : 3.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

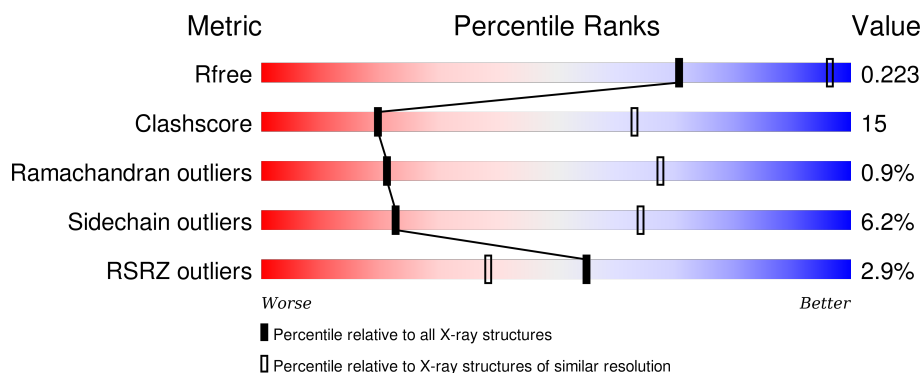
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1273 (4.06-3.50)
Clashscore	102246	1412 (4.06-3.50)
Ramachandran outliers	100387	1351 (4.06-3.50)
Sidechain outliers	100360	1347 (4.06-3.50)
RSRZ outliers	91569	1281 (4.06-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	<div> <div>2%</div> <div>68% 26% . .</div> </div>
1	B	548	<div> <div>%</div> <div>68% 26% . .</div> </div>
1	C	548	<div> <div>%</div> <div>67% 26% . .</div> </div>
1	D	548	<div> <div>%</div> <div>62% 30% . .</div> </div>
1	E	548	<div> <div>%</div> <div>65% 28% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	548	
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	
2	V	97	
2	W	97	
2	X	97	
2	Y	97	
2	Z	97	
2	a	97	
2	b	97	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 64540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	B	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	C	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	D	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	E	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	F	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	G	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	H	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	I	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	J	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	K	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	L	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	M	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			
1	N	524	Total	C	N	O	S	0	0	0
			3849	2395	665	769	20			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
B	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
B	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
C	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
C	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
D	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
D	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
E	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
E	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
F	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
F	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
G	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
G	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
H	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
H	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
I	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
I	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
J	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
J	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
K	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
K	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
L	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
L	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
M	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
M	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
N	52	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
N	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

- Molecule 2 is a protein called 10 kDa chaperonin.

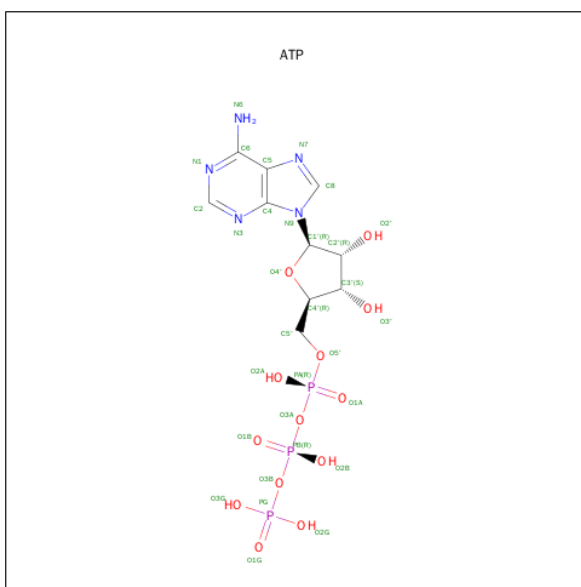
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	Q	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	R	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	S	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	T	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	97	Total 728	C 454	N 127	O 145	S 2	0	0	0
2	V	97	Total 728	C 454	N 127	O 145	S 2	0	0	0
2	W	97	Total 728	C 454	N 127	O 145	S 2	0	0	0
2	X	97	Total 728	C 454	N 127	O 145	S 2	0	0	0
2	Y	97	Total 728	C 454	N 127	O 145	S 2	0	0	0
2	Z	97	Total 728	C 454	N 127	O 145	S 2	0	0	0
2	a	97	Total 728	C 454	N 127	O 145	S 2	0	0	0
2	b	97	Total 728	C 454	N 127	O 145	S 2	0	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

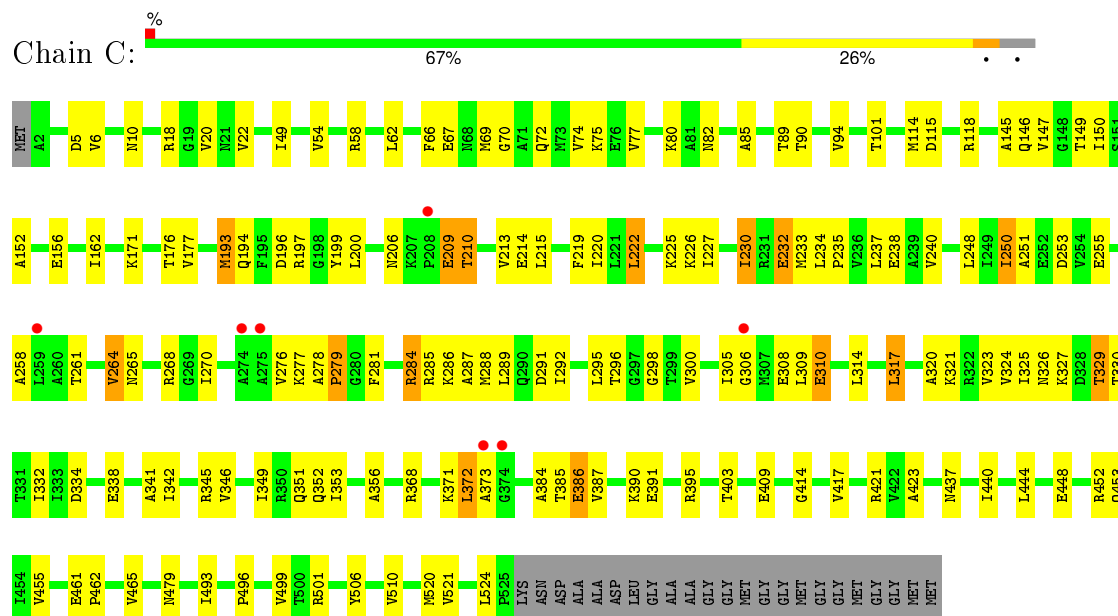
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	K 1	0	0
5	J	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0
5	K	1	Total 1	K 1	0	0
5	E	1	Total 1	K 1	0	0
5	H	1	Total 1	K 1	0	0
5	B	1	Total 1	K 1	0	0
5	I	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0
5	A	1	Total 1	K 1	0	0
5	N	1	Total 1	K 1	0	0
5	L	1	Total 1	K 1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

Continued on next page...

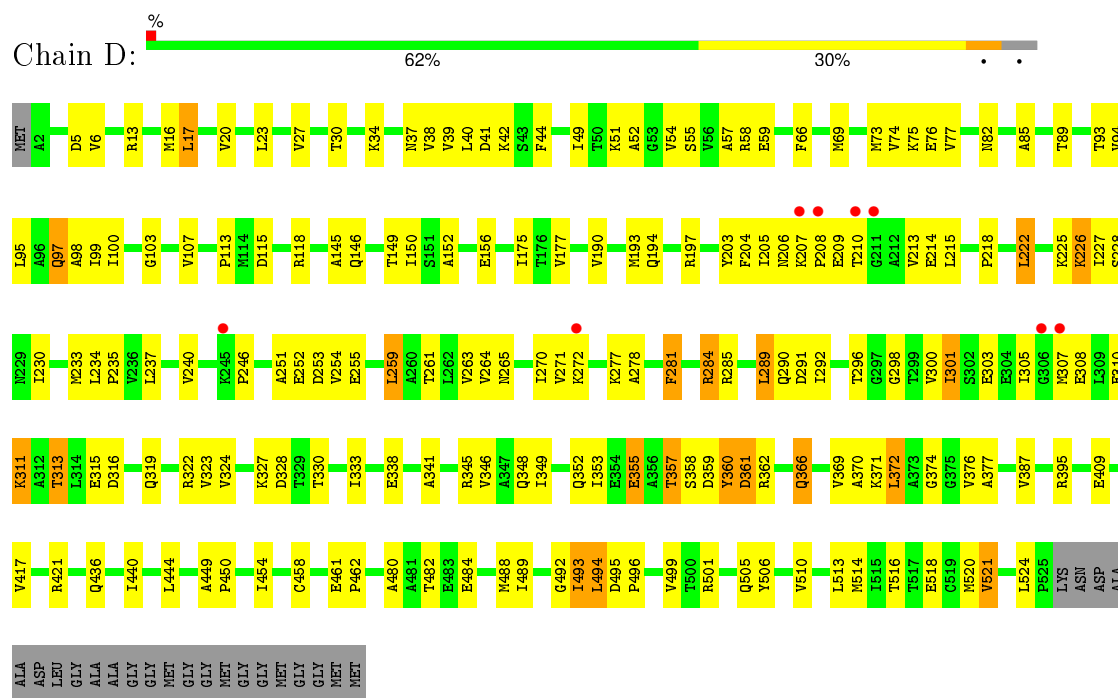
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	K	0	0
			1	1		

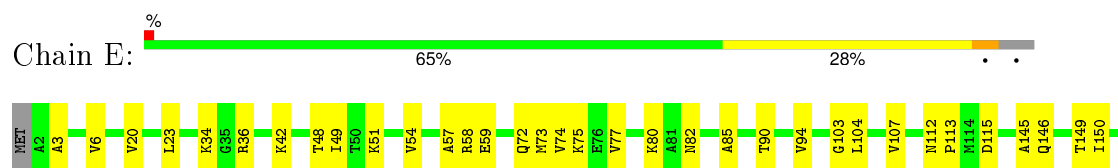
- Molecule 1: 60 kDa chaperonin

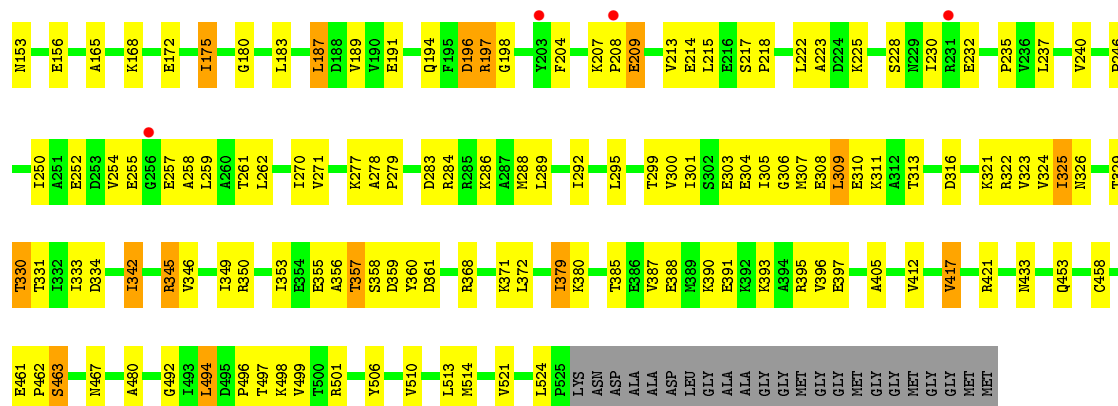


- Molecule 1: 60 kDa chaperonin

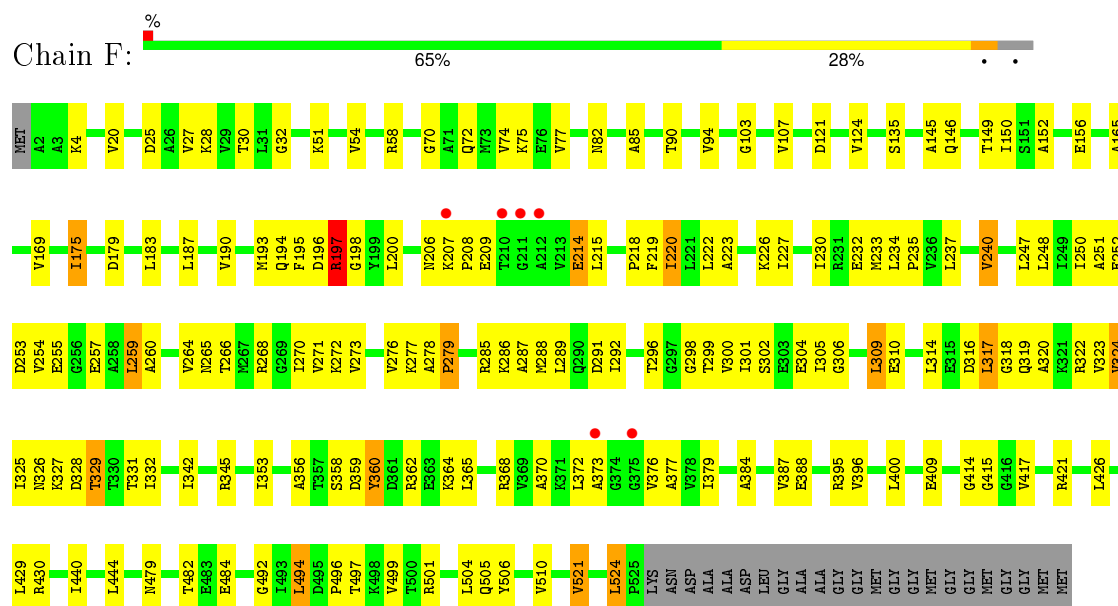


- Molecule 1: 60 kDa chaperonin

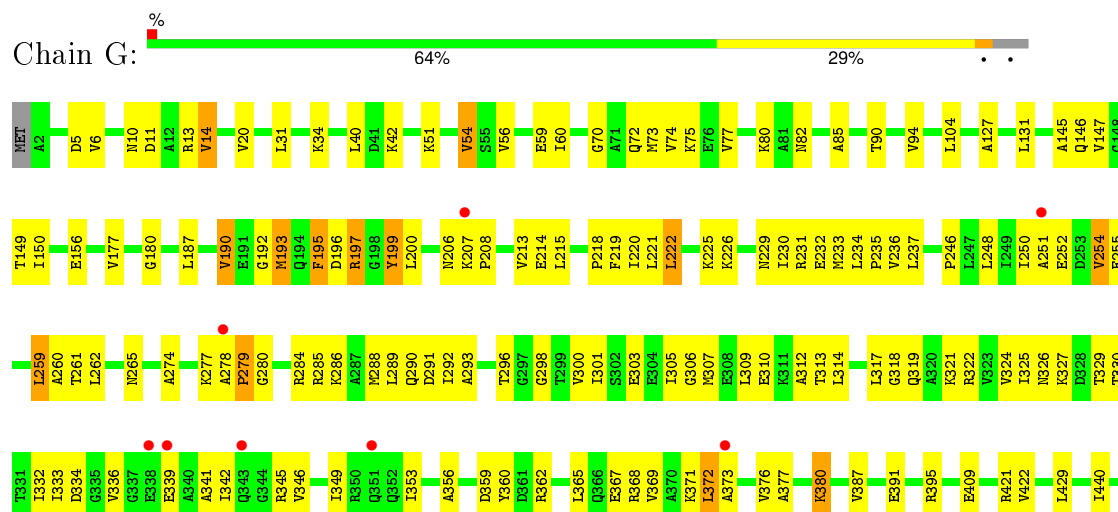




• Molecule 1: 60 kDa chaperonin

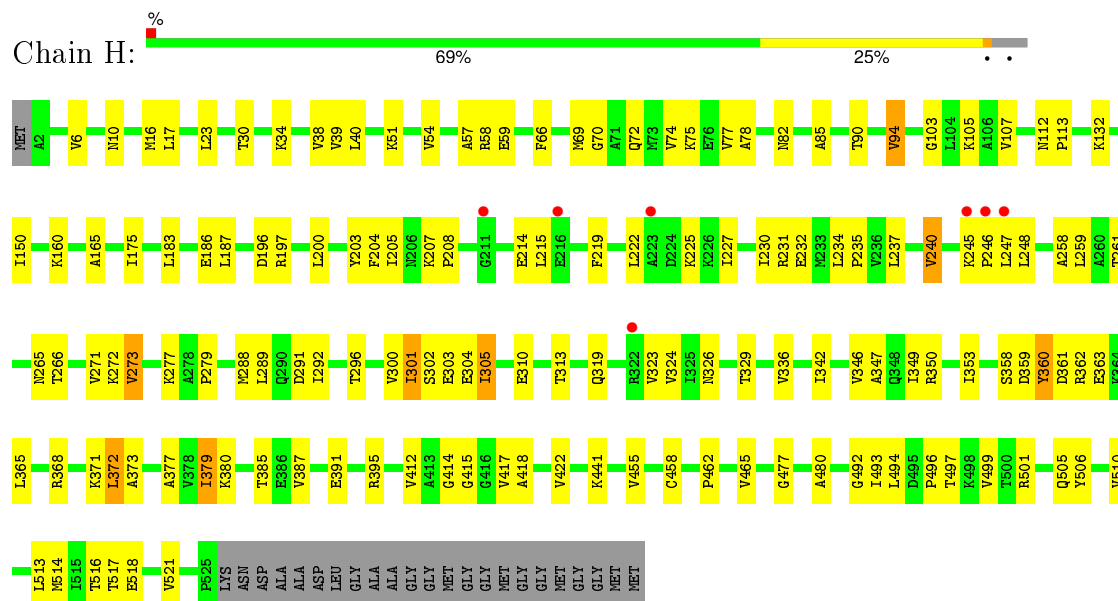


• Molecule 1: 60 kDa chaperonin

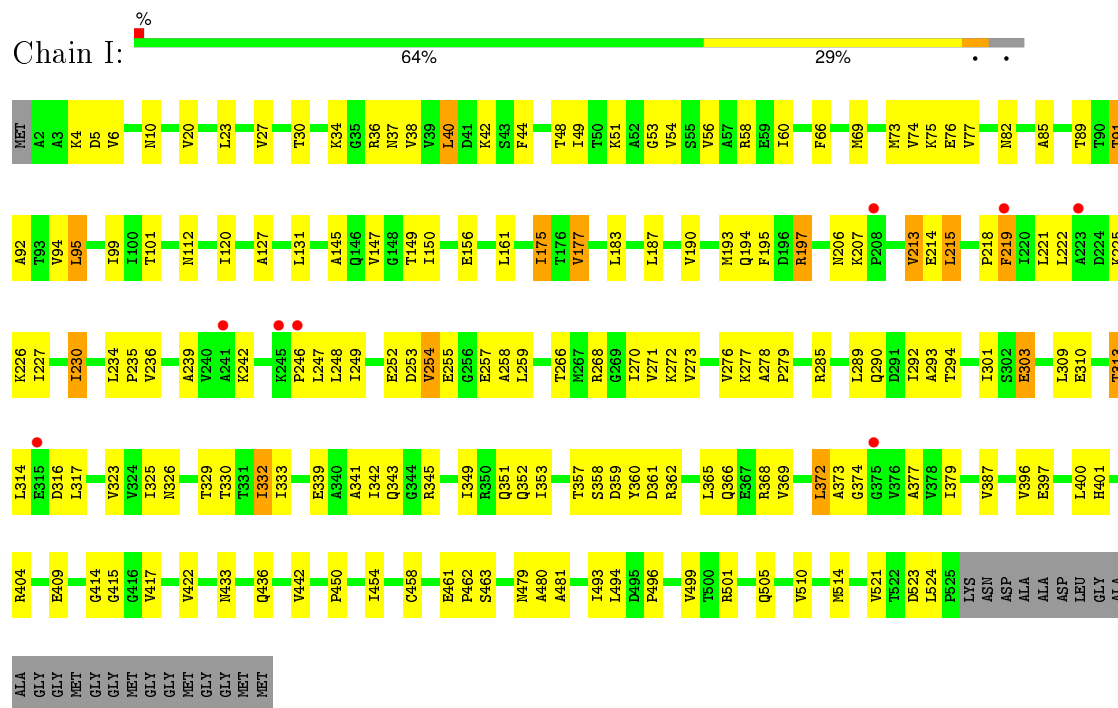




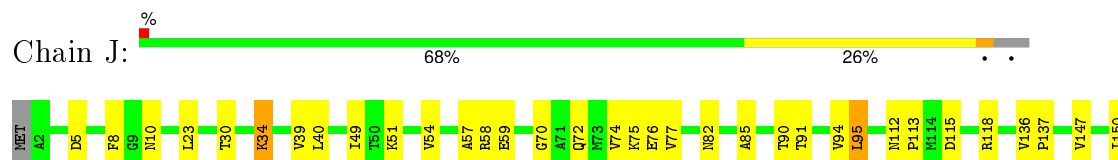
• Molecule 1: 60 kDa chaperonin

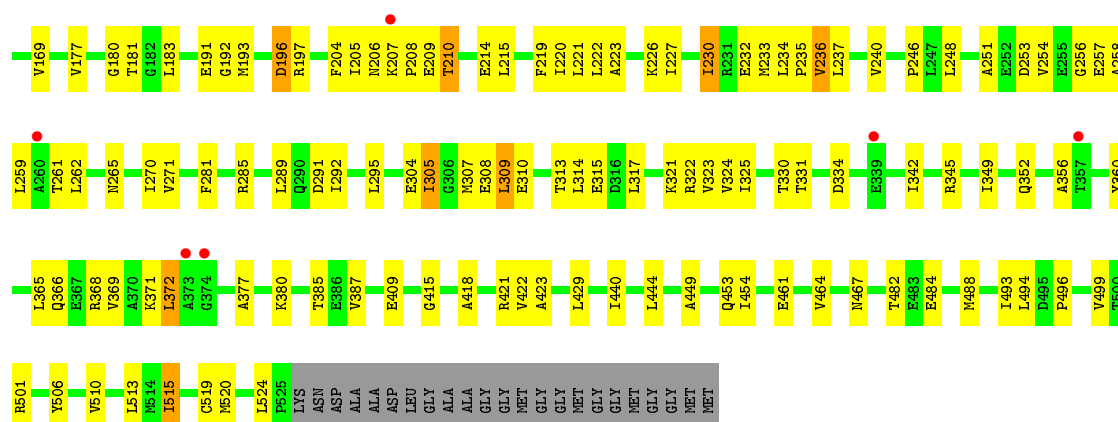


• Molecule 1: 60 kDa chaperonin

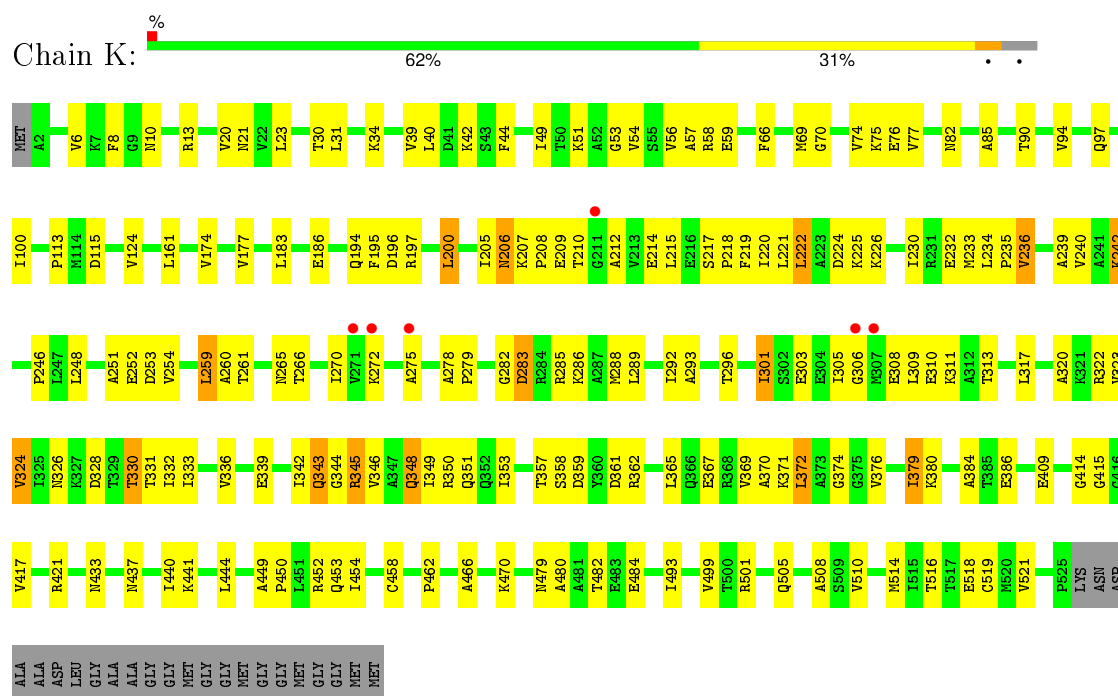


• Molecule 1: 60 kDa chaperonin

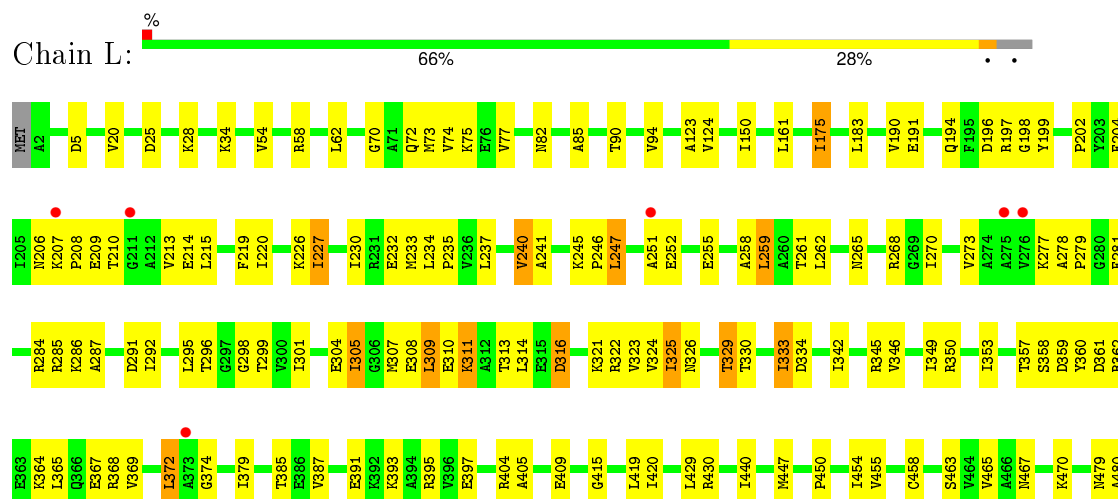




• Molecule 1: 60 kDa chaperonin

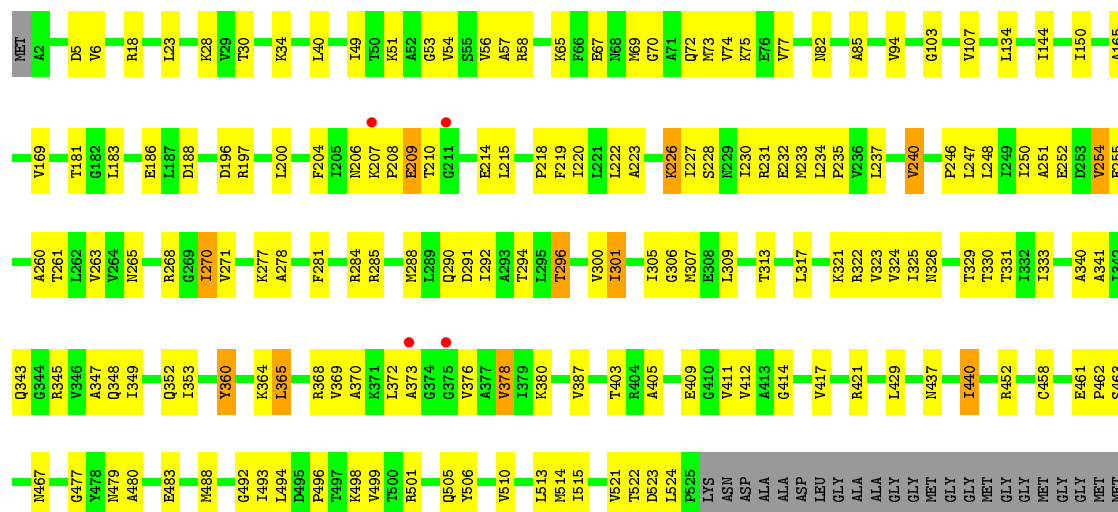


• Molecule 1: 60 kDa chaperonin

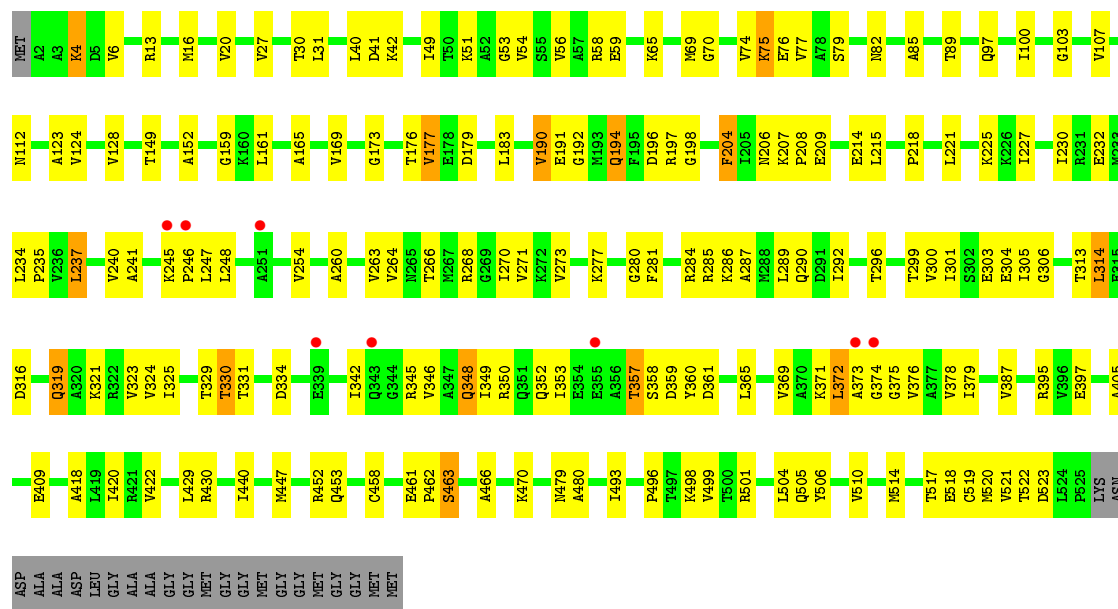




- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin

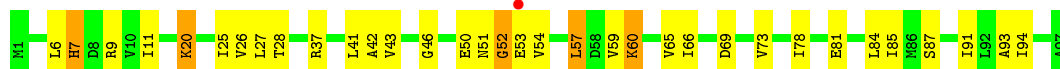


- Molecule 2: 10 kDa chaperonin

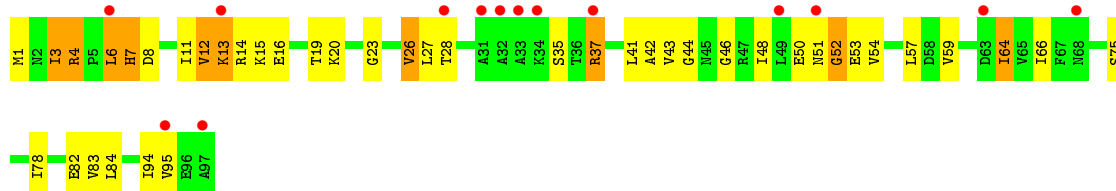




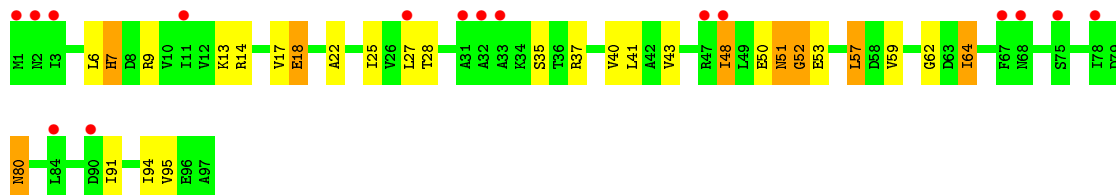
- Molecule 2: 10 kDa chaperonin



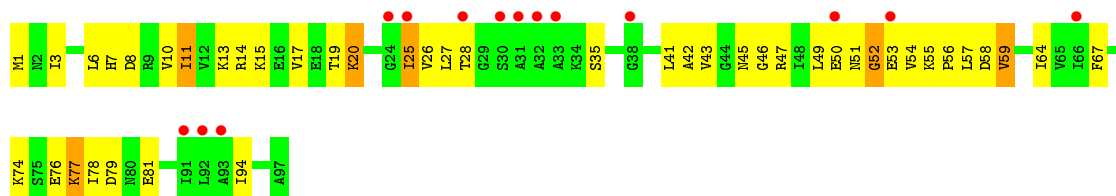
- Molecule 2: 10 kDa chaperonin



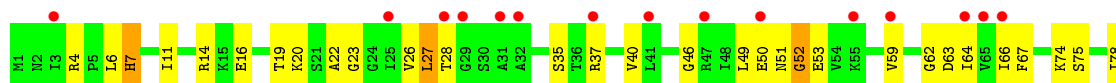
- Molecule 2: 10 kDa chaperonin

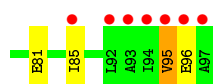


- Molecule 2: 10 kDa chaperonin

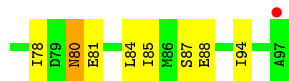
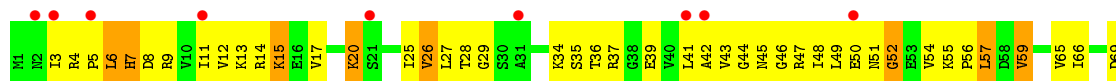


- Molecule 2: 10 kDa chaperonin





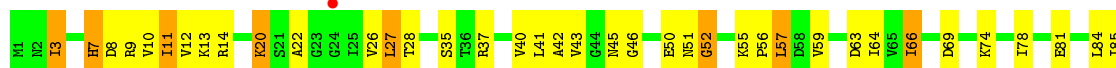
- Molecule 2: 10 kDa chaperonin



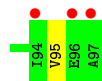
- Molecule 2: 10 kDa chaperonin



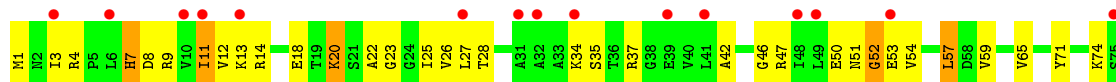
- Molecule 2: 10 kDa chaperonin

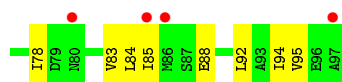


- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

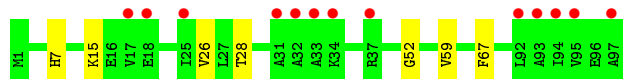
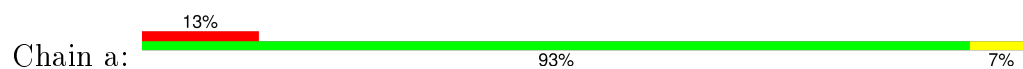




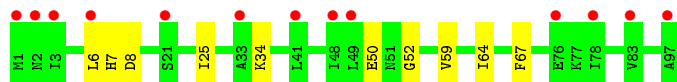
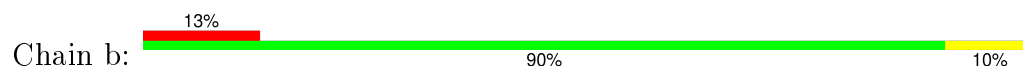
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	160.28Å 217.12Å 198.48Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	49.56 – 3.79 49.56 – 3.79	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.56-3.79) 83.4 (49.56-3.79)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1589)	Depositor
R, R_{free}	0.211 , 0.250 0.213 , 0.223	Depositor DCC
R_{free} test set	5551 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	112.4	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 148.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	4 of 122258 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	64540	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.02 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.8390e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

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: K, MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3877	0.43	0/5235
1	B	0.25	0/3877	0.45	0/5235
1	C	0.25	0/3877	0.44	0/5235
1	D	0.25	0/3877	0.46	1/5235 (0.0%)
1	E	0.25	0/3877	0.44	0/5235
1	F	0.25	0/3877	0.44	0/5235
1	G	0.25	0/3877	0.45	0/5235
1	H	0.25	0/3877	0.44	0/5235
1	I	0.25	0/3877	0.45	0/5235
1	J	0.25	0/3877	0.44	0/5235
1	K	0.25	0/3877	0.43	0/5235
1	L	0.25	0/3877	0.44	0/5235
1	M	0.25	0/3877	0.45	0/5235
1	N	0.25	0/3877	0.44	0/5235
2	O	0.19	0/732	0.38	0/983
2	P	0.19	0/732	0.38	0/983
2	Q	0.20	0/732	0.39	0/983
2	R	0.19	0/732	0.39	0/983
2	S	0.19	0/732	0.40	0/983
2	T	0.19	0/732	0.37	0/983
2	U	0.20	0/732	0.39	0/983
2	V	0.19	0/732	0.40	0/983
2	W	0.19	0/732	0.41	0/983
2	X	0.19	0/732	0.39	0/983
2	Y	0.20	0/732	0.38	0/983
2	Z	0.19	0/732	0.38	0/983
2	a	0.19	0/732	0.37	0/983
2	b	0.19	0/732	0.37	0/983
All	All	0.24	0/64526	0.44	1/87052 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3849	0	3978	108	0
1	B	3849	0	3978	107	0
1	C	3849	0	3978	109	0
1	D	3849	0	3977	133	0
1	E	3849	0	3978	111	0
1	F	3849	0	3978	128	0
1	G	3849	0	3978	120	0
1	H	3849	0	3978	109	0
1	I	3849	0	3978	143	0
1	J	3849	0	3978	106	0
1	K	3849	0	3978	126	0
1	L	3849	0	3978	113	0
1	M	3849	0	3978	123	0
1	N	3849	0	3978	126	0
2	O	728	0	762	27	0
2	P	728	0	762	35	0
2	Q	728	0	762	33	0
2	R	728	0	762	23	0
2	S	728	0	762	37	0
2	T	728	0	762	22	0
2	U	728	0	762	44	0
2	V	728	0	762	35	0
2	W	728	0	762	40	0
2	X	728	0	762	24	0
2	Y	728	0	762	26	0
2	Z	728	0	762	22	0
2	a	728	0	762	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	728	0	762	0	0
3	A	31	0	12	1	0
3	B	31	0	12	3	0
3	C	31	0	12	0	0
3	D	31	0	12	1	0
3	E	31	0	12	0	0
3	F	31	0	12	1	0
3	G	31	0	12	1	0
3	H	31	0	12	1	0
3	I	31	0	12	4	0
3	J	31	0	12	1	0
3	K	31	0	12	1	0
3	L	31	0	12	1	0
3	M	31	0	12	0	0
3	N	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	1	0	0	0	0
All	All	64540	0	66527	1902	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 15.

All (1902) 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:C:10:ASN:HD21	1:H:10:ASN:HD21	1.11	0.98
1:B:10:ASN:HD21	1:I:10:ASN:HD21	1.11	0.97
1:D:226:LYS:HZ3	1:D:252:GLU:H	1.12	0.92
1:G:10:ASN:HD21	1:K:10:ASN:HD21	1.19	0.90
1:G:77:VAL:HG22	1:G:510:VAL:HG21	1.54	0.90
1:A:77:VAL:HG22	1:A:510:VAL:HG21	1.54	0.89
1:F:345:ARG:HH22	1:F:372:LEU:HD11	1.38	0.88
1:M:215:LEU:HD23	1:M:246:PRO:HB2	1.55	0.88
1:F:197:ARG:HH22	1:F:250:ILE:HG23	1.37	0.88
1:I:77:VAL:HG22	1:I:510:VAL:HG21	1.56	0.88
1:H:77:VAL:HG22	1:H:510:VAL:HG21	1.53	0.87
1:N:77:VAL:HG22	1:N:510:VAL:HG21	1.55	0.86
1:C:479:ASN:HD22	1:C:493:ILE:HD11	1.41	0.86
1:A:10:ASN:HD21	1:J:10:ASN:HD21	1.21	0.85
1:L:215:LEU:HD23	1:L:246:PRO:HB2	1.55	0.85
1:D:16:MET:HB2	1:D:520:MET:HE1	1.58	0.84
1:D:372:LEU:HD13	1:D:374:GLY:H	1.42	0.84
1:H:368:ARG:NH1	1:H:368:ARG:O	2.11	0.84
1:F:265:ASN:HD21	2:P:26:VAL:HG13	1.42	0.84
1:M:77:VAL:HG22	1:M:510:VAL:HG21	1.60	0.84
1:L:77:VAL:HG22	1:L:510:VAL:HG21	1.60	0.84
1:C:149:THR:HG22	1:C:156:GLU:HA	1.60	0.83
1:E:215:LEU:HD23	1:E:246:PRO:HB2	1.57	0.83
1:D:37:ASN:HB3	1:D:49:ILE:HD11	1.59	0.83
2:R:59:VAL:HG22	2:R:94:ILE:HD11	1.60	0.83
1:F:197:ARG:NE	1:F:277:LYS:O	2.12	0.82
1:F:175:ILE:HG22	1:F:377:ALA:HB3	1.59	0.82
1:N:215:LEU:HD23	1:N:246:PRO:HB2	1.62	0.82
1:M:65:LYS:HB3	1:M:522:THR:HG21	1.62	0.81
1:J:77:VAL:HG22	1:J:510:VAL:HG21	1.60	0.81
1:H:6:VAL:HG12	1:H:521:VAL:HG12	1.62	0.81
1:F:149:THR:HG22	1:F:156:GLU:HA	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:215:LEU:HD11	1:I:323:VAL:HG22	1.63	0.81
2:Q:14:ARG:NH1	2:Q:37:ARG:O	2.15	0.80
1:D:149:THR:HG22	1:D:156:GLU:HA	1.62	0.80
1:C:345:ARG:HH21	1:C:368:ARG:HH22	1.28	0.80
1:I:372:LEU:HD12	1:I:374:GLY:H	1.47	0.80
1:A:49:ILE:HD11	1:G:73:MET:HE1	1.64	0.80
2:W:20:LYS:NZ	2:W:26:VAL:O	2.15	0.79
1:E:213:VAL:HG23	1:E:325:ILE:HG23	1.65	0.79
1:B:73:MET:HE1	1:C:49:ILE:HD11	1.65	0.79
1:B:6:VAL:HG12	1:B:521:VAL:HG12	1.65	0.79
2:T:14:ARG:NH1	2:T:35:SER:O	2.16	0.79
2:Y:3:ILE:HD11	2:Y:78:ILE:HG13	1.65	0.79
1:C:77:VAL:HG22	1:C:510:VAL:HG11	1.63	0.78
2:U:14:ARG:HH21	2:U:84:LEU:HD21	1.48	0.78
1:E:48:THR:HA	1:E:390:LYS:HE2	1.66	0.78
2:Z:40:VAL:HG13	2:Z:62:GLY:H	1.49	0.78
1:A:54:VAL:HG21	1:A:82:ASN:HB2	1.66	0.78
1:C:206:ASN:ND2	1:C:214:GLU:O	2.15	0.78
1:M:6:VAL:HG12	1:M:521:VAL:HG12	1.65	0.78
1:B:264:VAL:HG11	2:S:27:LEU:HB2	1.66	0.78
1:F:206:ASN:ND2	1:F:214:GLU:H	1.80	0.78
1:G:284:ARG:HD3	1:G:368:ARG:HH12	1.49	0.77
2:Q:14:ARG:NH1	2:Q:15:LYS:H	1.81	0.77
2:S:20:LYS:NZ	2:S:26:VAL:O	2.17	0.77
1:D:215:LEU:HD23	1:D:246:PRO:HB2	1.67	0.77
1:N:65:LYS:HB3	1:N:522:THR:HG21	1.68	0.76
1:F:222:LEU:HD11	1:F:300:VAL:HA	1.65	0.76
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.66	0.76
1:M:429:LEU:HD22	1:M:440:ILE:HG13	1.67	0.76
1:C:54:VAL:HG21	1:C:82:ASN:HB2	1.68	0.76
1:F:77:VAL:HG22	1:F:510:VAL:HG21	1.66	0.76
1:E:149:THR:HG22	1:E:156:GLU:HA	1.66	0.76
1:D:264:VAL:HG11	2:U:27:LEU:HD22	1.69	0.75
1:M:206:ASN:ND2	1:M:214:GLU:H	1.83	0.75
1:M:479:ASN:HD22	1:M:493:ILE:HD11	1.50	0.75
2:W:40:VAL:HG11	2:W:59:VAL:HG11	1.69	0.75
1:I:206:ASN:ND2	1:I:214:GLU:O	2.15	0.75
1:F:345:ARG:HH12	1:F:372:LEU:HD21	1.52	0.75
1:B:77:VAL:HG22	1:B:510:VAL:HG11	1.68	0.74
1:D:54:VAL:HG21	1:D:82:ASN:HB2	1.67	0.74
1:I:149:THR:HG22	1:I:156:GLU:HA	1.67	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:ILE:HD11	1:I:120:ILE:HD13	1.68	0.74
1:B:190:VAL:HG23	1:B:376:VAL:HG13	1.69	0.74
1:D:73:MET:HE1	1:E:49:ILE:HD11	1.69	0.74
2:O:14:ARG:NH2	2:O:35:SER:OG	2.19	0.74
1:D:77:VAL:HG22	1:D:510:VAL:HG21	1.67	0.74
1:K:200:LEU:HD11	1:K:275:ALA:HB3	1.69	0.74
1:G:455:VAL:HG11	1:G:465:VAL:HG11	1.69	0.74
2:S:52:GLY:HA3	2:T:51:ASN:HD22	1.53	0.74
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.70	0.74
1:F:200:LEU:HD11	1:F:277:LYS:HG3	1.69	0.74
1:M:294:THR:HB	1:M:341:ALA:HB1	1.68	0.74
1:D:209:GLU:HG2	1:D:210:THR:HG23	1.70	0.73
1:C:455:VAL:HG11	1:C:465:VAL:HG11	1.70	0.73
1:C:238:GLU:HG2	2:T:23:GLY:HA2	1.69	0.73
1:F:326:ASN:ND2	1:F:328:ASP:OD1	2.21	0.73
1:H:248:LEU:HD11	1:H:323:VAL:HG11	1.69	0.73
1:I:219:PHE:HE1	1:I:317:LEU:HD22	1.53	0.73
1:C:230:ILE:HD13	1:C:258:ALA:HA	1.71	0.73
1:H:518:GLU:HB2	1:I:36:ARG:HH11	1.53	0.73
1:E:54:VAL:HG21	1:E:82:ASN:HB2	1.71	0.73
1:I:23:LEU:HD12	1:I:60:ILE:HD12	1.70	0.73
1:M:150:ILE:HD13	1:M:494:LEU:H	1.54	0.72
1:B:248:LEU:HD11	1:B:323:VAL:HG11	1.70	0.72
1:M:222:LEU:HD11	1:M:300:VAL:HA	1.71	0.72
1:B:328:ASP:N	1:B:328:ASP:OD1	2.22	0.72
1:D:206:ASN:ND2	1:D:214:GLU:H	1.87	0.72
1:M:72:GLN:HA	1:M:75:LYS:HD3	1.70	0.72
2:X:14:ARG:NH2	2:X:37:ARG:O	2.22	0.72
1:E:72:GLN:HA	1:E:75:LYS:HD3	1.71	0.72
2:W:57:LEU:HD22	2:W:59:VAL:H	1.53	0.72
1:I:54:VAL:HG21	1:I:82:ASN:HB2	1.71	0.72
1:J:54:VAL:HG21	1:J:82:ASN:HB2	1.72	0.72
1:E:225:LYS:HE3	1:E:303:GLU:HG3	1.71	0.72
1:K:215:LEU:HD13	1:K:246:PRO:HB2	1.72	0.72
1:A:39:VAL:HG12	1:A:49:ILE:HG12	1.72	0.72
1:A:400:LEU:HD21	1:A:404:ARG:HH21	1.54	0.72
1:M:73:MET:HE1	1:N:49:ILE:HD11	1.72	0.71
1:M:261:THR:O	1:M:265:ASN:ND2	2.24	0.71
1:E:222:LEU:HD11	1:E:300:VAL:HA	1.73	0.71
2:W:20:LYS:HG2	2:W:27:LEU:HD13	1.72	0.71
2:W:14:ARG:NH1	2:W:35:SER:O	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:PHE:HE2	1:J:317:LEU:HD13	1.54	0.71
1:M:54:VAL:HG21	1:M:82:ASN:HB2	1.72	0.71
1:C:115:ASP:HA	1:C:118:ARG:HD2	1.73	0.71
1:I:187:LEU:HD13	1:I:379:ILE:HG22	1.73	0.71
1:J:308:GLU:HG3	1:J:309:LEU:HD23	1.73	0.71
1:N:479:ASN:HD22	1:N:493:ILE:HD11	1.55	0.71
1:A:207:LYS:HB2	1:A:208:PRO:HD3	1.72	0.71
1:I:278:ALA:HB3	1:I:285:ARG:HH11	1.56	0.70
1:F:326:ASN:HD21	1:F:329:THR:HG23	1.56	0.70
1:L:349:ILE:HD11	1:L:368:ARG:HG3	1.72	0.70
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.73	0.70
1:N:54:VAL:HG21	1:N:82:ASN:HB2	1.72	0.70
1:B:54:VAL:HG21	1:B:82:ASN:HB2	1.72	0.70
1:D:278:ALA:HB3	1:D:285:ARG:HH11	1.56	0.70
1:F:227:ILE:HD11	1:F:254:VAL:HG12	1.74	0.70
1:L:372:LEU:HD13	1:L:374:GLY:H	1.57	0.70
1:K:479:ASN:HD22	1:K:493:ILE:HD11	1.56	0.70
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.73	0.70
2:S:20:LYS:HD3	2:S:28:THR:H	1.56	0.70
1:K:54:VAL:HG21	1:K:82:ASN:HB2	1.73	0.70
1:C:325:ILE:HG22	1:C:330:THR:HG23	1.75	0.69
1:L:479:ASN:HD22	1:L:493:ILE:HD11	1.56	0.69
1:L:213:VAL:HG23	1:L:325:ILE:HG23	1.74	0.69
1:B:222:LEU:HD11	1:B:300:VAL:HA	1.72	0.69
1:J:34:LYS:HD3	1:J:34:LYS:H	1.57	0.69
2:P:57:LEU:O	2:P:60:LYS:NZ	2.26	0.69
1:G:131:LEU:HD12	1:G:422:VAL:HG11	1.75	0.69
1:M:207:LYS:HB2	1:M:208:PRO:HD3	1.73	0.69
1:I:415:GLY:N	3:I:601:ATP:O2'	2.24	0.69
1:J:206:ASN:ND2	1:J:214:GLU:O	2.25	0.69
1:A:200:LEU:HD21	1:A:277:LYS:HE3	1.75	0.69
1:C:72:GLN:HA	1:C:75:LYS:HD3	1.73	0.69
1:I:226:LYS:NZ	1:I:227:ILE:O	2.26	0.69
1:B:226:LYS:HA	1:B:226:LYS:HZ2	1.58	0.69
2:P:65:VAL:HG12	2:P:94:ILE:HG12	1.75	0.69
1:M:409:GLU:OE1	1:M:501:ARG:NH2	2.23	0.69
1:D:214:GLU:HG2	1:D:324:VAL:HG22	1.74	0.69
2:Z:20:LYS:HG3	2:Z:27:LEU:HA	1.73	0.69
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.74	0.68
2:V:67:PHE:O	2:W:74:LYS:NZ	2.27	0.68
1:L:455:VAL:HG11	1:L:465:VAL:HG11	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:14:ARG:HE	2:S:35:SER:HB3	1.59	0.68
1:J:233:MET:HE1	1:J:309:LEU:HB2	1.75	0.68
1:H:231:ARG:HG2	2:Y:22:ALA:HB1	1.76	0.68
1:N:292:ILE:O	1:N:296:THR:OG1	2.09	0.68
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.76	0.68
1:H:225:LYS:HE2	1:H:303:GLU:HG3	1.75	0.68
1:D:194:GLN:O	1:D:371:LYS:NZ	2.19	0.68
1:B:200:LEU:HD13	1:B:259:LEU:HD21	1.76	0.68
1:D:233:MET:HB3	1:D:237:LEU:HD13	1.75	0.68
1:L:262:LEU:HD22	1:L:273:VAL:HG11	1.75	0.68
1:I:479:ASN:HD22	1:I:493:ILE:HD11	1.58	0.68
2:V:52:GLY:O	2:V:55:LYS:NZ	2.27	0.68
2:P:20:LYS:HE2	2:P:20:LYS:HA	1.75	0.67
2:Y:20:LYS:HG2	2:Y:27:LEU:HG	1.75	0.67
1:F:58:ARG:HA	1:F:75:LYS:HE3	1.75	0.67
1:H:58:ARG:HA	1:H:75:LYS:HE3	1.76	0.67
2:S:15:LYS:NZ	2:S:19:THR:OG1	2.27	0.67
1:A:349:ILE:HD13	1:A:369:VAL:HG22	1.75	0.67
1:F:54:VAL:HG21	1:F:82:ASN:HB2	1.76	0.67
2:P:57:LEU:HD23	2:P:57:LEU:H	1.59	0.67
1:H:112:ASN:HD21	1:I:34:LYS:HD2	1.59	0.67
1:L:72:GLN:HA	1:L:75:LYS:HD3	1.75	0.67
1:C:296:THR:HG23	1:C:298:GLY:H	1.58	0.67
1:I:54:VAL:HG23	1:I:89:THR:HG21	1.77	0.67
1:J:34:LYS:NZ	1:J:454:ILE:O	2.27	0.67
2:Q:14:ARG:HE	2:Q:35:SER:HB3	1.60	0.67
1:L:265:ASN:HB2	1:L:270:ILE:HD11	1.77	0.67
1:I:37:ASN:HB3	1:I:49:ILE:HD11	1.76	0.67
2:U:34:LYS:NZ	2:U:69:ASP:OD2	2.27	0.67
1:F:207:LYS:HB2	1:F:208:PRO:HD3	1.77	0.67
2:S:13:LYS:HB2	2:S:41:LEU:HD11	1.77	0.67
1:H:412:VAL:HG13	1:H:497:THR:HG22	1.76	0.67
1:M:284:ARG:NH2	1:M:360:TYR:OH	2.28	0.67
2:P:20:LYS:NZ	2:P:26:VAL:O	2.27	0.66
1:F:309:LEU:H	1:F:309:LEU:HD23	1.60	0.66
1:K:100:ILE:HD11	1:K:514:MET:HE3	1.77	0.66
1:M:270:ILE:HG12	1:M:271:VAL:HG22	1.76	0.66
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.78	0.66
1:F:479:ASN:ND2	1:F:482:THR:OG1	2.29	0.66
2:U:20:LYS:HE2	2:U:20:LYS:HA	1.77	0.66
1:C:308:GLU:HG3	1:C:309:LEU:HD23	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:THR:HG22	1:F:316:ASP:HA	1.75	0.66
1:N:206:ASN:HD21	1:N:214:GLU:H	1.43	0.66
2:W:22:ALA:HA	2:X:77:LYS:HE2	1.76	0.66
1:G:353:ILE:HD12	1:G:365:LEU:HB3	1.77	0.66
1:L:287:ALA:O	1:L:368:ARG:NH2	2.29	0.66
1:B:270:ILE:HD13	2:S:25:ILE:HD11	1.77	0.66
1:L:54:VAL:HG21	1:L:82:ASN:HB2	1.75	0.66
1:J:265:ASN:HB2	1:J:270:ILE:HD11	1.78	0.66
1:H:261:THR:O	1:H:265:ASN:ND2	2.29	0.66
2:Q:75:SER:OG	2:Q:82:GLU:OE2	2.14	0.66
1:K:209:GLU:HG2	1:K:210:THR:HG23	1.77	0.66
1:A:479:ASN:HD22	1:A:493:ILE:HD11	1.60	0.66
1:L:207:LYS:HB2	1:L:208:PRO:HD3	1.78	0.66
1:I:95:LEU:O	1:I:99:ILE:HG22	1.96	0.65
2:P:43:VAL:HG13	2:P:57:LEU:HD11	1.77	0.65
1:G:149:THR:HG22	1:G:156:GLU:HA	1.76	0.65
1:F:219:PHE:CZ	1:F:317:LEU:HD13	2.30	0.65
1:K:345:ARG:NE	1:K:348:GLN:OE1	2.25	0.65
1:J:215:LEU:HD23	1:J:246:PRO:HB2	1.78	0.65
1:I:266:THR:HG23	1:I:272:LYS:HA	1.78	0.65
1:H:368:ARG:HH12	1:H:372:LEU:HD13	1.61	0.65
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.78	0.65
1:E:34:LYS:NZ	1:E:480:ALA:O	2.28	0.65
1:N:299:THR:HB	1:N:316:ASP:HA	1.79	0.65
2:Q:50:GLU:HG2	2:R:51:ASN:HB3	1.79	0.65
2:Z:14:ARG:NH2	2:Z:69:ASP:OD2	2.30	0.65
1:I:51:LYS:NZ	3:I:601:ATP:O1A	2.30	0.65
1:M:200:LEU:HD22	1:M:254:VAL:HG23	1.79	0.65
1:C:309:LEU:HD23	1:C:309:LEU:H	1.61	0.65
1:D:261:THR:HG22	2:U:29:GLY:H	1.62	0.65
1:H:54:VAL:HG21	1:H:82:ASN:HB2	1.79	0.65
2:V:66:ILE:HD11	2:V:95:VAL:HG23	1.79	0.64
2:V:13:LYS:HG3	2:V:83:VAL:HG12	1.77	0.64
1:L:220:ILE:HD11	1:L:296:THR:HG21	1.78	0.64
1:L:296:THR:HG23	1:L:298:GLY:H	1.62	0.64
1:C:287:ALA:O	1:C:368:ARG:NH2	2.29	0.64
1:A:265:ASN:HB2	1:A:270:ILE:HD11	1.78	0.64
1:C:214:GLU:HG2	1:C:324:VAL:HG22	1.80	0.64
2:U:20:LYS:NZ	2:U:26:VAL:O	2.30	0.64
1:C:321:LYS:HB3	1:C:334:ASP:HB3	1.79	0.64
1:A:197:ARG:HG2	1:A:277:LYS:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:THR:O	1:G:265:ASN:ND2	2.31	0.64
2:V:16:GLU:H	2:V:16:GLU:CD	2.01	0.64
2:W:14:ARG:NH2	2:W:69:ASP:OD1	2.29	0.64
1:J:309:LEU:H	1:J:309:LEU:HD23	1.61	0.64
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.80	0.64
1:D:296:THR:HG23	1:D:298:GLY:H	1.62	0.64
1:J:227:ILE:HD11	1:J:254:VAL:HG22	1.80	0.64
2:U:9:ARG:NH1	2:U:87:SER:OG	2.29	0.64
1:M:218:PRO:HG3	1:M:323:VAL:HG22	1.80	0.64
2:X:3:ILE:HD11	2:X:78:ILE:HG13	1.78	0.64
2:Q:4:ARG:HE	2:Q:4:ARG:HA	1.62	0.64
1:I:40:LEU:HD11	1:I:56:VAL:HG12	1.80	0.64
1:A:206:ASN:ND2	1:A:208:PRO:HD2	2.13	0.64
1:I:365:LEU:HG	1:I:368:ARG:HH21	1.63	0.64
1:D:226:LYS:HZ3	1:D:252:GLU:N	1.92	0.64
2:O:55:LYS:HD2	2:O:56:PRO:HD2	1.79	0.63
1:F:370:ALA:HB1	1:F:376:VAL:HG22	1.81	0.63
1:E:214:GLU:HG2	1:E:324:VAL:HG22	1.81	0.63
1:L:206:ASN:ND2	1:L:214:GLU:H	1.97	0.63
1:K:161:LEU:HD21	1:K:379:ILE:HD13	1.79	0.63
2:P:73:VAL:HG13	2:P:84:LEU:HD21	1.80	0.63
2:U:45:ASN:HD22	2:U:54:VAL:HG21	1.63	0.63
1:K:261:THR:O	1:K:265:ASN:ND2	2.32	0.63
1:I:131:LEU:HD12	1:I:422:VAL:HG21	1.81	0.63
2:P:50:GLU:O	2:P:52:GLY:N	2.31	0.62
1:M:220:ILE:HG12	1:M:296:THR:HG21	1.81	0.62
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.81	0.62
1:F:219:PHE:HE2	1:F:317:LEU:HD22	1.64	0.62
1:L:268:ARG:HD2	2:V:27:LEU:HD21	1.81	0.62
1:B:359:ASP:O	1:B:362:ARG:HG2	1.99	0.62
1:I:42:LYS:NZ	1:I:48:THR:OG1	2.30	0.62
1:F:248:LEU:HD11	1:F:325:ILE:HD11	1.81	0.62
1:E:379:ILE:HD11	1:E:396:VAL:HG11	1.81	0.62
2:R:40:VAL:HG13	2:R:62:GLY:H	1.64	0.62
1:K:207:LYS:HB2	1:K:208:PRO:HD3	1.80	0.62
1:E:20:VAL:HG13	1:E:74:VAL:HG21	1.81	0.62
1:M:134:LEU:HD22	1:M:412:VAL:HG23	1.82	0.62
1:E:51:LYS:NZ	1:E:391:GLU:OE2	2.29	0.62
2:U:43:VAL:HG11	2:U:57:LEU:HD11	1.81	0.62
1:B:10:ASN:ND2	1:I:10:ASN:HD21	1.92	0.62
1:D:265:ASN:HD21	2:U:26:VAL:HG23	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:48:ILE:HD13	2:R:48:ILE:H	1.65	0.62
1:E:194:GLN:OE1	1:E:331:THR:HG23	1.99	0.62
1:I:40:LEU:HB2	1:I:42:LYS:HZ2	1.64	0.62
1:C:194:GLN:O	1:C:371:LYS:NZ	2.23	0.62
1:E:412:VAL:HG13	1:E:497:THR:HG22	1.81	0.62
1:L:326:ASN:HD21	1:L:329:THR:HG23	1.65	0.62
2:U:37:ARG:HD3	2:U:66:ILE:HG22	1.82	0.62
1:D:338:GLU:HG2	1:D:341:ALA:H	1.65	0.62
2:P:37:ARG:HG2	2:P:66:ILE:HG22	1.82	0.61
2:X:55:LYS:HD2	2:X:56:PRO:HD2	1.82	0.61
1:K:20:VAL:HG13	1:K:74:VAL:HG21	1.81	0.61
1:D:27:VAL:HG21	1:D:93:THR:HG21	1.81	0.61
1:J:8:PHE:HE1	1:J:519:CYS:HG	1.47	0.61
2:Y:74:LYS:HD3	2:Y:85:ILE:HD11	1.83	0.61
1:I:175:ILE:HD13	1:I:400:LEU:HD11	1.81	0.61
1:I:409:GLU:OE1	1:I:501:ARG:NH2	2.32	0.61
2:V:16:GLU:OE2	2:V:19:THR:OG1	2.17	0.61
1:I:175:ILE:HD12	1:I:404:ARG:HH21	1.65	0.61
1:A:356:ALA:HB1	1:A:358:SER:HA	1.83	0.61
2:V:50:GLU:OE1	2:W:51:ASN:ND2	2.33	0.61
2:U:13:LYS:O	2:U:15:LYS:NZ	2.26	0.61
1:F:175:ILE:HG13	1:F:400:LEU:HD21	1.83	0.61
1:B:220:ILE:HG12	1:B:296:THR:HG21	1.81	0.61
1:J:115:ASP:OD1	1:J:118:ARG:NH1	2.34	0.61
1:J:72:GLN:HA	1:J:75:LYS:HD3	1.82	0.61
1:F:206:ASN:ND2	1:F:208:PRO:HD2	2.16	0.61
1:I:197:ARG:HD2	1:I:277:LYS:HE3	1.82	0.61
1:J:209:GLU:N	1:J:209:GLU:OE1	2.28	0.61
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.82	0.61
2:O:47:ARG:HE	2:O:49:LEU:HD12	1.64	0.61
1:B:294:THR:HG21	1:B:345:ARG:NE	2.16	0.61
1:H:222:LEU:HD11	1:H:301:ILE:H	1.65	0.61
1:G:20:VAL:HG13	1:G:74:VAL:HG21	1.83	0.61
1:I:323:VAL:HG12	1:I:332:ILE:HB	1.82	0.60
1:A:321:LYS:O	1:A:322:ARG:NH1	2.32	0.60
1:H:234:LEU:HD12	2:Y:23:GLY:HA2	1.83	0.60
1:K:224:ASP:OD1	1:K:286:LYS:NZ	2.28	0.60
2:V:14:ARG:HH11	2:V:14:ARG:HA	1.65	0.60
1:K:251:ALA:O	1:K:278:ALA:N	2.34	0.60
1:C:326:ASN:HD21	1:C:329:THR:HG22	1.66	0.60
1:C:145:ALA:O	1:C:149:THR:HG23	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:262:LEU:HA	1:J:265:ASN:ND2	2.15	0.60
1:L:308:GLU:H	1:L:311:LYS:HE3	1.64	0.60
1:C:281:PHE:O	1:C:284:ARG:HG3	2.01	0.60
2:U:55:LYS:HD2	2:U:56:PRO:HD2	1.83	0.60
1:C:448:GLU:OE1	1:C:452:ARG:NH2	2.34	0.60
1:A:72:GLN:HA	1:A:75:LYS:HD3	1.83	0.60
1:K:452:ARG:HG3	1:K:462:PRO:HB2	1.84	0.60
1:H:415:GLY:N	3:H:601:ATP:O2'	2.33	0.60
2:V:14:ARG:HH21	2:V:35:SER:HB3	1.67	0.60
1:H:385:THR:OG1	1:N:76:GLU:OE2	2.18	0.60
1:I:294:THR:HB	1:I:345:ARG:HH11	1.65	0.60
1:I:193:MET:HB3	1:I:332:ILE:HG23	1.84	0.60
1:K:206:ASN:ND2	1:K:214:GLU:H	1.98	0.60
1:K:358:SER:O	1:K:362:ARG:NH2	2.34	0.60
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.83	0.60
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.83	0.60
1:I:248:LEU:HD11	1:I:325:ILE:HD11	1.83	0.60
1:G:72:GLN:HA	1:G:75:LYS:HD3	1.83	0.60
1:H:150:ILE:HD11	1:H:492:GLY:O	2.02	0.60
1:H:360:TYR:O	1:H:363:GLU:HG2	2.02	0.60
1:L:206:ASN:ND2	1:L:208:PRO:HD2	2.16	0.60
2:U:13:LYS:HB3	2:U:41:LEU:HD11	1.82	0.60
1:G:349:ILE:O	1:G:353:ILE:HG12	2.02	0.60
2:O:14:ARG:NH2	2:O:35:SER:O	2.35	0.60
1:D:13:ARG:NH2	1:D:518:GLU:OE1	2.33	0.60
1:F:152:ALA:O	1:F:395:ARG:NH1	2.35	0.60
1:M:18:ARG:NH1	1:M:67:GLU:OE2	2.35	0.59
1:M:165:ALA:O	1:M:169:VAL:HG12	2.03	0.59
2:T:51:ASN:O	2:T:53:GLU:N	2.35	0.59
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.85	0.59
1:J:409:GLU:OE1	1:J:501:ARG:NH2	2.28	0.59
1:M:206:ASN:ND2	1:M:208:PRO:HD2	2.18	0.59
1:I:227:ILE:HD11	1:I:254:VAL:HB	1.84	0.59
1:I:303:GLU:OE1	1:I:303:GLU:N	2.35	0.59
1:E:393:LYS:NZ	1:E:397:GLU:OE1	2.35	0.59
2:X:50:GLU:O	2:X:52:GLY:N	2.31	0.59
2:Q:12:VAL:HG22	2:Q:84:LEU:HD11	1.85	0.59
1:K:209:GLU:OE1	1:K:209:GLU:N	2.35	0.59
1:N:349:ILE:O	1:N:352:GLN:HG2	2.02	0.59
2:S:11:ILE:HG23	2:S:42:ALA:HB3	1.84	0.59
1:C:345:ARG:HH21	1:C:368:ARG:NH2	1.99	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ARG:O	1:A:349:ILE:HG13	2.02	0.59
1:K:265:ASN:HA	1:K:270:ILE:HD12	1.85	0.59
1:B:225:LYS:NZ	1:B:304:GLU:OE2	2.33	0.59
2:R:13:LYS:HB2	2:R:41:LEU:HD11	1.84	0.59
1:M:40:LEU:HD21	1:M:56:VAL:HG12	1.83	0.59
1:F:230:ILE:HD11	2:P:28:THR:HG23	1.84	0.59
1:H:214:GLU:HG2	1:H:324:VAL:HG22	1.84	0.59
1:D:58:ARG:HA	1:D:75:LYS:HD3	1.85	0.59
2:V:11:ILE:HB	2:V:42:ALA:HB3	1.85	0.59
1:M:452:ARG:HG3	1:M:462:PRO:HB2	1.85	0.59
1:G:237:LEU:HD13	2:Q:26:VAL:HG11	1.85	0.59
2:X:8:ASP:HA	2:X:57:LEU:HD21	1.85	0.59
2:T:20:LYS:HB3	2:T:27:LEU:HA	1.84	0.59
1:I:254:VAL:HG22	1:I:259:LEU:HG	1.84	0.59
1:I:325:ILE:HG12	1:I:330:THR:HG23	1.85	0.59
1:G:225:LYS:HE2	1:G:303:GLU:HG3	1.84	0.59
1:D:409:GLU:OE1	1:D:501:ARG:NH2	2.35	0.59
1:B:51:LYS:NZ	3:B:601:ATP:O1A	2.36	0.58
1:M:364:LYS:HE2	1:M:368:ARG:HH21	1.68	0.58
1:M:188:ASP:HB2	1:M:378:VAL:HG13	1.85	0.58
1:N:372:LEU:HD12	1:N:374:GLY:H	1.68	0.58
1:B:353:ILE:HG13	1:B:365:LEU:HB3	1.84	0.58
2:O:11:ILE:HB	2:O:42:ALA:HB3	1.85	0.58
2:R:50:GLU:O	2:R:52:GLY:N	2.31	0.58
2:O:50:GLU:HG2	2:P:51:ASN:HB2	1.84	0.58
1:E:391:GLU:OE2	1:E:395:ARG:NE	2.35	0.58
1:B:214:GLU:HG2	1:B:324:VAL:HG22	1.85	0.58
1:E:145:ALA:O	1:E:149:THR:HG23	2.04	0.58
1:K:206:ASN:ND2	1:K:208:PRO:HD2	2.17	0.58
2:Y:7:HIS:HB2	2:Y:46:GLY:O	2.03	0.58
1:G:10:ASN:ND2	1:K:10:ASN:HD21	1.97	0.58
2:Q:16:GLU:HB2	2:Q:19:THR:HG22	1.84	0.58
1:E:197:ARG:NH1	1:E:279:PRO:O	2.36	0.58
1:L:358:SER:O	1:L:362:ARG:NH1	2.36	0.58
1:L:214:GLU:HG2	1:L:324:VAL:HB	1.86	0.58
1:K:206:ASN:ND2	1:K:214:GLU:HG2	2.19	0.58
1:L:237:LEU:O	1:L:240:VAL:HG22	2.04	0.58
1:G:259:LEU:HD12	1:G:262:LEU:HD21	1.86	0.58
2:Y:50:GLU:O	2:Y:52:GLY:N	2.32	0.58
1:G:195:PHE:CE2	1:G:279:PRO:HB3	2.39	0.58
1:I:252:GLU:O	1:I:277:LYS:HG3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:LEU:HB3	1:H:273:VAL:HG13	1.85	0.58
1:K:232:GLU:HB2	1:K:310:GLU:HG3	1.85	0.58
2:T:7:HIS:HB2	2:T:46:GLY:O	2.04	0.58
1:K:357:THR:HG22	1:K:358:SER:H	1.68	0.57
2:T:11:ILE:HD12	2:T:85:ILE:HG12	1.86	0.57
1:J:349:ILE:O	1:J:352:GLN:HG2	2.04	0.57
1:D:246:PRO:HB3	1:D:272:LYS:HG3	1.87	0.57
1:H:113:PRO:HG2	1:I:36:ARG:HE	1.68	0.57
1:C:58:ARG:O	1:C:75:LYS:NZ	2.38	0.57
1:K:370:ALA:HB1	1:K:376:VAL:HG22	1.86	0.57
2:Z:59:VAL:HG12	2:Z:94:ILE:HD11	1.86	0.57
1:G:6:VAL:HG12	1:G:521:VAL:HG22	1.85	0.57
1:N:227:ILE:HD11	1:N:254:VAL:HG12	1.85	0.57
2:U:50:GLU:O	2:U:52:GLY:N	2.33	0.57
2:P:37:ARG:HH22	2:Q:78:ILE:HG13	1.70	0.57
1:F:415:GLY:N	3:F:601:ATP:O2'	2.31	0.57
1:G:187:LEU:HD11	1:G:377:ALA:HB1	1.84	0.57
2:Q:14:ARG:NH2	2:Q:35:SER:OG	2.37	0.57
1:M:411:VAL:HG21	1:M:494:LEU:HD21	1.86	0.57
1:J:324:VAL:HG13	1:J:331:THR:HB	1.84	0.57
1:F:145:ALA:O	1:F:149:THR:HG23	2.04	0.57
1:B:226:LYS:NZ	1:B:253:ASP:H	2.02	0.57
1:L:150:ILE:HD13	1:L:494:LEU:H	1.69	0.57
2:W:50:GLU:O	2:W:52:GLY:N	2.34	0.57
2:Z:10:VAL:HG13	2:Z:43:VAL:HG23	1.85	0.57
2:R:43:VAL:HG13	2:R:57:LEU:HD11	1.85	0.57
1:M:292:ILE:O	1:M:296:THR:OG1	2.23	0.57
1:N:198:GLY:HA2	1:N:325:ILE:HD11	1.86	0.57
1:D:6:VAL:HG12	1:D:521:VAL:HB	1.86	0.57
1:L:20:VAL:HG13	1:L:74:VAL:HG21	1.85	0.57
1:H:326:ASN:HD21	1:H:329:THR:HG1	1.51	0.57
1:B:409:GLU:OE1	1:B:501:ARG:NH2	2.38	0.57
1:G:190:VAL:HG13	1:G:376:VAL:HG23	1.87	0.57
2:W:66:ILE:O	2:W:92:LEU:HG	2.04	0.57
2:Y:11:ILE:HB	2:Y:85:ILE:HG22	1.86	0.57
1:B:200:LEU:HD11	1:B:275:ALA:HB3	1.86	0.57
1:I:496:PRO:O	1:I:499:VAL:HG22	2.04	0.57
1:L:233:MET:HB3	1:L:237:LEU:HD13	1.87	0.57
1:L:150:ILE:CD1	1:L:494:LEU:H	2.17	0.57
1:N:221:LEU:HD11	1:N:301:ILE:HD12	1.86	0.57
1:G:319:GLN:HG2	1:G:336:VAL:HG21	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:MET:HB3	1:G:332:ILE:HG13	1.86	0.57
1:D:97:GLN:HG3	1:D:98:ALA:N	2.20	0.57
1:D:328:ASP:N	1:D:328:ASP:OD1	2.38	0.57
1:M:150:ILE:CD1	1:M:494:LEU:H	2.18	0.56
1:B:220:ILE:HD11	1:B:222:LEU:HD23	1.87	0.56
1:I:254:VAL:HG23	1:I:258:ALA:HB3	1.87	0.56
1:B:338:GLU:HG2	1:B:341:ALA:H	1.69	0.56
2:W:3:ILE:HD12	2:W:78:ILE:HG21	1.87	0.56
2:Y:11:ILE:HG23	2:Y:42:ALA:HB3	1.86	0.56
2:V:57:LEU:HD21	2:V:88:GLU:HG3	1.87	0.56
1:H:359:ASP:O	1:H:362:ARG:N	2.38	0.56
1:L:405:ALA:HB1	1:L:498:LYS:HD3	1.86	0.56
1:K:415:GLY:N	3:K:601:ATP:O2'	2.32	0.56
1:H:207:LYS:HB2	1:H:208:PRO:HD3	1.86	0.56
1:I:215:LEU:HD13	1:I:218:PRO:HG3	1.86	0.56
1:D:145:ALA:O	1:D:149:THR:HG23	2.04	0.56
1:M:513:LEU:HB3	1:N:49:ILE:HD12	1.87	0.56
2:U:49:LEU:O	2:U:50:GLU:HG2	2.05	0.56
1:G:42:LYS:NZ	1:G:59:GLU:OE2	2.33	0.56
1:E:150:ILE:HD13	1:E:494:LEU:H	1.70	0.56
2:W:55:LYS:HD2	2:W:56:PRO:HD2	1.86	0.56
1:E:196:ASP:OD1	1:E:196:ASP:N	2.38	0.56
1:J:365:LEU:O	1:J:369:VAL:HG13	2.05	0.56
1:L:150:ILE:HD11	1:L:492:GLY:O	2.05	0.56
1:I:4:LYS:NZ	1:I:523:ASP:OD1	2.34	0.56
2:S:20:LYS:HG2	2:S:27:LEU:HA	1.85	0.56
1:K:34:LYS:NZ	1:K:480:ALA:O	2.38	0.56
1:B:10:ASN:HD21	1:I:10:ASN:ND2	1.93	0.56
1:M:69:MET:SD	1:N:41:ASP:HB2	2.46	0.56
1:B:207:LYS:HB2	1:B:208:PRO:HD3	1.87	0.56
1:N:165:ALA:O	1:N:169:VAL:HG12	2.06	0.56
2:U:20:LYS:HZ2	2:U:27:LEU:HA	1.70	0.56
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.87	0.56
1:N:409:GLU:OE1	1:N:501:ARG:NH2	2.36	0.56
1:C:226:LYS:HG2	1:C:227:ILE:H	1.71	0.56
1:C:265:ASN:ND2	1:C:270:ILE:HD11	2.20	0.56
1:D:237:LEU:O	1:D:240:VAL:HG22	2.06	0.56
1:N:206:ASN:ND2	1:N:214:GLU:H	2.04	0.56
1:I:20:VAL:HG13	1:I:74:VAL:HG21	1.88	0.56
1:C:409:GLU:OE1	1:C:501:ARG:NH2	2.34	0.56
1:K:58:ARG:HA	1:K:75:LYS:HD3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:LYS:HD3	1:I:253:ASP:OD1	2.06	0.56
1:M:231:ARG:HH22	2:X:77:LYS:HZ3	1.53	0.56
1:H:361:ASP:OD1	1:H:362:ARG:N	2.39	0.56
1:N:241:ALA:HB1	2:X:25:ILE:HD11	1.88	0.56
1:F:296:THR:HG23	1:F:298:GLY:H	1.71	0.56
2:Z:49:LEU:O	2:Z:50:GLU:HG2	2.06	0.56
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.88	0.56
1:H:72:GLN:HA	1:H:75:LYS:HD3	1.88	0.55
1:I:339:GLU:O	1:I:343:GLN:NE2	2.39	0.55
2:S:45:ASN:OD1	2:S:46:GLY:N	2.37	0.55
1:B:226:LYS:HZ3	1:B:253:ASP:H	1.52	0.55
1:M:231:ARG:HH12	2:X:77:LYS:HZ2	1.53	0.55
1:E:150:ILE:HD11	1:E:492:GLY:O	2.06	0.55
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.88	0.55
1:F:165:ALA:O	1:F:169:VAL:HG12	2.05	0.55
1:J:342:ILE:HG13	1:J:345:ARG:NH1	2.21	0.55
1:B:261:THR:HG22	2:S:28:THR:HA	1.88	0.55
1:D:207:LYS:HB2	1:D:208:PRO:HD3	1.87	0.55
1:K:206:ASN:HD22	1:K:214:GLU:HG2	1.71	0.55
2:U:65:VAL:HG12	2:U:94:ILE:HG12	1.88	0.55
2:W:45:ASN:OD1	2:W:46:GLY:N	2.37	0.55
1:J:461:GLU:HB2	1:J:464:VAL:HG22	1.87	0.55
1:D:23:LEU:HD11	1:D:57:ALA:HA	1.88	0.55
1:C:20:VAL:HG13	1:C:74:VAL:HG21	1.87	0.55
1:B:165:ALA:O	1:B:169:VAL:HG12	2.05	0.55
2:Z:45:ASN:OD1	2:Z:46:GLY:N	2.39	0.55
2:O:51:ASN:O	2:O:53:GLU:N	2.39	0.55
1:F:20:VAL:HG13	1:F:74:VAL:HG21	1.88	0.55
1:B:115:ASP:OD1	1:B:118:ARG:NH1	2.39	0.55
1:D:281:PHE:O	1:D:284:ARG:HG2	2.06	0.55
1:K:195:PHE:CE1	1:K:279:PRO:HG3	2.41	0.55
1:K:279:PRO:HB2	1:K:288:MET:SD	2.47	0.55
1:H:417:VAL:HG11	1:H:477:GLY:HA3	1.88	0.55
1:F:314:LEU:HD13	1:F:317:LEU:HD21	1.87	0.55
2:Q:50:GLU:O	2:Q:52:GLY:N	2.35	0.55
2:T:96:GLU:OE1	2:U:4:ARG:NH1	2.40	0.55
1:A:247:LEU:HD21	1:A:249:ILE:HD11	1.88	0.55
1:A:303:GLU:N	1:A:303:GLU:OE1	2.40	0.55
1:J:215:LEU:HD13	1:J:323:VAL:HG13	1.87	0.55
1:A:357:THR:HB	1:A:361:ASP:HB2	1.87	0.55
1:L:359:ASP:O	1:L:362:ARG:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:219:PHE:CE2	1:H:245:LYS:HE2	2.42	0.55
1:A:248:LEU:HD11	1:A:325:ILE:HD11	1.89	0.55
1:L:34:LYS:NZ	1:L:480:ALA:O	2.40	0.55
1:M:226:LYS:NZ	1:M:227:ILE:O	2.25	0.55
1:G:341:ALA:O	1:G:345:ARG:HG2	2.07	0.55
1:C:6:VAL:HG12	1:C:521:VAL:HG22	1.88	0.55
1:L:409:GLU:OE1	1:L:501:ARG:NH2	2.32	0.55
1:K:328:ASP:OD1	1:K:328:ASP:N	2.40	0.55
1:J:58:ARG:HA	1:J:75:LYS:HE3	1.89	0.55
2:Y:47:ARG:NH2	2:Y:88:GLU:OE2	2.36	0.55
1:G:215:LEU:HD23	1:G:246:PRO:HB2	1.88	0.55
1:B:326:ASN:HD21	1:B:329:THR:HG22	1.71	0.55
1:D:115:ASP:OD1	1:D:118:ARG:NH1	2.40	0.55
1:N:192:GLY:O	1:N:194:GLN:NE2	2.40	0.55
1:M:34:LYS:NZ	1:M:483:GLU:OE2	2.31	0.55
1:H:16:MET:HE1	1:H:514:MET:HG2	1.88	0.54
1:G:251:ALA:O	1:G:278:ALA:N	2.40	0.54
2:Q:48:ILE:HG22	2:Q:54:VAL:HG22	1.88	0.54
1:F:251:ALA:O	1:F:278:ALA:N	2.41	0.54
1:M:30:THR:OG1	1:M:51:LYS:HG3	2.07	0.54
1:E:307:MET:HA	1:E:311:LYS:HD3	1.88	0.54
1:D:359:ASP:O	1:D:362:ARG:N	2.40	0.54
1:I:215:LEU:HD11	1:I:323:VAL:CG2	2.35	0.54
1:I:145:ALA:O	1:I:149:THR:HG23	2.07	0.54
1:M:226:LYS:HE3	1:M:254:VAL:HA	1.88	0.54
1:B:305:ILE:HG23	1:B:307:MET:H	1.73	0.54
1:D:289:LEU:HD12	1:D:292:ILE:HD12	1.89	0.54
2:W:11:ILE:HB	2:W:85:ILE:HG12	1.89	0.54
1:D:290:GLN:HE22	1:D:300:VAL:HG11	1.71	0.54
1:N:42:LYS:NZ	1:N:59:GLU:OE2	2.39	0.54
1:E:150:ILE:CD1	1:E:494:LEU:H	2.21	0.54
1:G:326:ASN:HD21	1:G:329:THR:HG23	1.73	0.54
1:M:251:ALA:O	1:M:278:ALA:N	2.41	0.54
1:F:124:VAL:HG23	1:F:504:LEU:HG	1.90	0.54
2:T:50:GLU:O	2:T:52:GLY:N	2.38	0.54
1:I:225:LYS:N	1:I:303:GLU:OE2	2.39	0.54
1:I:341:ALA:O	1:I:345:ARG:HG2	2.08	0.54
1:D:362:ARG:O	1:D:366:GLN:HB2	2.07	0.54
1:H:346:VAL:HG22	1:H:372:LEU:HD23	1.90	0.54
1:J:314:LEU:HA	1:J:317:LEU:HD12	1.90	0.54
2:P:94:ILE:HG13	2:Q:6:LEU:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:ILE:HD11	1:J:209:GLU:HA	1.90	0.54
1:B:194:GLN:HG2	1:B:331:THR:HG23	1.88	0.54
1:N:215:LEU:HD22	1:N:248:LEU:HD11	1.89	0.54
1:D:218:PRO:HA	1:D:246:PRO:HG2	1.89	0.54
1:F:328:ASP:N	1:F:328:ASP:OD1	2.41	0.54
1:N:207:LYS:HB2	1:N:208:PRO:HD3	1.89	0.54
1:A:517:THR:HG21	1:A:520:MET:HE3	1.89	0.54
1:M:370:ALA:HB1	1:M:376:VAL:HG22	1.89	0.54
1:E:304:GLU:O	1:F:260:ALA:HA	2.07	0.54
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.90	0.54
1:K:409:GLU:OE1	1:K:501:ARG:NH2	2.39	0.54
2:U:14:ARG:HD2	2:U:35:SER:HB3	1.90	0.54
1:H:112:ASN:ND2	1:I:34:LYS:HD2	2.23	0.54
1:K:286:LYS:HD3	1:K:289:LEU:HD21	1.90	0.54
1:D:290:GLN:NE2	1:D:300:VAL:HG11	2.22	0.54
1:H:237:LEU:O	1:H:240:VAL:HG12	2.08	0.54
1:K:226:LYS:NZ	1:K:252:GLU:OE2	2.39	0.54
1:N:325:ILE:HD13	1:N:330:THR:HB	1.90	0.54
1:M:305:ILE:HD13	1:N:263:VAL:HG11	1.90	0.54
1:B:230:ILE:HD13	1:B:261:THR:HG21	1.90	0.53
1:B:496:PRO:O	1:B:499:VAL:HG22	2.07	0.53
1:M:306:GLY:N	1:N:260:ALA:HB1	2.23	0.53
1:B:39:VAL:HG22	1:B:49:ILE:HD12	1.90	0.53
1:F:501:ARG:O	1:F:505:GLN:HG3	2.08	0.53
2:S:55:LYS:NZ	2:T:51:ASN:O	2.30	0.53
1:H:496:PRO:O	1:H:499:VAL:HG22	2.07	0.53
1:G:145:ALA:O	1:G:149:THR:HG23	2.08	0.53
1:B:353:ILE:HG13	1:B:365:LEU:HD13	1.90	0.53
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.91	0.53
1:M:353:ILE:HD13	1:M:365:LEU:HD23	1.91	0.53
1:K:174:VAL:HB	1:K:370:ALA:HB2	1.90	0.53
1:L:333:ILE:HG13	1:L:334:ASP:N	2.23	0.53
2:V:7:HIS:HB2	2:V:46:GLY:O	2.07	0.53
1:L:305:ILE:CG2	1:L:307:MET:HG2	2.38	0.53
1:N:466:ALA:O	1:N:470:LYS:HG3	2.08	0.53
1:I:73:MET:HB2	1:I:514:MET:HE3	1.91	0.53
1:H:455:VAL:HG11	1:H:465:VAL:HG11	1.90	0.53
2:W:20:LYS:HD3	2:W:28:THR:H	1.72	0.53
2:X:78:ILE:O	2:X:81:GLU:HG2	2.09	0.53
1:G:321:LYS:HB3	1:G:334:ASP:HB3	1.90	0.53
1:D:305:ILE:HG13	1:D:307:MET:HG2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:ASP:HB2	1:F:345:ARG:NH1	2.24	0.53
2:O:14:ARG:HE	2:O:34:LYS:HE2	1.73	0.53
1:M:349:ILE:HD11	1:M:368:ARG:HD2	1.89	0.53
1:C:284:ARG:O	1:C:288:MET:HG2	2.09	0.53
1:G:229:ASN:OD1	1:G:231:ARG:HG2	2.09	0.53
2:Q:7:HIS:HB2	2:Q:46:GLY:O	2.09	0.53
1:F:345:ARG:NH1	1:F:372:LEU:HD21	2.23	0.53
1:I:112:ASN:HD21	1:J:34:LYS:HB2	1.73	0.53
1:A:346:VAL:HA	1:A:349:ILE:HD12	1.91	0.53
1:M:200:LEU:HD11	1:M:277:LYS:HG3	1.90	0.53
2:U:3:ILE:HG13	2:U:78:ILE:HG13	1.91	0.53
1:H:418:ALA:O	1:H:422:VAL:HG12	2.09	0.53
1:M:522:THR:HG22	1:M:523:ASP:H	1.74	0.53
1:I:218:PRO:HA	1:I:246:PRO:HG2	1.90	0.53
1:G:254:VAL:HG22	1:G:259:LEU:HD13	1.91	0.53
1:H:353:ILE:HG22	1:H:365:LEU:HB3	1.90	0.53
2:W:10:VAL:HG13	2:W:43:VAL:HG12	1.90	0.53
1:G:367:GLU:O	1:G:371:LYS:HG3	2.09	0.53
1:E:204:PHE:HD1	1:E:213:VAL:HG11	1.74	0.53
1:N:69:MET:SD	1:N:522:THR:OG1	2.62	0.53
1:K:200:LEU:HD13	1:K:259:LEU:HG	1.90	0.53
1:F:429:LEU:O	1:F:430:ARG:NH1	2.37	0.53
1:C:222:LEU:HD13	1:C:300:VAL:HA	1.91	0.53
2:W:94:ILE:HD13	2:X:4:ARG:HH21	1.73	0.53
1:C:279:PRO:HB2	1:C:288:MET:SD	2.48	0.52
1:I:289:LEU:HA	1:I:292:ILE:HG22	1.90	0.52
2:V:78:ILE:O	2:V:81:GLU:HG2	2.08	0.52
1:C:417:VAL:O	1:C:421:ARG:HG2	2.08	0.52
1:C:437:ASN:O	1:C:440:ILE:HG12	2.08	0.52
1:C:506:TYR:O	1:C:510:VAL:HG12	2.09	0.52
1:D:251:ALA:O	1:D:278:ALA:N	2.42	0.52
1:M:237:LEU:O	1:M:240:VAL:HG13	2.08	0.52
1:M:347:ALA:CB	1:N:209:GLU:HG2	2.40	0.52
1:D:76:GLU:OE2	1:E:385:THR:OG1	2.25	0.52
1:I:352:GLN:OE1	1:I:368:ARG:NH2	2.42	0.52
1:E:194:GLN:NE2	1:E:331:THR:OG1	2.30	0.52
1:N:169:VAL:HG22	1:N:173:GLY:HA3	1.91	0.52
1:K:30:THR:OG1	1:K:51:LYS:HG3	2.10	0.52
1:K:437:ASN:O	1:K:440:ILE:HG13	2.09	0.52
1:H:34:LYS:HD3	1:N:112:ASN:HD22	1.73	0.52
1:A:39:VAL:CG2	1:G:520:MET:HG2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:455:VAL:HG21	1:L:465:VAL:HG11	1.90	0.52
1:D:518:GLU:OE1	1:E:36:ARG:NH1	2.42	0.52
1:E:326:ASN:HD21	1:E:329:THR:HG23	1.73	0.52
1:L:247:LEU:HB3	1:L:273:VAL:HG23	1.91	0.52
1:M:227:ILE:HD12	1:M:309:LEU:HD23	1.90	0.52
1:A:262:LEU:HA	1:A:265:ASN:ND2	2.24	0.52
1:N:353:ILE:HG22	1:N:365:LEU:HD13	1.91	0.52
1:A:251:ALA:O	1:A:278:ALA:N	2.43	0.52
1:I:34:LYS:HE2	1:I:481:ALA:HA	1.91	0.52
1:N:350:ARG:O	1:N:353:ILE:HG12	2.09	0.52
1:I:6:VAL:HG12	1:I:521:VAL:HG22	1.91	0.52
1:B:349:ILE:HA	1:B:352:GLN:HG2	1.92	0.52
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.49	0.52
1:C:146:GLN:O	1:C:149:THR:OG1	2.22	0.52
1:M:58:ARG:O	1:M:75:LYS:NZ	2.42	0.52
1:L:322:ARG:O	1:L:333:ILE:HG23	2.09	0.52
1:J:520:MET:HG2	1:K:39:VAL:CG1	2.40	0.52
1:E:6:VAL:HG12	1:E:521:VAL:HG22	1.89	0.52
1:B:218:PRO:HA	1:B:246:PRO:HG2	1.92	0.52
1:I:230:ILE:HD11	1:I:257:GLU:OE1	2.09	0.52
1:E:405:ALA:HB1	1:E:498:LYS:HD3	1.92	0.52
1:I:351:GLN:HG2	1:J:210:THR:OG1	2.09	0.52
1:G:206:ASN:HB2	1:G:213:VAL:HG12	1.90	0.52
1:N:522:THR:HG22	1:N:523:ASP:H	1.74	0.52
1:I:92:ALA:HA	1:I:95:LEU:HD22	1.92	0.52
1:M:290:GLN:OE1	1:M:345:ARG:NH1	2.43	0.52
1:A:51:LYS:NZ	3:A:601:ATP:O1A	2.43	0.52
1:G:222:LEU:HD13	1:G:300:VAL:HA	1.91	0.52
1:A:165:ALA:O	1:A:169:VAL:HG12	2.09	0.52
2:U:20:LYS:CE	2:U:28:THR:H	2.22	0.52
2:U:43:VAL:CG1	2:U:57:LEU:HD11	2.40	0.52
1:I:58:ARG:HA	1:I:75:LYS:HD3	1.91	0.52
2:Z:78:ILE:O	2:Z:81:GLU:HG2	2.10	0.52
2:X:11:ILE:HG23	2:X:42:ALA:HB3	1.92	0.52
1:M:340:ALA:HA	1:M:343:GLN:HG2	1.90	0.52
1:H:66:PHE:HA	1:H:69:MET:HE3	1.92	0.52
1:H:368:ARG:NH1	1:H:371:LYS:HB2	2.25	0.52
1:L:77:VAL:CG2	1:L:510:VAL:HG21	2.35	0.52
2:W:50:GLU:HG2	2:X:51:ASN:HB2	1.91	0.52
2:S:47:ARG:NE	2:S:49:LEU:HD21	2.25	0.52
1:F:379:ILE:HD11	1:F:396:VAL:HG11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:321:LYS:HB3	1:J:334:ASP:HB2	1.91	0.52
2:U:80:ASN:O	2:U:80:ASN:ND2	2.40	0.52
1:H:291:ASP:OD1	1:H:368:ARG:NH2	2.38	0.51
1:H:215:LEU:HB2	1:H:323:VAL:HG12	1.91	0.51
1:B:20:VAL:HG13	1:B:74:VAL:HG21	1.91	0.51
1:F:214:GLU:OE2	1:F:322:ARG:NH2	2.41	0.51
1:G:199:TYR:HB3	1:G:325:ILE:CD1	2.41	0.51
1:N:345:ARG:O	1:N:348:GLN:HG2	2.11	0.51
1:A:193:MET:SD	1:A:371:LYS:HB3	2.50	0.51
1:N:30:THR:OG1	1:N:51:LYS:HG3	2.10	0.51
1:B:415:GLY:N	3:B:601:ATP:O2'	2.31	0.51
1:D:34:LYS:NZ	1:D:480:ALA:O	2.42	0.51
2:T:74:LYS:HG2	2:T:75:SER:N	2.26	0.51
1:D:355:GLU:HG2	1:D:357:THR:HG22	1.93	0.51
1:B:308:GLU:HG2	1:B:309:LEU:H	1.75	0.51
1:K:239:ALA:HA	1:K:242:LYS:HE3	1.92	0.51
1:K:222:LEU:HD21	1:K:293:ALA:HB2	1.91	0.51
2:T:78:ILE:O	2:T:81:GLU:HG2	2.10	0.51
1:N:20:VAL:HG13	1:N:74:VAL:HG21	1.92	0.51
2:V:84:LEU:HD13	2:V:86:MET:HE3	1.91	0.51
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.92	0.51
2:Z:13:LYS:HB2	2:Z:41:LEU:HD11	1.92	0.51
1:N:169:VAL:HG23	1:N:375:GLY:O	2.11	0.51
2:W:11:ILE:HG23	2:W:42:ALA:HB3	1.92	0.51
1:K:501:ARG:O	1:K:505:GLN:HG3	2.10	0.51
1:M:305:ILE:HG22	1:N:264:VAL:HG23	1.93	0.51
2:Q:8:ASP:HA	2:Q:57:LEU:HD21	1.92	0.51
2:Z:51:ASN:O	2:Z:53:GLU:N	2.44	0.51
1:I:91:THR:OG1	3:I:601:ATP:O2B	2.28	0.51
1:L:391:GLU:OE2	1:L:395:ARG:NE	2.43	0.51
2:S:74:LYS:NZ	2:S:76:GLU:OE2	2.38	0.51
1:E:49:ILE:H	1:E:390:LYS:NZ	2.08	0.51
1:D:510:VAL:HG13	1:E:385:THR:HG21	1.91	0.51
2:Q:3:ILE:HD13	2:Q:11:ILE:HD13	1.91	0.51
1:L:393:LYS:NZ	1:L:397:GLU:OE1	2.42	0.51
1:J:429:LEU:HG	1:J:440:ILE:HD13	1.92	0.51
1:F:222:LEU:HA	1:F:250:ILE:HB	1.93	0.51
2:V:34:LYS:HG3	2:V:35:SER:H	1.76	0.51
1:L:513:LEU:HB3	1:M:49:ILE:HD12	1.92	0.51
1:E:165:ALA:HB2	1:E:187:LEU:HD11	1.92	0.51
2:V:14:ARG:HH21	2:V:35:SER:CB	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:310:GLU:OE1	1:L:311:LYS:HG2	2.11	0.51
1:J:369:VAL:O	1:J:372:LEU:HG	2.10	0.51
1:N:218:PRO:HG2	1:N:323:VAL:HG12	1.93	0.51
1:B:368:ARG:O	1:B:371:LYS:HG2	2.11	0.51
1:C:251:ALA:O	1:C:278:ALA:N	2.44	0.51
1:H:40:LEU:HD13	1:H:59:GLU:HG3	1.92	0.51
1:A:196:ASP:OD1	1:A:196:ASP:N	2.42	0.51
2:W:20:LYS:HE2	2:W:20:LYS:HA	1.93	0.51
1:J:34:LYS:HD3	1:J:34:LYS:N	2.26	0.51
1:N:214:GLU:HG2	1:N:324:VAL:HB	1.93	0.51
1:F:219:PHE:CE2	1:F:317:LEU:HD22	2.45	0.51
1:M:226:LYS:HZ1	1:M:255:GLU:HB2	1.75	0.51
1:A:16:MET:HB2	1:A:520:MET:HE1	1.92	0.51
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.93	0.51
1:F:306:GLY:N	1:G:260:ALA:HB1	2.26	0.51
2:Y:57:LEU:HD12	2:Y:57:LEU:H	1.75	0.51
1:A:479:ASN:ND2	1:A:493:ILE:HD11	2.26	0.50
2:R:50:GLU:HG2	2:S:51:ASN:HA	1.92	0.50
1:K:350:ARG:O	1:K:353:ILE:HG22	2.11	0.50
1:H:513:LEU:O	1:H:516:THR:OG1	2.21	0.50
1:D:252:GLU:O	1:D:277:LYS:HG3	2.11	0.50
1:E:197:ARG:HD3	1:E:277:LYS:HB2	1.91	0.50
2:W:12:VAL:HG12	2:W:40:VAL:HG12	1.93	0.50
1:D:113:PRO:HB2	1:D:516:THR:HG22	1.92	0.50
1:D:346:VAL:O	1:D:349:ILE:HG22	2.12	0.50
1:H:379:ILE:HG13	1:H:379:ILE:O	2.10	0.50
1:M:77:VAL:CG2	1:M:510:VAL:HG21	2.37	0.50
1:J:506:TYR:O	1:J:510:VAL:HG22	2.12	0.50
2:U:7:HIS:HB2	2:U:46:GLY:O	2.11	0.50
1:G:341:ALA:O	1:G:345:ARG:NH1	2.45	0.50
2:T:40:VAL:HG12	2:T:63:ASP:O	2.12	0.50
1:J:196:ASP:N	1:J:196:ASP:OD1	2.44	0.50
2:P:20:LYS:CE	2:P:28:THR:H	2.24	0.50
1:D:215:LEU:HB2	1:D:323:VAL:HG12	1.92	0.50
1:C:455:VAL:HG21	1:C:465:VAL:HG11	1.94	0.50
2:W:37:ARG:NH2	2:X:77:LYS:O	2.45	0.50
2:Z:59:VAL:HG11	2:Z:91:ILE:HD12	1.93	0.50
1:G:214:GLU:HG2	1:G:324:VAL:HG22	1.94	0.50
1:M:321:LYS:HG2	1:M:322:ARG:HG3	1.93	0.50
1:K:225:LYS:HE2	1:K:303:GLU:HG3	1.93	0.50
1:N:16:MET:HB2	1:N:520:MET:HE1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:190:VAL:HG13	1:N:376:VAL:HG23	1.92	0.50
1:A:54:VAL:HG22	1:A:78:ALA:HB1	1.94	0.50
1:D:206:ASN:ND2	1:D:208:PRO:HD2	2.26	0.50
1:I:91:THR:O	1:I:94:VAL:HG12	2.11	0.50
1:I:379:ILE:HD11	1:I:396:VAL:HG11	1.93	0.50
1:G:70:GLY:O	1:G:74:VAL:HG23	2.12	0.50
1:N:194:GLN:OE1	1:N:371:LYS:NZ	2.39	0.50
1:B:124:VAL:HG21	1:B:508:ALA:HB2	1.92	0.50
2:U:11:ILE:HB	2:U:42:ALA:HB3	1.94	0.50
2:P:11:ILE:HG12	2:P:85:ILE:HG23	1.94	0.50
2:P:20:LYS:HE3	2:P:28:THR:HB	1.94	0.50
1:G:365:LEU:HD23	1:G:368:ARG:HH21	1.77	0.50
1:E:496:PRO:O	1:E:499:VAL:HG22	2.11	0.50
1:F:219:PHE:O	1:F:248:LEU:N	2.44	0.50
1:H:326:ASN:ND2	1:H:329:THR:HG1	2.10	0.50
1:A:222:LEU:HD22	1:A:289:LEU:HD22	1.93	0.50
1:J:222:LEU:HB3	1:J:289:LEU:HD21	1.92	0.50
1:G:305:ILE:HG13	1:G:307:MET:HG2	1.92	0.50
1:B:204:PHE:HB2	1:B:266:THR:HG21	1.93	0.50
1:N:452:ARG:HH12	1:N:463:SER:HA	1.77	0.50
1:M:219:PHE:CE1	1:M:317:LEU:HD13	2.46	0.50
1:J:315:GLU:OE1	1:J:315:GLU:N	2.44	0.50
1:H:77:VAL:CG2	1:H:510:VAL:HG21	2.33	0.50
1:H:506:TYR:O	1:H:510:VAL:HG22	2.12	0.50
1:M:220:ILE:HG22	1:M:248:LEU:HB3	1.93	0.50
2:V:20:LYS:HE2	2:V:26:VAL:O	2.12	0.50
1:J:349:ILE:HG23	1:J:352:GLN:NE2	2.26	0.50
1:D:42:LYS:HD3	1:D:44:PHE:CE1	2.46	0.50
2:W:13:LYS:HE3	2:W:41:LEU:HD21	1.92	0.50
1:A:20:VAL:HG13	1:A:74:VAL:HG21	1.93	0.50
2:W:20:LYS:HZ2	2:W:28:THR:H	1.59	0.50
1:K:254:VAL:HG23	1:K:259:LEU:HD11	1.92	0.50
1:D:366:GLN:O	1:D:369:VAL:HG12	2.11	0.50
1:E:232:GLU:HG3	1:E:309:LEU:HD13	1.94	0.50
1:G:54:VAL:HG11	1:G:82:ASN:HB2	1.92	0.50
1:K:196:ASP:N	1:K:196:ASP:OD1	2.42	0.50
1:G:195:PHE:CD2	1:G:279:PRO:HB3	2.47	0.50
2:U:43:VAL:HG12	2:U:44:GLY:O	2.12	0.50
1:A:53:GLY:O	1:A:56:VAL:HG22	2.12	0.50
2:Y:65:VAL:HG12	2:Y:94:ILE:HG12	1.93	0.50
1:A:150:ILE:HD11	1:A:492:GLY:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:PRO:HG2	1:E:323:VAL:HG12	1.94	0.50
1:M:227:ILE:HG12	1:M:228:SER:H	1.77	0.49
1:J:496:PRO:O	1:J:499:VAL:HG22	2.12	0.49
2:S:8:ASP:HA	2:S:57:LEU:HD21	1.93	0.49
1:J:415:GLY:N	3:J:601:ATP:O2'	2.42	0.49
1:D:322:ARG:O	1:D:333:ILE:HG22	2.12	0.49
1:N:506:TYR:O	1:N:510:VAL:HG22	2.12	0.49
1:L:214:GLU:HA	1:L:323:VAL:O	2.13	0.49
1:M:325:ILE:HG12	1:M:330:THR:HG23	1.93	0.49
1:F:323:VAL:HG12	1:F:332:ILE:HG23	1.95	0.49
1:C:305:ILE:HD12	1:D:263:VAL:HG11	1.94	0.49
1:A:463:SER:O	1:A:467:ASN:ND2	2.35	0.49
1:L:415:GLY:N	3:L:601:ATP:O2'	2.41	0.49
1:H:113:PRO:HG2	1:I:36:ARG:NE	2.27	0.49
2:V:27:LEU:HD12	2:V:27:LEU:H	1.76	0.49
1:H:150:ILE:CD1	1:H:494:LEU:H	2.25	0.49
1:H:103:GLY:O	1:H:107:VAL:HG23	2.12	0.49
1:M:345:ARG:O	1:M:349:ILE:HG12	2.13	0.49
1:N:324:VAL:HG13	1:N:331:THR:HB	1.94	0.49
2:T:40:VAL:HG13	2:T:62:GLY:H	1.77	0.49
1:G:409:GLU:OE1	1:G:501:ARG:NH2	2.36	0.49
1:L:175:ILE:O	1:L:404:ARG:NH2	2.45	0.49
1:K:8:PHE:HE1	1:K:519:CYS:HG	1.59	0.49
1:E:237:LEU:O	1:E:240:VAL:HG22	2.12	0.49
1:I:89:THR:HG22	3:I:601:ATP:O2G	2.12	0.49
1:K:242:LYS:O	1:K:242:LYS:HG2	2.11	0.49
1:L:292:ILE:O	1:L:295:LEU:HG	2.13	0.49
1:F:150:ILE:CD1	1:F:494:LEU:H	2.26	0.49
1:I:359:ASP:O	1:I:362:ARG:HG2	2.12	0.49
1:F:198:GLY:O	1:F:276:VAL:HG12	2.13	0.49
2:U:15:LYS:HZ3	2:U:39:GLU:N	2.11	0.49
1:E:356:ALA:O	1:E:357:THR:OG1	2.25	0.49
1:L:353:ILE:HD11	1:L:365:LEU:HB3	1.95	0.49
1:F:30:THR:OG1	1:F:51:LYS:HG3	2.10	0.49
1:L:463:SER:O	1:L:467:ASN:ND2	2.39	0.49
1:C:237:LEU:O	1:C:240:VAL:HG22	2.12	0.49
1:E:235:PRO:HG3	1:E:310:GLU:O	2.12	0.49
1:I:215:LEU:HD12	1:I:215:LEU:H	1.77	0.49
2:Q:13:LYS:HE2	2:Q:83:VAL:HB	1.95	0.49
1:F:324:VAL:HG13	1:F:331:THR:OG1	2.13	0.49
1:N:124:VAL:O	1:N:128:VAL:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ALA:HB1	1:D:376:VAL:HG22	1.94	0.49
1:L:255:GLU:N	1:L:255:GLU:OE1	2.39	0.49
1:L:255:GLU:O	1:L:259:LEU:HD22	2.13	0.49
1:C:152:ALA:O	1:C:395:ARG:NH1	2.45	0.49
1:F:226:LYS:HG2	1:F:253:ASP:HB3	1.95	0.49
2:P:78:ILE:O	2:P:81:GLU:HG2	2.13	0.49
1:B:458:CYS:SG	1:B:480:ALA:HB1	2.53	0.49
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.95	0.49
2:V:50:GLU:O	2:V:52:GLY:N	2.38	0.49
1:F:496:PRO:O	1:F:499:VAL:HG22	2.12	0.49
1:L:70:GLY:O	1:L:74:VAL:HG23	2.13	0.49
1:C:226:LYS:HG2	1:C:227:ILE:N	2.28	0.49
1:G:206:ASN:HB3	1:G:208:PRO:HD2	1.94	0.49
2:S:78:ILE:O	2:S:81:GLU:HG2	2.13	0.49
1:B:30:THR:OG1	1:B:51:LYS:HG3	2.12	0.49
2:Z:20:LYS:HD2	2:Z:27:LEU:HD23	1.95	0.49
1:C:222:LEU:HA	1:C:250:ILE:HG13	1.93	0.49
1:N:70:GLY:O	1:N:74:VAL:HG23	2.13	0.49
1:G:220:ILE:HD11	1:G:250:ILE:HG13	1.94	0.49
1:A:232:GLU:HG2	1:A:310:GLU:OE1	2.13	0.49
1:G:236:VAL:HG22	1:G:312:ALA:HB3	1.95	0.49
2:V:45:ASN:O	2:V:56:PRO:HA	2.13	0.49
1:H:132:LYS:HZ2	1:H:501:ARG:HG3	1.77	0.49
2:O:57:LEU:HD21	2:O:88:GLU:HB2	1.95	0.49
1:K:115:ASP:OD2	1:K:433:ASN:ND2	2.46	0.49
2:U:47:ARG:HH21	2:U:88:GLU:HB3	1.78	0.49
1:G:127:ALA:O	1:G:131:LEU:HD13	2.12	0.48
1:E:208:PRO:HG3	1:E:214:GLU:HG3	1.93	0.48
1:M:53:GLY:O	1:M:56:VAL:HG22	2.13	0.48
2:S:43:VAL:HG13	2:S:57:LEU:HD12	1.94	0.48
1:N:280:GLY:C	1:N:285:ARG:HB3	2.33	0.48
1:G:506:TYR:O	1:G:510:VAL:HG22	2.13	0.48
1:N:206:ASN:ND2	1:N:214:GLU:O	2.46	0.48
1:I:175:ILE:HG23	1:I:377:ALA:HB3	1.94	0.48
1:H:150:ILE:HD13	1:H:494:LEU:H	1.78	0.48
1:M:305:ILE:HG22	1:M:306:GLY:H	1.78	0.48
1:B:343:GLN:O	1:B:346:VAL:HG12	2.13	0.48
1:B:368:ARG:HA	1:B:371:LYS:HE3	1.95	0.48
1:E:359:ASP:OD1	1:E:360:TYR:N	2.46	0.48
1:D:30:THR:HB	1:D:51:LYS:HD2	1.95	0.48
1:C:232:GLU:HB2	1:C:310:GLU:CD	2.34	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TYR:O	1:A:363:GLU:HG2	2.13	0.48
1:D:296:THR:OG1	1:D:319:GLN:N	2.46	0.48
2:S:47:ARG:HG2	2:S:49:LEU:HG	1.94	0.48
1:H:39:VAL:CG1	1:N:520:MET:HG2	2.43	0.48
1:N:58:ARG:HG2	1:N:75:LYS:NZ	2.28	0.48
2:R:64:ILE:HB	2:R:95:VAL:HG23	1.95	0.48
1:I:433:ASN:ND2	1:I:436:GLN:OE1	2.46	0.48
1:I:76:GLU:OE2	1:J:385:THR:OG1	2.27	0.48
2:P:20:LYS:NZ	2:P:28:THR:H	2.12	0.48
2:R:91:ILE:HG13	2:S:6:LEU:HD13	1.95	0.48
1:E:49:ILE:H	1:E:390:LYS:HZ1	1.60	0.48
2:O:50:GLU:O	2:O:52:GLY:N	2.41	0.48
2:U:59:VAL:HG12	2:U:94:ILE:HD11	1.95	0.48
2:T:95:VAL:HG13	2:U:3:ILE:HD12	1.96	0.48
1:D:270:ILE:HG13	1:D:271:VAL:HG22	1.94	0.48
1:D:66:PHE:O	1:D:69:MET:HB2	2.13	0.48
1:L:161:LEU:HD21	1:L:379:ILE:HD11	1.95	0.48
1:A:266:THR:HG23	1:A:272:LYS:HA	1.95	0.48
1:I:510:VAL:HG13	1:J:385:THR:HG21	1.94	0.48
1:H:16:MET:HG3	1:H:17:LEU:N	2.27	0.48
1:I:215:LEU:HD22	1:I:218:PRO:HB3	1.95	0.48
1:I:99:ILE:HD12	1:I:442:VAL:HG12	1.96	0.48
1:I:127:ALA:O	1:I:131:LEU:HD13	2.14	0.48
1:B:357:THR:HA	1:B:358:SER:HA	1.59	0.48
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.95	0.48
1:G:391:GLU:OE2	1:G:395:ARG:NE	2.45	0.48
2:S:52:GLY:HA3	2:T:51:ASN:ND2	2.25	0.48
1:J:308:GLU:HG3	1:J:309:LEU:H	1.78	0.48
2:S:14:ARG:HH22	2:S:17:VAL:HG13	1.79	0.48
1:C:220:ILE:HD11	1:C:296:THR:HG21	1.94	0.48
1:H:222:LEU:HD11	1:H:300:VAL:HA	1.94	0.48
1:A:56:VAL:O	1:A:60:ILE:HG12	2.13	0.48
1:F:233:MET:HB3	1:F:237:LEU:HD13	1.95	0.48
1:G:232:GLU:HG3	1:G:309:LEU:HD13	1.95	0.48
1:N:6:VAL:HG22	1:N:521:VAL:HG12	1.95	0.48
1:M:103:GLY:O	1:M:107:VAL:HG23	2.14	0.48
1:J:23:LEU:HD11	1:J:57:ALA:HA	1.94	0.48
1:L:90:THR:O	1:L:94:VAL:HG23	2.13	0.48
1:M:150:ILE:HD11	1:M:492:GLY:O	2.14	0.48
1:I:278:ALA:HB3	1:I:285:ARG:NH1	2.28	0.48
1:J:34:LYS:CD	1:J:34:LYS:H	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:11:ILE:HG12	2:V:85:ILE:HD13	1.94	0.48
1:L:305:ILE:HG22	1:L:307:MET:HG2	1.95	0.48
1:E:228:SER:HA	1:E:255:GLU:OE1	2.14	0.48
2:Z:37:ARG:HG2	2:Z:66:ILE:HG12	1.94	0.48
1:M:506:TYR:O	1:M:510:VAL:HG22	2.14	0.48
1:F:150:ILE:HD11	1:F:492:GLY:O	2.14	0.48
1:G:429:LEU:HG	1:G:440:ILE:HD13	1.94	0.48
1:E:115:ASP:OD2	1:E:433:ASN:ND2	2.43	0.48
1:D:254:VAL:HG23	1:D:259:LEU:HD21	1.96	0.48
1:M:226:LYS:NZ	1:M:255:GLU:HB2	2.28	0.48
2:P:69:ASP:HA	2:P:73:VAL:HG21	1.96	0.48
1:K:222:LEU:O	1:K:301:ILE:HG23	2.14	0.48
1:H:271:VAL:HG22	1:H:273:VAL:HG22	1.95	0.48
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.54	0.48
1:A:342:ILE:HG23	1:A:372:LEU:HD22	1.96	0.48
2:P:9:ARG:HH11	2:P:87:SER:HB3	1.77	0.48
1:I:147:VAL:O	1:I:150:ILE:HG13	2.14	0.48
1:J:94:VAL:HG12	1:J:449:ALA:HB1	1.95	0.48
1:G:280:GLY:C	1:G:285:ARG:HB3	2.34	0.48
2:S:14:ARG:HH21	2:S:35:SER:N	2.12	0.48
1:C:225:LYS:NZ	1:C:309:LEU:HD22	2.29	0.48
1:K:351:GLN:HG2	1:L:210:THR:H	1.79	0.48
1:M:322:ARG:O	1:M:333:ILE:HG22	2.14	0.48
1:D:270:ILE:HG13	1:D:271:VAL:N	2.29	0.48
1:K:94:VAL:HG12	1:K:449:ALA:HB1	1.95	0.48
1:J:207:LYS:HB2	1:J:208:PRO:HD3	1.96	0.48
1:D:150:ILE:HD11	1:D:492:GLY:O	2.14	0.48
1:K:510:VAL:HG22	1:L:385:THR:HG21	1.96	0.48
1:K:417:VAL:O	1:K:421:ARG:HG2	2.14	0.48
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.54	0.48
1:A:506:TYR:O	1:A:510:VAL:HG22	2.13	0.47
1:E:387:VAL:HG12	1:E:390:LYS:HE3	1.95	0.47
1:B:56:VAL:O	1:B:60:ILE:HG12	2.14	0.47
1:M:248:LEU:HD11	1:M:325:ILE:HD11	1.95	0.47
1:B:345:ARG:HA	1:B:345:ARG:HD3	1.69	0.47
1:G:200:LEU:HD22	1:G:254:VAL:HG13	1.96	0.47
1:F:409:GLU:OE1	1:F:501:ARG:HD3	2.14	0.47
1:F:324:VAL:O	1:F:331:THR:OG1	2.17	0.47
1:J:39:VAL:HG22	1:J:49:ILE:HG12	1.95	0.47
1:M:301:ILE:HA	1:M:307:MET:SD	2.53	0.47
1:I:270:ILE:HD13	2:Z:25:ILE:HD13	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:12:VAL:HG13	2:V:39:GLU:O	2.13	0.47
1:E:197:ARG:HD2	1:E:278:ALA:O	2.14	0.47
1:C:206:ASN:HD21	1:C:215:LEU:HD23	1.79	0.47
1:A:349:ILE:HG23	1:A:365:LEU:HD11	1.95	0.47
1:C:496:PRO:O	1:C:499:VAL:HG22	2.13	0.47
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.54	0.47
2:O:48:ILE:HG22	2:O:54:VAL:HG22	1.95	0.47
1:N:305:ILE:HG22	1:N:306:GLY:H	1.79	0.47
1:B:321:LYS:HE3	1:B:322:ARG:CZ	2.44	0.47
1:I:77:VAL:CG2	1:I:510:VAL:HG21	2.35	0.47
2:W:20:LYS:HZ1	2:W:28:THR:HG23	1.79	0.47
1:G:288:MET:O	1:G:292:ILE:HG23	2.13	0.47
1:H:518:GLU:OE1	1:I:36:ARG:NH1	2.46	0.47
1:C:114:MET:O	1:C:118:ARG:HG3	2.14	0.47
2:Z:20:LYS:HE2	2:Z:27:LEU:HB2	1.97	0.47
1:J:270:ILE:HG13	1:J:271:VAL:N	2.29	0.47
1:E:194:GLN:HE22	1:E:331:THR:HG1	1.56	0.47
1:K:292:ILE:HG13	1:K:293:ALA:N	2.29	0.47
1:A:496:PRO:O	1:A:499:VAL:HG22	2.14	0.47
2:X:11:ILE:HD11	2:X:41:LEU:HD22	1.96	0.47
1:A:229:ASN:HB3	1:A:232:GLU:HB3	1.96	0.47
1:F:232:GLU:OE2	1:F:233:MET:HG2	2.14	0.47
1:A:326:ASN:OD1	1:A:329:THR:HG22	2.14	0.47
1:M:28:LYS:HG2	1:M:94:VAL:HG22	1.96	0.47
1:C:193:MET:HB3	1:C:332:ILE:HG22	1.95	0.47
1:H:368:ARG:HD2	1:H:368:ARG:HA	1.71	0.47
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.96	0.47
1:L:58:ARG:O	1:L:75:LYS:NZ	2.46	0.47
1:A:230:ILE:HD12	1:A:261:THR:OG1	2.15	0.47
1:J:292:ILE:O	1:J:295:LEU:HG	2.14	0.47
1:N:89:THR:OG1	3:N:601:ATP:O2G	2.28	0.47
1:M:348:GLN:O	1:M:352:GLN:HG3	2.14	0.47
1:J:305:ILE:HD11	1:J:307:MET:HG2	1.97	0.47
1:N:77:VAL:CG2	1:N:510:VAL:HG21	2.37	0.47
1:L:215:LEU:HD13	1:L:323:VAL:HG23	1.96	0.47
1:F:146:GLN:O	1:F:149:THR:OG1	2.24	0.47
2:W:20:LYS:NZ	2:W:28:THR:HG23	2.29	0.47
1:G:353:ILE:CD1	1:G:365:LEU:HB3	2.43	0.47
2:X:14:ARG:NH1	2:X:35:SER:O	2.47	0.47
1:L:232:GLU:HG3	1:L:309:LEU:HD13	1.96	0.47
1:A:73:MET:SD	1:B:49:ILE:HD11	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:LEU:HG	1:F:440:ILE:HD13	1.97	0.47
2:T:74:LYS:HG2	2:T:75:SER:H	1.79	0.47
1:G:214:GLU:HG2	1:G:324:VAL:HG13	1.96	0.47
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.45	0.47
1:K:76:GLU:OE2	1:L:385:THR:OG1	2.29	0.47
1:D:52:ALA:O	1:D:55:SER:OG	2.32	0.47
1:G:339:GLU:HA	1:G:342:ILE:HG22	1.96	0.47
1:B:353:ILE:HA	1:B:365:LEU:HD13	1.97	0.47
1:C:265:ASN:HD21	1:C:270:ILE:HD11	1.80	0.47
1:J:90:THR:O	1:J:94:VAL:HG23	2.15	0.47
1:B:95:LEU:O	1:B:99:ILE:HG13	2.15	0.47
1:G:221:LEU:HD11	1:G:301:ILE:HD12	1.97	0.47
1:A:409:GLU:OE1	1:A:501:ARG:NH2	2.38	0.47
1:B:234:LEU:N	1:B:235:PRO:HD2	2.29	0.47
2:O:13:LYS:HB2	2:O:41:LEU:HD11	1.97	0.47
1:F:183:LEU:HD22	1:F:384:ALA:HA	1.97	0.47
1:D:308:GLU:H	1:D:311:LYS:HG3	1.78	0.47
1:J:418:ALA:O	1:J:422:VAL:HG12	2.14	0.47
1:D:372:LEU:HD12	1:D:372:LEU:H	1.80	0.47
1:D:214:GLU:HA	1:D:323:VAL:O	2.14	0.47
1:H:215:LEU:HD13	1:H:246:PRO:HB2	1.97	0.47
1:J:233:MET:O	1:J:236:VAL:HG13	2.14	0.47
1:D:278:ALA:HB3	1:D:285:ARG:NH1	2.28	0.47
1:J:258:ALA:O	1:J:262:LEU:HD13	2.15	0.47
2:O:45:ASN:O	2:O:56:PRO:HA	2.14	0.47
1:D:222:LEU:HD13	1:D:300:VAL:HA	1.97	0.47
1:F:135:SER:OG	1:F:409:GLU:O	2.29	0.47
1:H:349:ILE:O	1:H:353:ILE:HG23	2.15	0.47
1:J:220:ILE:HG12	1:J:248:LEU:HD21	1.96	0.47
2:S:1:MET:N	2:S:79:ASP:OD1	2.45	0.47
1:A:149:THR:HG22	1:A:154:SER:HA	1.96	0.47
1:K:186:GLU:HG3	1:K:380:LYS:HB2	1.97	0.47
1:I:222:LEU:HD21	1:I:293:ALA:HB2	1.95	0.47
1:H:200:LEU:HD23	1:H:259:LEU:HD11	1.97	0.47
1:H:291:ASP:OD1	1:H:292:ILE:N	2.48	0.47
2:R:59:VAL:HG21	2:R:91:ILE:HD12	1.97	0.47
2:S:14:ARG:NH2	2:S:17:VAL:HG13	2.29	0.47
1:I:349:ILE:O	1:I:353:ILE:HG12	2.15	0.47
1:M:496:PRO:O	1:M:499:VAL:HG22	2.15	0.47
1:D:175:ILE:HG12	1:D:377:ALA:HB3	1.97	0.47
1:A:218:PRO:HG2	1:A:323:VAL:HG13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:PRO:O	1:A:454:ILE:HG13	2.14	0.47
1:E:305:ILE:HG22	1:E:306:GLY:H	1.80	0.47
1:E:342:ILE:O	1:E:346:VAL:HG23	2.15	0.47
1:N:103:GLY:O	1:N:107:VAL:HG23	2.15	0.47
1:I:112:ASN:ND2	1:J:34:LYS:HB2	2.30	0.47
1:A:270:ILE:HG13	1:A:271:VAL:N	2.29	0.47
2:Y:14:ARG:HG3	2:Y:84:LEU:HD13	1.97	0.47
1:F:359:ASP:O	1:F:362:ARG:N	2.48	0.47
1:C:219:PHE:CE2	1:C:317:LEU:HB3	2.50	0.47
1:N:161:LEU:HD21	1:N:379:ILE:HD11	1.96	0.47
1:K:343:GLN:HG2	1:K:344:GLY:N	2.29	0.47
1:G:289:LEU:HA	1:G:292:ILE:HG12	1.97	0.47
1:L:496:PRO:O	1:L:499:VAL:HG22	2.15	0.47
1:F:482:THR:OG1	1:F:484:GLU:HG2	2.15	0.47
1:J:352:GLN:HE22	1:J:368:ARG:HH12	1.63	0.47
1:C:520:MET:HG2	1:D:39:VAL:CG2	2.45	0.47
1:K:6:VAL:HG12	1:K:521:VAL:HG22	1.96	0.47
1:N:268:ARG:HG3	2:X:27:LEU:HD11	1.96	0.47
1:M:463:SER:O	1:M:467:ASN:ND2	2.42	0.47
1:B:463:SER:O	1:B:467:ASN:ND2	2.42	0.47
1:E:258:ALA:O	1:E:261:THR:OG1	2.30	0.47
1:F:187:LEU:HD12	1:F:379:ILE:HG22	1.96	0.46
1:I:270:ILE:HG13	1:I:271:VAL:N	2.30	0.46
1:M:232:GLU:OE2	1:M:233:MET:HG3	2.15	0.46
1:J:5:ASP:HB2	1:J:524:LEU:HD23	1.96	0.46
1:B:292:ILE:HG13	1:B:293:ALA:N	2.29	0.46
1:F:288:MET:HA	1:F:291:ASP:OD2	2.14	0.46
1:I:510:VAL:O	1:I:514:MET:HB2	2.15	0.46
1:G:290:GLN:HG3	1:G:291:ASP:OD1	2.15	0.46
1:K:322:ARG:O	1:K:333:ILE:HG22	2.15	0.46
1:N:206:ASN:ND2	1:N:208:PRO:HD2	2.30	0.46
1:E:208:PRO:HG3	1:E:214:GLU:CG	2.45	0.46
1:G:496:PRO:O	1:G:499:VAL:HG22	2.15	0.46
1:K:409:GLU:CD	1:K:501:ARG:HH21	2.18	0.46
1:G:309:LEU:HD12	1:G:310:GLU:HG2	1.97	0.46
1:H:302:SER:O	1:H:305:ILE:HG22	2.15	0.46
1:D:152:ALA:O	1:D:395:ARG:NH1	2.48	0.46
1:B:262:LEU:HD11	1:B:273:VAL:HB	1.97	0.46
1:G:286:LYS:HA	1:G:289:LEU:HG	1.97	0.46
1:D:207:LYS:H	1:D:207:LYS:HD2	1.80	0.46
1:H:517:THR:O	1:I:36:ARG:NH1	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:13:LYS:HE3	2:U:41:LEU:HD21	1.98	0.46
2:W:78:ILE:O	2:W:81:GLU:HG2	2.15	0.46
2:S:45:ASN:O	2:S:56:PRO:HA	2.15	0.46
1:D:113:PRO:HB2	1:D:516:THR:HA	1.98	0.46
1:G:226:LYS:HG2	1:G:252:GLU:HB2	1.97	0.46
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.73	0.46
1:N:204:PHE:O	1:N:204:PHE:HD1	1.99	0.46
1:H:342:ILE:O	1:H:346:VAL:HG23	2.16	0.46
1:M:223:ALA:N	1:M:250:ILE:O	2.44	0.46
1:M:347:ALA:HB3	1:N:209:GLU:HG2	1.96	0.46
1:E:270:ILE:HG13	1:E:271:VAL:HG12	1.98	0.46
1:N:97:GLN:O	1:N:100:ILE:HG13	2.16	0.46
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.98	0.46
1:B:53:GLY:O	1:B:56:VAL:HG22	2.15	0.46
1:K:252:GLU:HG2	1:K:253:ASP:N	2.30	0.46
1:N:75:LYS:NZ	1:N:79:SER:HB2	2.30	0.46
1:K:66:PHE:O	1:K:69:MET:HB2	2.16	0.46
1:L:281:PHE:HD2	1:L:284:ARG:HE	1.64	0.46
1:G:197:ARG:HB3	1:G:277:LYS:HE3	1.96	0.46
1:F:103:GLY:O	1:F:107:VAL:HG23	2.16	0.46
1:I:290:GLN:N	1:I:290:GLN:OE1	2.49	0.46
2:W:14:ARG:HH21	2:W:84:LEU:HD21	1.80	0.46
1:H:54:VAL:HG22	1:H:78:ALA:HB1	1.98	0.46
1:C:261:THR:O	1:C:265:ASN:HB2	2.16	0.46
2:W:11:ILE:CG2	2:W:42:ALA:HB3	2.45	0.46
1:C:232:GLU:OE1	1:C:233:MET:HG2	2.16	0.46
1:E:255:GLU:N	1:E:255:GLU:OE2	2.47	0.46
1:K:90:THR:O	1:K:94:VAL:HG23	2.16	0.46
1:K:266:THR:HG23	1:K:272:LYS:HA	1.98	0.46
1:L:342:ILE:HG23	1:L:345:ARG:HH21	1.80	0.46
1:D:488:MET:HB3	1:D:493:ILE:HG13	1.97	0.46
1:F:270:ILE:HG13	1:F:271:VAL:HG22	1.98	0.46
1:J:256:GLY:O	1:J:259:LEU:HG	2.15	0.46
1:L:226:LYS:HG2	1:L:227:ILE:H	1.79	0.46
1:D:226:LYS:HE2	1:D:253:ASP:H	1.80	0.46
1:F:372:LEU:HB3	1:F:373:ALA:H	1.50	0.46
1:H:288:MET:HA	1:H:291:ASP:OD2	2.16	0.46
1:I:366:GLN:O	1:I:369:VAL:HG12	2.16	0.46
1:E:198:GLY:HA2	1:E:325:ILE:HD11	1.98	0.46
1:I:294:THR:HB	1:I:345:ARG:NH1	2.29	0.46
1:L:258:ALA:O	1:L:261:THR:OG1	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:314:LEU:HD23	1:N:314:LEU:H	1.80	0.46
1:M:214:GLU:HG2	1:M:324:VAL:HG12	1.97	0.46
2:P:50:GLU:HG2	2:Q:51:ASN:HB2	1.98	0.46
1:J:349:ILE:HG23	1:J:352:GLN:HE21	1.81	0.46
1:J:366:GLN:O	1:J:369:VAL:HG22	2.15	0.46
1:B:246:PRO:HB3	1:B:272:LYS:HG3	1.98	0.46
1:J:285:ARG:O	1:J:289:LEU:HB2	2.16	0.46
1:A:90:THR:O	1:A:94:VAL:HG23	2.16	0.46
1:L:450:PRO:O	1:L:454:ILE:HG13	2.16	0.46
1:I:239:ALA:O	1:I:242:LYS:HG2	2.16	0.46
1:M:103:GLY:HA3	1:M:515:ILE:HD13	1.97	0.46
1:M:209:GLU:CD	1:M:209:GLU:H	2.18	0.46
1:G:199:TYR:CE2	1:G:327:LYS:HA	2.50	0.46
1:L:219:PHE:CZ	1:L:247:LEU:HG	2.51	0.46
1:K:177:VAL:HB	1:K:379:ILE:HG23	1.98	0.46
1:C:268:ARG:HD2	2:T:27:LEU:HD22	1.97	0.46
1:L:251:ALA:O	1:L:278:ALA:N	2.49	0.46
1:N:270:ILE:HG13	1:N:271:VAL:N	2.31	0.46
1:B:285:ARG:O	1:B:289:LEU:HG	2.16	0.46
1:K:13:ARG:NH1	1:K:518:GLU:OE1	2.50	0.46
1:G:195:PHE:N	1:G:195:PHE:CD1	2.83	0.45
1:K:218:PRO:HA	1:K:246:PRO:HG2	1.97	0.45
1:H:90:THR:O	1:H:94:VAL:HG22	2.15	0.45
1:D:313:THR:HG23	1:D:316:ASP:OD2	2.16	0.45
1:I:195:PHE:CE2	1:I:279:PRO:HG3	2.51	0.45
1:E:506:TYR:O	1:E:510:VAL:HG23	2.16	0.45
1:L:196:ASP:OD1	1:L:196:ASP:N	2.40	0.45
2:P:51:ASN:O	2:P:53:GLU:N	2.50	0.45
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.99	0.45
1:M:234:LEU:N	1:M:235:PRO:HD2	2.31	0.45
1:K:372:LEU:HD12	1:K:374:GLY:H	1.80	0.45
1:C:461:GLU:HA	1:C:462:PRO:HD3	1.72	0.45
1:K:40:LEU:HD13	1:K:59:GLU:HG3	1.97	0.45
2:Q:64:ILE:HG23	2:Q:95:VAL:O	2.16	0.45
1:C:199:TYR:OH	1:C:327:LYS:HG2	2.16	0.45
1:C:5:ASP:HB2	1:C:524:LEU:HD23	1.98	0.45
1:H:186:GLU:HG3	1:H:380:LYS:HB2	1.98	0.45
1:E:299:THR:HB	1:E:316:ASP:HA	1.97	0.45
1:N:247:LEU:HG	1:N:248:LEU:N	2.31	0.45
1:J:77:VAL:CG2	1:J:510:VAL:HG21	2.39	0.45
2:Y:74:LYS:HB3	2:Y:85:ILE:HG13	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:506:TYR:O	1:F:510:VAL:HG22	2.16	0.45
1:D:190:VAL:HG11	1:D:194:GLN:HB3	1.98	0.45
1:H:266:THR:HG22	1:H:273:VAL:H	1.80	0.45
1:J:291:ASP:OD2	1:J:368:ARG:NH2	2.50	0.45
1:J:349:ILE:HG21	1:J:369:VAL:HG12	1.97	0.45
1:L:321:LYS:HB3	1:L:334:ASP:HB3	1.97	0.45
1:E:305:ILE:HG22	1:E:306:GLY:N	2.30	0.45
1:B:179:ASP:OD1	1:B:179:ASP:N	2.50	0.45
1:G:284:ARG:HD3	1:G:368:ARG:NH1	2.26	0.45
1:D:458:CYS:SG	1:D:480:ALA:HB1	2.57	0.45
2:Q:11:ILE:HB	2:Q:42:ALA:HB3	1.98	0.45
1:N:75:LYS:HZ3	1:N:79:SER:HB2	1.81	0.45
1:I:177:VAL:HG11	1:I:397:GLU:HG2	1.98	0.45
1:J:234:LEU:N	1:J:235:PRO:HD2	2.31	0.45
1:N:176:THR:HG23	1:N:378:VAL:HG13	1.99	0.45
1:N:53:GLY:O	1:N:56:VAL:HG22	2.16	0.45
1:H:248:LEU:HD11	1:H:323:VAL:HG21	1.98	0.45
1:J:232:GLU:OE2	1:J:233:MET:HG2	2.15	0.45
1:M:364:LYS:HE2	1:M:368:ARG:NH2	2.31	0.45
1:G:146:GLN:O	1:G:149:THR:OG1	2.28	0.45
1:J:366:GLN:HA	1:J:369:VAL:HG22	1.98	0.45
1:H:350:ARG:O	1:H:353:ILE:HG12	2.16	0.45
1:F:32:GLY:O	1:F:51:LYS:NZ	2.50	0.45
1:H:501:ARG:O	1:H:505:GLN:HG3	2.17	0.45
1:J:234:LEU:HA	1:J:234:LEU:HD23	1.85	0.45
2:S:59:VAL:HG12	2:S:94:ILE:HD11	1.99	0.45
1:K:183:LEU:HD22	1:K:384:ALA:HA	1.98	0.45
1:E:463:SER:O	1:E:467:ASN:ND2	2.42	0.45
1:K:53:GLY:O	1:K:56:VAL:HG22	2.15	0.45
1:K:482:THR:OG1	1:K:484:GLU:HG2	2.16	0.45
1:C:234:LEU:N	1:C:235:PRO:HD2	2.32	0.45
1:B:432:GLN:HG2	1:B:436:GLN:OE1	2.16	0.45
2:O:34:LYS:HG2	2:O:35:SER:H	1.82	0.45
1:D:506:TYR:O	1:D:510:VAL:HG22	2.16	0.45
1:B:221:LEU:N	1:B:248:LEU:O	2.46	0.45
1:D:349:ILE:HD12	1:D:352:GLN:CD	2.37	0.45
1:E:357:THR:HB	1:E:361:ASP:CG	2.37	0.45
1:B:80:LYS:NZ	1:C:384:ALA:O	2.44	0.45
1:E:353:ILE:C	1:E:355:GLU:H	2.19	0.45
1:C:66:PHE:O	1:C:69:MET:HB2	2.17	0.45
1:G:322:ARG:HG3	1:G:333:ILE:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:GLU:HA	1:E:462:PRO:HD3	1.83	0.45
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.98	0.45
1:I:30:THR:OG1	1:I:51:LYS:HG3	2.17	0.45
2:S:11:ILE:CG2	2:S:42:ALA:HB3	2.46	0.45
1:D:97:GLN:O	1:D:100:ILE:HG13	2.16	0.45
1:F:497:THR:O	1:F:501:ARG:HG2	2.17	0.45
1:B:346:VAL:HA	1:B:349:ILE:HG12	1.98	0.45
1:A:169:VAL:HG22	1:A:173:GLY:HA3	1.99	0.45
1:C:314:LEU:HA	1:C:317:LEU:HD22	1.98	0.45
1:J:30:THR:HB	1:J:51:LYS:HG3	1.98	0.45
1:L:234:LEU:N	1:L:235:PRO:HD2	2.32	0.45
1:K:234:LEU:N	1:K:235:PRO:HD2	2.32	0.45
1:M:215:LEU:HD13	1:M:323:VAL:HG23	1.99	0.45
1:C:80:LYS:HG2	1:C:506:TYR:CZ	2.52	0.45
2:S:50:GLU:O	2:S:52:GLY:N	2.45	0.45
1:L:369:VAL:O	1:L:372:LEU:HG	2.16	0.45
1:I:227:ILE:HG22	1:I:309:LEU:HD23	1.98	0.45
1:D:190:VAL:CG1	1:D:194:GLN:HB3	2.47	0.45
1:B:206:ASN:HB2	1:B:213:VAL:HG13	1.99	0.45
1:D:359:ASP:O	1:D:362:ARG:HG2	2.16	0.45
1:B:76:GLU:OE2	1:C:385:THR:OG1	2.33	0.45
1:F:360:TYR:CZ	1:F:364:LYS:HD3	2.52	0.45
1:J:304:GLU:O	1:K:260:ALA:HA	2.17	0.45
1:D:234:LEU:N	1:D:235:PRO:HD2	2.32	0.45
1:K:323:VAL:HG22	1:K:332:ILE:HG12	1.99	0.45
1:H:372:LEU:HB3	1:H:373:ALA:H	1.52	0.45
1:A:214:GLU:HG2	1:A:324:VAL:HG22	1.99	0.45
1:K:479:ASN:ND2	1:K:493:ILE:HD11	2.28	0.45
1:E:214:GLU:HG2	1:E:324:VAL:HG13	1.98	0.45
2:W:13:LYS:HE3	2:W:41:LEU:HD11	1.99	0.45
1:H:505:GLN:HE22	1:I:183:LEU:HD22	1.80	0.45
1:G:90:THR:O	1:G:94:VAL:HG23	2.16	0.45
2:R:17:VAL:O	2:R:18:GLU:HG2	2.16	0.45
1:G:219:PHE:O	1:G:248:LEU:N	2.48	0.45
1:C:248:LEU:HD22	1:C:323:VAL:HG21	1.97	0.45
1:I:206:ASN:CG	1:I:213:VAL:HG23	2.36	0.45
1:I:221:LEU:HD12	1:I:317:LEU:HD21	1.99	0.45
1:L:479:ASN:ND2	1:L:493:ILE:HD11	2.29	0.45
1:F:72:GLN:HA	1:F:75:LYS:HD3	1.99	0.45
2:Q:7:HIS:O	2:Q:8:ASP:HB3	2.16	0.45
2:W:96:GLU:OE2	2:X:4:ARG:NE	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:GLY:O	1:C:417:VAL:HG12	2.17	0.45
1:J:91:THR:O	1:J:95:LEU:HD22	2.17	0.45
1:F:286:LYS:NZ	1:F:304:GLU:OE2	2.48	0.45
1:I:207:LYS:H	1:I:207:LYS:HD2	1.81	0.45
1:L:73:MET:HE2	1:L:73:MET:HB3	1.77	0.45
1:F:214:GLU:HG3	1:F:215:LEU:N	2.32	0.44
1:F:70:GLY:O	1:F:74:VAL:HG23	2.17	0.44
1:M:73:MET:HB3	1:M:73:MET:HE2	1.88	0.44
1:I:85:ALA:O	1:I:401:HIS:HB3	2.17	0.44
2:Q:13:LYS:HD2	2:Q:41:LEU:HD12	1.98	0.44
1:N:40:LEU:HD21	1:N:56:VAL:HG12	1.99	0.44
1:G:5:ASP:HB2	1:G:524:LEU:HD12	1.99	0.44
1:I:414:GLY:O	1:I:417:VAL:HG12	2.17	0.44
1:H:230:ILE:HD13	1:H:230:ILE:HA	1.88	0.44
1:B:372:LEU:HB2	1:B:373:ALA:H	1.56	0.44
1:D:226:LYS:N	1:D:226:LYS:HD2	2.32	0.44
1:A:365:LEU:HD13	1:A:368:ARG:HH21	1.82	0.44
2:V:15:LYS:HE2	2:V:16:GLU:OE2	2.18	0.44
1:G:255:GLU:O	1:G:259:LEU:HD22	2.18	0.44
1:E:217:SER:N	1:E:218:PRO:HD3	2.32	0.44
1:G:232:GLU:N	1:G:232:GLU:OE1	2.47	0.44
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.57	0.44
1:K:359:ASP:O	1:K:361:ASP:N	2.38	0.44
1:L:299:THR:HB	1:L:316:ASP:HA	2.00	0.44
1:H:70:GLY:O	1:H:74:VAL:HG23	2.18	0.44
2:S:20:LYS:HZ1	2:S:28:THR:HG23	1.82	0.44
1:L:175:ILE:O	1:L:175:ILE:HG13	2.15	0.44
2:R:14:ARG:NH1	2:R:35:SER:O	2.50	0.44
1:D:204:PHE:CE1	1:D:213:VAL:HG11	2.52	0.44
1:E:333:ILE:HG13	1:E:334:ASP:N	2.32	0.44
1:I:450:PRO:O	1:I:454:ILE:HG13	2.18	0.44
1:I:40:LEU:HB2	1:I:42:LYS:NZ	2.33	0.44
1:A:284:ARG:HH22	1:A:368:ARG:HD3	1.82	0.44
1:E:207:LYS:N	1:E:208:PRO:HD2	2.31	0.44
1:I:501:ARG:O	1:I:505:GLN:HG3	2.18	0.44
1:D:496:PRO:O	1:D:499:VAL:HG22	2.17	0.44
1:H:302:SER:OG	1:H:304:GLU:HG2	2.17	0.44
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.47	0.44
1:N:13:ARG:NH2	1:N:518:GLU:OE1	2.44	0.44
1:A:305:ILE:HD11	1:B:203:TYR:CE1	2.52	0.44
1:M:252:GLU:HG2	1:M:285:ARG:CZ	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:458:CYS:SG	1:N:480:ALA:HB1	2.58	0.44
1:K:217:SER:HA	1:K:320:ALA:O	2.17	0.44
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.99	0.44
2:Z:7:HIS:C	2:Z:9:ARG:H	2.21	0.44
2:U:20:LYS:HE3	2:U:28:THR:OG1	2.18	0.44
1:C:261:THR:O	1:C:264:VAL:HG12	2.18	0.44
2:V:7:HIS:C	2:V:9:ARG:H	2.21	0.44
1:K:361:ASP:O	1:K:365:LEU:HD13	2.17	0.44
1:K:466:ALA:O	1:K:470:LYS:HG3	2.17	0.44
1:D:103:GLY:O	1:D:107:VAL:HG23	2.18	0.44
1:G:11:ASP:O	1:G:14:VAL:HG12	2.18	0.44
1:K:23:LEU:HD11	1:K:57:ALA:HA	1.99	0.44
1:F:414:GLY:O	1:F:417:VAL:HG12	2.18	0.44
2:Y:34:LYS:HG3	2:Y:35:SER:H	1.82	0.44
1:E:345:ARG:O	1:E:349:ILE:HG13	2.17	0.44
1:H:30:THR:HB	1:H:51:LYS:HG3	1.99	0.44
1:E:421:ARG:HD3	1:E:421:ARG:HA	1.79	0.44
1:B:370:ALA:HB1	1:B:376:VAL:HB	2.00	0.44
1:B:220:ILE:HG13	1:B:220:ILE:O	2.17	0.44
1:M:284:ARG:HG3	1:M:364:LYS:HE3	1.99	0.44
1:I:294:THR:CB	1:I:345:ARG:HD2	2.48	0.44
1:N:369:VAL:O	1:N:372:LEU:HG	2.18	0.44
1:J:220:ILE:HG23	1:J:248:LEU:HD11	2.00	0.44
1:D:94:VAL:HG12	1:D:449:ALA:HB1	1.99	0.44
1:M:326:ASN:ND2	1:M:329:THR:OG1	2.41	0.44
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.99	0.44
1:A:24:ALA:O	1:A:28:LYS:HG3	2.18	0.44
1:F:234:LEU:N	1:F:235:PRO:HD2	2.32	0.44
1:F:218:PRO:HD2	1:F:320:ALA:O	2.18	0.44
1:N:522:THR:HG22	1:N:523:ASP:N	2.33	0.44
1:D:77:VAL:CG2	1:D:510:VAL:HG21	2.42	0.44
1:I:219:PHE:CZ	1:I:247:LEU:HD13	2.53	0.44
1:F:194:GLN:HG3	1:F:331:THR:HG22	2.00	0.44
1:C:391:GLU:OE2	1:C:395:ARG:NE	2.51	0.44
1:M:186:GLU:HG3	1:M:380:LYS:HB2	1.99	0.44
1:C:18:ARG:HD2	1:C:67:GLU:OE2	2.18	0.44
1:M:477:GLY:HA3	1:M:488:MET:SD	2.58	0.44
1:K:212:ALA:HB2	1:K:326:ASN:HB3	2.00	0.44
2:P:20:LYS:CE	2:P:20:LYS:HA	2.43	0.44
2:R:51:ASN:O	2:R:53:GLU:N	2.51	0.44
2:Q:51:ASN:O	2:Q:53:GLU:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:345:ARG:O	1:N:349:ILE:HG12	2.16	0.44
2:Z:50:GLU:O	2:Z:52:GLY:N	2.44	0.44
1:K:339:GLU:HA	1:K:342:ILE:HG12	2.00	0.44
1:K:69:MET:HE3	1:K:521:VAL:O	2.18	0.44
1:E:270:ILE:HG13	1:E:271:VAL:N	2.33	0.44
1:N:270:ILE:HG13	1:N:271:VAL:HG22	2.00	0.44
1:D:461:GLU:HA	1:D:462:PRO:HD3	1.79	0.44
1:F:255:GLU:O	1:F:259:LEU:HD22	2.18	0.44
1:F:266:THR:HG23	1:F:272:LYS:HA	2.00	0.44
1:M:372:LEU:HB3	1:M:373:ALA:H	1.49	0.44
1:B:196:ASP:CG	1:B:197:ARG:H	2.21	0.44
2:R:37:ARG:NH2	2:S:77:LYS:HE3	2.33	0.44
2:W:40:VAL:HG22	2:W:63:ASP:O	2.18	0.44
2:P:57:LEU:HD12	2:P:59:VAL:HG13	2.00	0.44
1:C:70:GLY:O	1:C:74:VAL:HG23	2.18	0.44
1:D:150:ILE:CD1	1:D:494:LEU:H	2.31	0.44
1:N:290:GLN:OE1	1:N:300:VAL:HG21	2.17	0.44
2:Z:18:GLU:OE2	2:Z:33:ALA:HB3	2.18	0.44
1:J:325:ILE:HD13	1:J:330:THR:OG1	2.18	0.44
1:A:296:THR:O	1:A:336:VAL:HG22	2.18	0.44
2:R:80:ASN:O	2:R:80:ASN:ND2	2.49	0.44
1:E:325:ILE:HD13	1:E:330:THR:HB	1.99	0.43
1:A:206:ASN:ND2	1:A:214:GLU:H	2.16	0.43
1:I:225:LYS:HG3	1:I:226:LYS:O	2.18	0.43
1:B:349:ILE:HD12	1:B:369:VAL:HG22	2.00	0.43
1:G:220:ILE:HG21	1:G:296:THR:HG21	1.99	0.43
1:D:417:VAL:O	1:D:421:ARG:HG2	2.18	0.43
1:G:56:VAL:O	1:G:60:ILE:HG12	2.18	0.43
1:J:191:GLU:N	1:J:191:GLU:OE1	2.36	0.43
1:B:219:PHE:O	1:B:248:LEU:N	2.50	0.43
1:H:234:LEU:N	1:H:235:PRO:HD2	2.33	0.43
2:T:7:HIS:ND1	2:T:7:HIS:O	2.50	0.43
1:C:421:ARG:HG3	1:C:421:ARG:HH11	1.83	0.43
1:N:124:VAL:HG22	1:N:504:LEU:HD21	1.99	0.43
1:L:304:GLU:O	1:M:260:ALA:HA	2.19	0.43
1:N:342:ILE:O	1:N:346:VAL:HG23	2.18	0.43
1:D:149:THR:CG2	1:D:156:GLU:HA	2.43	0.43
2:O:14:ARG:HH11	2:O:14:ARG:HA	1.83	0.43
1:B:226:LYS:HA	1:B:226:LYS:NZ	2.30	0.43
1:B:226:LYS:NZ	1:B:253:ASP:O	2.44	0.43
1:A:345:ARG:O	1:A:348:GLN:HG2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:HA	1:A:268:ARG:HG2	1.99	0.43
2:S:53:GLU:HG3	2:S:54:VAL:H	1.83	0.43
1:J:352:GLN:HG3	1:J:365:LEU:HD13	2.00	0.43
1:G:215:LEU:HB3	1:G:218:PRO:HB3	1.99	0.43
1:H:347:ALA:O	1:H:350:ARG:HG2	2.18	0.43
1:K:353:ILE:HD12	1:K:353:ILE:HA	1.85	0.43
2:P:11:ILE:O	2:P:41:LEU:HG	2.18	0.43
1:I:358:SER:OG	1:I:359:ASP:N	2.50	0.43
1:D:255:GLU:N	1:D:255:GLU:OE1	2.48	0.43
1:J:40:LEU:HD13	1:J:59:GLU:HG3	1.99	0.43
1:N:429:LEU:O	1:N:430:ARG:NH1	2.43	0.43
1:E:42:LYS:NZ	1:E:59:GLU:OE2	2.45	0.43
1:K:346:VAL:HA	1:K:349:ILE:HG22	1.98	0.43
1:J:513:LEU:HB3	1:K:49:ILE:HD12	2.00	0.43
2:Y:37:ARG:NH2	2:Z:77:LYS:O	2.51	0.43
1:F:206:ASN:N	1:F:206:ASN:OD1	2.52	0.43
1:G:195:PHE:CE1	1:G:330:THR:HB	2.54	0.43
1:I:53:GLY:O	1:I:56:VAL:HG22	2.19	0.43
1:C:276:VAL:HG21	1:C:330:THR:OG1	2.18	0.43
1:N:296:THR:HG22	1:N:319:GLN:N	2.33	0.43
2:R:7:HIS:C	2:R:9:ARG:H	2.22	0.43
1:G:207:LYS:N	1:G:208:PRO:HD2	2.34	0.43
1:M:219:PHE:CE1	1:M:247:LEU:HD13	2.53	0.43
1:N:287:ALA:O	1:N:290:GLN:HB2	2.19	0.43
1:G:356:ALA:HB3	1:G:362:ARG:HG2	1.98	0.43
1:D:348:GLN:HA	1:E:209:GLU:OE2	2.18	0.43
1:F:195:PHE:CE1	1:F:279:PRO:HG3	2.53	0.43
1:G:455:VAL:HG21	1:G:465:VAL:HG11	2.01	0.43
1:B:288:MET:O	1:B:292:ILE:HG23	2.19	0.43
1:E:321:LYS:HG2	1:E:333:ILE:HD11	2.01	0.43
1:L:25:ASP:HA	1:L:28:LYS:HD3	2.00	0.43
1:K:283:ASP:N	1:K:283:ASP:OD1	2.49	0.43
1:D:146:GLN:O	1:D:149:THR:OG1	2.28	0.43
1:J:232:GLU:OE1	1:J:232:GLU:N	2.52	0.43
1:A:324:VAL:HG23	1:A:333:ILE:HD11	2.01	0.43
1:E:34:LYS:HD2	1:E:458:CYS:HA	1.99	0.43
2:R:57:LEU:H	2:R:57:LEU:HD23	1.84	0.43
1:G:232:GLU:OE2	1:G:233:MET:HG3	2.18	0.43
2:V:12:VAL:HG22	2:V:40:VAL:HA	2.00	0.43
1:N:177:VAL:HG11	1:N:397:GLU:HG2	2.01	0.43
1:B:414:GLY:O	1:B:417:VAL:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ARG:O	1:F:289:LEU:HG	2.19	0.43
1:D:227:ILE:HD12	1:D:227:ILE:HA	1.82	0.43
1:C:209:GLU:O	1:C:210:THR:HG22	2.18	0.43
1:M:204:PHE:HD2	1:M:263:VAL:HG12	1.83	0.43
1:E:191:GLU:N	1:E:191:GLU:OE1	2.33	0.43
1:H:232:GLU:OE1	1:H:232:GLU:N	2.51	0.43
1:G:286:LYS:O	1:G:290:GLN:HG2	2.19	0.43
1:M:206:ASN:OD1	1:M:206:ASN:N	2.50	0.43
1:K:206:ASN:N	1:K:206:ASN:OD1	2.52	0.43
2:P:37:ARG:NH2	2:Q:78:ILE:HG13	2.32	0.43
1:K:70:GLY:O	1:K:74:VAL:HG23	2.19	0.43
2:W:7:HIS:C	2:W:9:ARG:H	2.22	0.43
1:A:16:MET:HB2	1:A:520:MET:CE	2.49	0.43
2:V:7:HIS:CG	2:V:48:ILE:HD11	2.54	0.43
2:Z:78:ILE:HD13	2:Z:83:VAL:HG21	2.00	0.43
1:L:361:ASP:O	1:L:365:LEU:HD13	2.18	0.43
1:F:353:ILE:HG12	1:F:365:LEU:HB3	2.01	0.43
1:C:90:THR:O	1:C:94:VAL:HG23	2.18	0.43
1:G:482:THR:OG1	1:G:484:GLU:HG2	2.19	0.43
1:C:345:ARG:O	1:C:349:ILE:HG12	2.19	0.43
2:Y:11:ILE:O	2:Y:11:ILE:HG12	2.18	0.43
1:A:321:LYS:HG2	1:A:322:ARG:HG2	2.00	0.43
1:D:175:ILE:HG23	1:D:377:ALA:HB3	2.01	0.43
1:K:31:LEU:HD23	1:K:453:GLN:HB3	2.01	0.43
2:Y:13:LYS:HD2	2:Y:83:VAL:HG12	2.01	0.43
1:B:103:GLY:O	1:B:107:VAL:HG23	2.19	0.43
1:E:292:ILE:O	1:E:295:LEU:HG	2.19	0.43
1:N:266:THR:HG22	1:N:273:VAL:H	1.81	0.43
1:K:305:ILE:HG22	1:K:306:GLY:H	1.83	0.43
1:C:352:GLN:HG2	1:D:327:LYS:HE3	2.01	0.43
1:E:223:ALA:N	1:E:250:ILE:O	2.50	0.43
1:G:298:GLY:HA3	1:G:318:GLY:HA2	2.00	0.43
1:K:194:GLN:HA	1:K:330:THR:O	2.19	0.43
1:G:147:VAL:O	1:G:150:ILE:HG22	2.19	0.43
1:D:440:ILE:O	1:D:444:LEU:HG	2.19	0.43
1:B:479:ASN:HD21	3:B:601:ATP:HN62	1.67	0.43
1:A:206:ASN:OD1	1:A:206:ASN:N	2.51	0.43
1:I:38:VAL:O	1:I:49:ILE:HD12	2.19	0.43
2:X:50:GLU:HG2	2:Y:51:ASN:HB2	2.01	0.43
1:F:121:ASP:O	1:F:124:VAL:HG12	2.18	0.43
1:A:165:ALA:HB1	1:A:175:ILE:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:47:ARG:NE	2:U:88:GLU:OE1	2.52	0.43
1:F:237:LEU:O	1:F:240:VAL:HG22	2.19	0.43
1:G:440:ILE:O	1:G:444:LEU:HG	2.18	0.43
2:P:7:HIS:C	2:P:9:ARG:H	2.21	0.43
1:H:203:TYR:CD1	1:N:305:ILE:HD11	2.53	0.43
1:E:322:ARG:HB3	1:E:333:ILE:HD11	2.00	0.43
1:G:314:LEU:HD23	1:G:317:LEU:HD12	1.99	0.43
1:M:417:VAL:O	1:M:421:ARG:HG2	2.19	0.43
1:E:112:ASN:HA	1:E:113:PRO:HD3	1.88	0.43
1:H:165:ALA:HB1	1:H:175:ILE:HD13	2.00	0.43
1:E:90:THR:O	1:E:94:VAL:HG23	2.19	0.43
1:N:232:GLU:OE1	1:N:232:GLU:N	2.52	0.43
1:H:196:ASP:OD1	1:H:196:ASP:N	2.41	0.43
1:E:146:GLN:O	1:E:149:THR:OG1	2.30	0.43
1:M:349:ILE:HG21	1:M:369:VAL:HG23	2.01	0.43
1:L:209:GLU:HB3	1:L:210:THR:H	1.62	0.43
2:Y:51:ASN:O	2:Y:53:GLU:N	2.52	0.43
2:Y:7:HIS:O	2:Y:8:ASP:HB3	2.19	0.43
1:J:520:MET:HG2	1:K:39:VAL:HG13	2.01	0.43
1:E:168:LYS:CD	1:E:189:VAL:HG21	2.49	0.43
1:A:123:ALA:HB2	1:A:440:ILE:HD13	2.00	0.43
2:X:69:ASP:HA	2:X:73:VAL:HG21	2.00	0.43
1:G:369:VAL:O	1:G:372:LEU:HG	2.18	0.43
1:F:421:ARG:HA	1:F:421:ARG:HD3	1.78	0.43
1:M:74:VAL:O	1:M:77:VAL:HG23	2.19	0.42
2:W:12:VAL:HG12	2:W:40:VAL:HA	2.01	0.42
1:B:294:THR:HG21	1:B:345:ARG:HE	1.82	0.42
1:N:365:LEU:O	1:N:369:VAL:HG23	2.19	0.42
1:C:200:LEU:HD11	1:C:277:LYS:HG3	1.99	0.42
1:H:391:GLU:OE2	1:H:395:ARG:NE	2.52	0.42
1:D:20:VAL:HG13	1:D:74:VAL:HG21	2.01	0.42
1:C:342:ILE:O	1:C:346:VAL:HG23	2.19	0.42
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.59	0.42
1:J:371:LYS:HA	1:J:371:LYS:HD2	1.81	0.42
1:I:369:VAL:O	1:I:372:LEU:HG	2.18	0.42
1:E:286:LYS:HD3	1:E:289:LEU:HD21	2.01	0.42
1:N:496:PRO:O	1:N:499:VAL:HG22	2.19	0.42
2:U:6:LEU:O	2:U:7:HIS:CG	2.72	0.42
1:M:288:MET:HA	1:M:291:ASP:OD2	2.19	0.42
1:A:356:ALA:HA	1:A:357:THR:HB	2.01	0.42
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:372:LEU:HB2	1:G:373:ALA:H	1.60	0.42
2:X:15:LYS:HB3	2:X:16:GLU:H	1.62	0.42
1:A:414:GLY:O	1:A:417:VAL:HG12	2.20	0.42
1:J:226:LYS:HD3	1:J:253:ASP:HB3	2.01	0.42
1:D:225:LYS:HD3	1:D:303:GLU:HG3	2.00	0.42
1:F:220:ILE:HG23	1:F:318:GLY:C	2.39	0.42
1:E:175:ILE:O	1:E:175:ILE:HG13	2.15	0.42
1:F:197:ARG:NH2	1:F:276:VAL:HG23	2.35	0.42
1:M:70:GLY:O	1:M:74:VAL:HG23	2.19	0.42
1:G:40:LEU:HD13	1:G:59:GLU:HG3	2.01	0.42
1:D:359:ASP:O	1:D:361:ASP:N	2.53	0.42
1:K:342:ILE:HG13	1:K:343:GLN:N	2.34	0.42
1:K:305:ILE:HG22	1:K:306:GLY:N	2.35	0.42
1:N:149:THR:OG1	1:N:159:GLY:HA3	2.20	0.42
2:O:94:ILE:HG13	2:P:6:LEU:HD11	2.00	0.42
1:G:450:PRO:O	1:G:454:ILE:HG13	2.20	0.42
1:B:195:PHE:CD2	1:B:279:PRO:HB3	2.53	0.42
1:F:196:ASP:OD1	1:F:196:ASP:N	2.43	0.42
2:S:20:LYS:NZ	2:S:28:THR:HG23	2.34	0.42
1:G:195:PHE:HD1	1:G:195:PHE:N	2.18	0.42
1:B:77:VAL:CG2	1:B:510:VAL:HG11	2.44	0.42
1:J:236:VAL:HG22	1:J:237:LEU:N	2.34	0.42
2:V:67:PHE:C	2:V:67:PHE:HD1	2.22	0.42
1:A:349:ILE:CG2	1:A:365:LEU:HD11	2.49	0.42
1:K:289:LEU:HA	1:K:292:ILE:HG12	2.02	0.42
1:F:190:VAL:CG1	1:F:194:GLN:HB3	2.48	0.42
1:K:248:LEU:HD22	1:K:323:VAL:HG11	2.01	0.42
2:O:7:HIS:O	2:O:7:HIS:ND1	2.51	0.42
2:O:15:LYS:HD3	2:O:37:ARG:HB3	1.99	0.42
1:F:264:VAL:O	1:F:268:ARG:HG2	2.20	0.42
1:L:524:LEU:HA	1:L:525:PRO:HD3	1.85	0.42
1:B:251:ALA:O	1:B:278:ALA:N	2.52	0.42
1:F:223:ALA:N	1:F:250:ILE:O	2.52	0.42
1:D:510:VAL:O	1:D:514:MET:HG3	2.19	0.42
2:V:67:PHE:C	2:V:67:PHE:CD1	2.92	0.42
1:K:348:GLN:O	1:K:351:GLN:HB3	2.20	0.42
2:V:20:LYS:HD3	2:V:27:LEU:HB3	2.01	0.42
1:I:276:VAL:HG21	1:I:325:ILE:HD13	2.01	0.42
1:K:285:ARG:HA	1:K:288:MET:HG2	2.01	0.42
2:P:7:HIS:HB2	2:P:46:GLY:O	2.20	0.42
1:H:230:ILE:HD11	1:H:258:ALA:HB1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:15:LYS:HB3	2:O:16:GLU:H	1.65	0.42
1:H:296:THR:O	1:H:336:VAL:HG22	2.20	0.42
1:B:360:TYR:OH	1:B:364:LYS:NZ	2.38	0.42
1:D:513:LEU:HD11	1:E:388:GLU:HA	2.02	0.42
1:M:405:ALA:HB1	1:M:498:LYS:HB3	2.02	0.42
1:D:301:ILE:HG13	1:D:301:ILE:O	2.14	0.42
1:C:54:VAL:HG23	1:C:89:THR:HG21	2.02	0.42
1:E:222:LEU:HD13	1:E:289:LEU:HD13	2.01	0.42
1:I:226:LYS:NZ	1:I:255:GLU:HB3	2.35	0.42
1:K:351:GLN:HG2	1:L:210:THR:HA	2.01	0.42
1:A:258:ALA:O	1:A:262:LEU:HD13	2.20	0.42
1:D:349:ILE:O	1:D:353:ILE:HG13	2.20	0.42
2:U:11:ILE:HG12	2:U:85:ILE:HG12	2.02	0.42
1:C:305:ILE:HG22	1:C:306:GLY:H	1.84	0.42
1:C:320:ALA:CB	1:C:332:ILE:HD11	2.50	0.42
1:H:200:LEU:HD11	1:H:277:LYS:HG3	2.02	0.42
1:E:368:ARG:HA	1:E:371:LYS:HE3	2.01	0.42
1:F:247:LEU:HB3	1:F:273:VAL:HG22	2.01	0.42
1:A:103:GLY:O	1:A:107:VAL:HG23	2.20	0.42
1:A:156:GLU:CD	1:A:156:GLU:H	2.23	0.42
1:A:270:ILE:HG13	1:A:271:VAL:HG22	2.01	0.42
2:U:78:ILE:HA	2:U:78:ILE:HD13	1.92	0.42
1:B:349:ILE:O	1:B:352:GLN:HG2	2.19	0.42
1:K:77:VAL:HG22	1:K:510:VAL:HG21	2.02	0.42
1:B:355:GLU:OE2	1:C:210:THR:OG1	2.38	0.42
1:C:292:ILE:O	1:C:295:LEU:HG	2.19	0.42
1:I:66:PHE:O	1:I:69:MET:HB2	2.19	0.42
1:A:231:ARG:HG2	2:R:22:ALA:HB1	2.02	0.42
1:J:482:THR:OG1	1:J:484:GLU:HG2	2.20	0.42
1:I:461:GLU:HA	1:I:462:PRO:HD3	1.90	0.42
1:G:359:ASP:OD2	1:G:360:TYR:N	2.45	0.42
1:C:285:ARG:HG3	1:C:286:LYS:N	2.34	0.42
2:X:7:HIS:HB2	2:X:46:GLY:O	2.19	0.42
1:J:169:VAL:HG21	1:J:377:ALA:HB2	2.01	0.42
1:E:252:GLU:N	1:E:252:GLU:OE1	2.51	0.42
1:A:80:LYS:HG2	1:A:506:TYR:CZ	2.55	0.42
1:F:278:ALA:HA	1:F:279:PRO:HD3	1.84	0.42
1:D:372:LEU:HD13	1:D:374:GLY:N	2.21	0.42
2:S:51:ASN:O	2:S:53:GLU:N	2.52	0.42
1:K:440:ILE:O	1:K:444:LEU:HG	2.20	0.42
1:F:302:SER:HB3	1:F:305:ILE:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:GLU:O	1:K:343:GLN:HB3	2.19	0.42
2:O:7:HIS:HB2	2:O:46:GLY:O	2.20	0.42
1:L:5:ASP:HB2	1:L:524:LEU:HD12	2.02	0.42
1:L:241:ALA:HB1	2:V:25:ILE:HD11	2.02	0.42
2:V:51:ASN:O	2:V:53:GLU:N	2.53	0.42
1:D:495:ASP:OD2	3:D:601:ATP:O3'	2.34	0.42
1:F:4:LYS:HB3	1:F:521:VAL:HG23	2.01	0.42
1:F:291:ASP:OD1	1:F:292:ILE:N	2.53	0.42
1:L:265:ASN:HD22	1:L:270:ILE:HD11	1.84	0.42
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.94	0.42
1:I:268:ARG:HG3	1:I:270:ILE:HG12	2.02	0.42
1:C:69:MET:HE3	1:D:41:ASP:HB2	2.01	0.42
2:O:59:VAL:HG12	2:O:94:ILE:HD11	2.02	0.42
1:N:359:ASP:O	1:N:361:ASP:N	2.53	0.42
1:D:450:PRO:O	1:D:454:ILE:HG13	2.19	0.42
1:D:205:ILE:HA	1:D:205:ILE:HD12	1.90	0.42
1:G:196:ASP:N	1:G:196:ASP:OD1	2.43	0.42
1:C:171:LYS:HA	1:C:171:LYS:HD2	1.92	0.42
1:L:206:ASN:N	1:L:206:ASN:OD1	2.52	0.42
1:M:522:THR:HG22	1:M:523:ASP:N	2.35	0.42
2:Y:3:ILE:HD12	2:Y:11:ILE:HD12	2.01	0.42
2:Y:3:ILE:HG22	2:Y:4:ARG:H	1.85	0.42
2:Q:13:LYS:HD3	2:Q:83:VAL:HG12	2.02	0.42
1:F:440:ILE:O	1:F:444:LEU:HG	2.20	0.42
1:H:34:LYS:HD3	1:N:112:ASN:ND2	2.34	0.42
1:N:27:VAL:O	1:N:30:THR:HG22	2.20	0.42
1:F:305:ILE:HG22	1:F:306:GLY:H	1.85	0.42
1:A:229:ASN:OD1	1:A:230:ILE:N	2.53	0.42
1:N:285:ARG:HG3	1:N:286:LYS:N	2.34	0.42
1:N:305:ILE:HG22	1:N:306:GLY:N	2.35	0.42
1:M:414:GLY:O	1:M:417:VAL:HG12	2.20	0.42
1:D:303:GLU:OE1	1:D:303:GLU:N	2.53	0.42
1:F:25:ASP:HA	1:F:28:LYS:HD3	2.01	0.42
1:J:112:ASN:HA	1:J:113:PRO:HD3	1.90	0.42
1:H:38:VAL:HG22	1:N:519:CYS:HB3	2.02	0.42
1:E:3:ALA:O	1:E:524:LEU:HD13	2.20	0.42
1:M:23:LEU:HD11	1:M:57:ALA:HA	2.00	0.42
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.87	0.42
1:A:66:PHE:O	1:A:69:MET:HB2	2.20	0.42
1:H:23:LEU:HD11	1:H:57:ALA:HA	2.01	0.42
1:H:227:ILE:HA	1:H:227:ILE:HD12	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:GLU:N	1:N:191:GLU:OE1	2.35	0.42
1:C:77:VAL:CG2	1:C:510:VAL:HG11	2.41	0.41
1:L:346:VAL:O	1:L:350:ARG:HG3	2.20	0.41
1:N:296:THR:HG22	1:N:319:GLN:H	1.85	0.41
1:A:349:ILE:HG21	1:A:369:VAL:CG2	2.50	0.41
1:I:349:ILE:O	1:I:352:GLN:HG2	2.20	0.41
1:B:302:SER:O	1:B:305:ILE:HG22	2.20	0.41
2:O:11:ILE:HD12	2:O:85:ILE:HG12	2.02	0.41
1:C:226:LYS:HG3	1:C:253:ASP:O	2.20	0.41
1:K:441:LYS:HD3	1:K:444:LEU:HD12	2.02	0.41
1:D:357:THR:O	1:D:358:SER:OG	2.33	0.41
2:Y:57:LEU:HD12	2:Y:57:LEU:N	2.35	0.41
1:E:510:VAL:HG12	1:E:514:MET:CE	2.50	0.41
1:E:77:VAL:HG22	1:E:510:VAL:HG21	2.01	0.41
1:D:227:ILE:HG13	1:D:228:SER:H	1.84	0.41
1:G:234:LEU:N	1:G:235:PRO:HD2	2.35	0.41
1:A:429:LEU:O	1:A:430:ARG:NH1	2.45	0.41
1:C:162:ILE:HD13	1:C:403:THR:HG21	2.02	0.41
1:A:226:LYS:HB3	1:A:226:LYS:HE2	1.80	0.41
1:J:74:VAL:O	1:J:77:VAL:HG23	2.20	0.41
1:G:288:MET:HB3	1:G:368:ARG:HD3	2.02	0.41
1:I:56:VAL:O	1:I:60:ILE:HG13	2.19	0.41
1:I:226:LYS:HE2	1:I:254:VAL:HA	2.02	0.41
1:F:482:THR:HG1	1:F:484:GLU:HG2	1.85	0.41
1:C:371:LYS:HA	1:C:371:LYS:HD2	1.83	0.41
1:J:115:ASP:HA	1:J:118:ARG:HD2	2.03	0.41
1:B:409:GLU:CD	1:B:501:ARG:HH21	2.24	0.41
1:K:440:ILE:HG13	1:K:441:LYS:N	2.35	0.41
1:D:150:ILE:HD13	1:D:494:LEU:H	1.85	0.41
1:N:204:PHE:CD1	1:N:204:PHE:O	2.73	0.41
1:E:355:GLU:OE1	1:F:327:LYS:HD3	2.20	0.41
1:C:386:GLU:O	1:C:390:LYS:HG2	2.20	0.41
1:A:234:LEU:N	1:A:235:PRO:HD2	2.35	0.41
1:B:299:THR:N	1:B:316:ASP:O	2.51	0.41
1:E:103:GLY:O	1:E:107:VAL:HG23	2.21	0.41
1:I:234:LEU:N	1:I:235:PRO:HD2	2.35	0.41
1:K:324:VAL:HG13	1:K:331:THR:OG1	2.20	0.41
1:D:5:ASP:HB2	1:D:524:LEU:HD23	2.02	0.41
1:G:421:ARG:HA	1:G:421:ARG:HD3	1.82	0.41
1:H:74:VAL:O	1:H:77:VAL:HG23	2.20	0.41
1:F:326:ASN:ND2	1:F:329:THR:HG23	2.30	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:VAL:O	1:I:30:THR:HG22	2.21	0.41
1:L:287:ALA:HB1	1:L:368:ARG:HH12	1.85	0.41
1:M:501:ARG:O	1:M:505:GLN:HG3	2.20	0.41
2:Q:78:ILE:HD13	2:Q:83:VAL:HG21	2.02	0.41
1:L:501:ARG:HD3	1:L:505:GLN:NE2	2.36	0.41
1:K:414:GLY:O	1:K:417:VAL:HG12	2.20	0.41
1:G:342:ILE:O	1:G:346:VAL:HG23	2.20	0.41
1:A:135:SER:OG	1:A:409:GLU:O	2.36	0.41
1:G:150:ILE:HG21	1:G:494:LEU:O	2.20	0.41
1:N:225:LYS:HE2	1:N:303:GLU:HG3	2.02	0.41
1:N:321:LYS:HD3	1:N:334:ASP:HB3	2.03	0.41
1:L:190:VAL:HG11	1:L:194:GLN:NE2	2.36	0.41
2:W:20:LYS:HZ2	2:W:28:THR:N	2.19	0.41
1:C:213:VAL:HG23	1:C:325:ILE:HG13	2.02	0.41
1:I:225:LYS:HD2	1:I:303:GLU:HG2	2.02	0.41
1:I:226:LYS:HD2	1:I:227:ILE:H	1.85	0.41
1:B:302:SER:OG	1:B:304:GLU:OE1	2.38	0.41
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.88	0.41
1:A:16:MET:SD	1:A:514:MET:HG2	2.61	0.41
1:F:379:ILE:CD1	1:F:396:VAL:HG11	2.51	0.41
1:F:270:ILE:HG13	1:F:271:VAL:N	2.35	0.41
2:Q:20:LYS:HD3	2:Q:27:LEU:HD13	2.02	0.41
1:I:313:THR:HG23	1:I:316:ASP:OD2	2.19	0.41
1:N:240:VAL:HG13	1:N:245:LYS:O	2.20	0.41
1:J:136:VAL:HA	1:J:137:PRO:HD3	1.90	0.41
1:E:513:LEU:HD11	1:F:388:GLU:HA	2.03	0.41
1:C:147:VAL:O	1:C:150:ILE:HG22	2.21	0.41
1:C:338:GLU:HG2	1:C:341:ALA:H	1.85	0.41
1:M:524:LEU:HA	1:M:524:LEU:HD23	1.90	0.41
1:M:5:ASP:HB2	1:M:524:LEU:HD23	2.02	0.41
1:A:291:ASP:OD1	1:A:292:ILE:N	2.53	0.41
1:C:255:GLU:OE1	1:C:255:GLU:N	2.45	0.41
1:F:342:ILE:HG12	1:F:345:ARG:HH21	1.85	0.41
1:M:522:THR:HG23	1:N:41:ASP:CG	2.41	0.41
1:H:112:ASN:HA	1:H:113:PRO:HD3	1.80	0.41
1:E:58:ARG:O	1:E:75:LYS:NZ	2.53	0.41
1:L:495:ASP:HA	1:L:496:PRO:HD2	1.96	0.41
1:L:494:LEU:HA	1:L:494:LEU:HD23	1.88	0.41
2:W:7:HIS:HB2	2:W:46:GLY:O	2.20	0.41
1:M:305:ILE:HG22	1:M:306:GLY:N	2.36	0.41
2:O:15:LYS:HD3	2:O:37:ARG:CB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:HG2	1:A:253:ASP:N	2.35	0.41
1:G:77:VAL:CG2	1:G:510:VAL:HG21	2.38	0.41
1:G:80:LYS:HG2	1:G:506:TYR:CZ	2.55	0.41
1:F:195:PHE:HE1	1:F:279:PRO:HG3	1.86	0.41
1:C:349:ILE:O	1:C:353:ILE:HG13	2.21	0.41
2:U:20:LYS:HD3	2:U:27:LEU:HG	2.03	0.41
1:L:346:VAL:O	1:L:349:ILE:HG22	2.20	0.41
1:M:291:ASP:OD1	1:M:292:ILE:N	2.54	0.41
1:D:501:ARG:O	1:D:505:GLN:HG3	2.20	0.41
1:G:200:LEU:HD22	1:G:254:VAL:CG1	2.51	0.41
1:B:206:ASN:ND2	1:B:207:LYS:H	2.17	0.41
1:D:361:ASP:OD1	1:D:361:ASP:N	2.54	0.41
1:E:73:MET:HE1	1:E:514:MET:HG3	2.02	0.41
1:C:285:ARG:O	1:C:289:LEU:HB2	2.20	0.41
1:F:90:THR:O	1:F:94:VAL:HG23	2.20	0.41
1:K:450:PRO:O	1:K:454:ILE:HG13	2.20	0.41
2:S:58:ASP:HB2	2:T:6:LEU:HD22	2.02	0.41
2:U:34:LYS:HG2	2:U:35:SER:H	1.86	0.41
1:G:289:LEU:O	1:G:292:ILE:HG12	2.21	0.41
1:L:198:GLY:HA2	1:L:325:ILE:HD11	2.02	0.41
2:Q:23:GLY:HA3	2:Q:26:VAL:HG13	2.03	0.41
1:F:193:MET:HB3	1:F:332:ILE:HB	2.03	0.41
1:L:342:ILE:HG23	1:L:345:ARG:NH2	2.35	0.41
1:D:436:GLN:O	1:D:440:ILE:HG13	2.20	0.41
1:L:429:LEU:O	1:L:430:ARG:NH1	2.45	0.41
1:K:21:ASN:OD1	1:K:97:GLN:NE2	2.36	0.41
1:D:482:THR:OG1	1:D:484:GLU:HG2	2.21	0.41
1:K:113:PRO:HB2	1:K:516:THR:HA	2.02	0.41
1:G:292:ILE:HG13	1:G:293:ALA:N	2.35	0.41
1:A:345:ARG:HA	1:A:345:ARG:HD2	1.85	0.41
2:R:7:HIS:CE1	2:R:48:ILE:HD12	2.55	0.41
1:B:346:VAL:O	1:B:350:ARG:HG2	2.21	0.41
1:N:20:VAL:HG22	1:N:74:VAL:HG21	2.02	0.41
1:B:351:GLN:HG3	1:C:209:GLU:HB3	2.03	0.41
1:I:5:ASP:HB2	1:I:524:LEU:HD23	2.03	0.41
1:M:144:ILE:HG23	1:M:403:THR:CG2	2.50	0.41
2:Q:43:VAL:HG12	2:Q:44:GLY:O	2.20	0.41
1:I:326:ASN:HD21	1:I:329:THR:HG22	1.85	0.41
2:P:20:LYS:HZ2	2:P:27:LEU:HA	1.86	0.41
1:L:506:TYR:O	1:L:510:VAL:HG22	2.20	0.41
2:Q:15:LYS:HB3	2:Q:16:GLU:H	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:LYS:HG3	1:N:522:THR:O	2.21	0.41
1:M:437:ASN:O	1:M:440:ILE:HG23	2.20	0.41
1:H:113:PRO:CG	1:I:36:ARG:HE	2.33	0.41
1:C:225:LYS:HZ1	1:C:309:LEU:HD22	1.85	0.41
1:M:226:LYS:HZ1	1:M:255:GLU:N	2.18	0.41
1:A:268:ARG:CZ	2:R:27:LEU:HD21	2.50	0.41
2:U:7:HIS:C	2:U:9:ARG:H	2.24	0.41
1:H:222:LEU:HB2	1:H:289:LEU:HD11	2.03	0.41
1:K:282:GLY:O	1:K:286:LYS:HG2	2.21	0.41
1:L:308:GLU:HG3	1:L:309:LEU:H	1.85	0.41
1:H:358:SER:OG	1:H:359:ASP:N	2.53	0.41
1:F:296:THR:OG1	1:F:319:GLN:N	2.54	0.41
1:B:169:VAL:HG22	1:B:173:GLY:HA3	2.03	0.41
1:E:308:GLU:H	1:E:311:LYS:HD3	1.85	0.41
1:N:517:THR:HG21	1:N:520:MET:HE2	2.03	0.41
2:P:11:ILE:HB	2:P:42:ALA:HB3	2.03	0.41
1:A:70:GLY:O	1:A:74:VAL:HG23	2.21	0.41
1:D:270:ILE:HG21	2:U:25:ILE:HB	2.01	0.41
2:Z:6:LEU:O	2:Z:7:HIS:CG	2.73	0.41
2:Y:18:GLU:H	2:Y:35:SER:HB2	1.85	0.41
1:D:225:LYS:HB3	1:D:303:GLU:OE2	2.20	0.41
2:O:7:HIS:C	2:O:9:ARG:H	2.24	0.41
1:H:187:LEU:HD11	1:H:377:ALA:HB1	2.02	0.41
1:N:281:PHE:O	1:N:284:ARG:HG2	2.19	0.41
1:K:233:MET:O	1:K:236:VAL:HG13	2.20	0.41
1:N:405:ALA:HB1	1:N:498:LYS:HD3	2.02	0.41
1:L:252:GLU:O	1:L:277:LYS:HG3	2.20	0.41
1:N:422:VAL:HG23	1:N:447:MET:CE	2.50	0.41
1:C:423:ALA:HA	1:C:444:LEU:HD22	2.03	0.41
1:K:220:ILE:HG12	1:K:296:THR:HG21	2.02	0.41
1:J:423:ALA:HA	1:J:444:LEU:HD22	2.03	0.41
1:F:524:LEU:HA	1:F:524:LEU:HD22	1.89	0.41
1:L:191:GLU:OE1	1:L:191:GLU:N	2.32	0.41
1:H:441:LYS:HA	1:H:441:LYS:HD3	1.84	0.41
1:N:510:VAL:O	1:N:514:MET:HB2	2.21	0.41
1:L:245:LYS:HG2	1:L:246:PRO:HD2	2.02	0.41
1:I:215:LEU:HD13	1:I:218:PRO:CG	2.50	0.41
1:M:268:ARG:NH1	2:W:27:LEU:HD21	2.36	0.41
1:E:149:THR:CG2	1:E:156:GLU:HA	2.44	0.41
1:I:99:ILE:HD11	1:I:120:ILE:CD1	2.46	0.41
2:W:37:ARG:NH1	2:X:76:GLU:OE2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:THR:O	1:E:501:ARG:HG2	2.20	0.41
2:P:66:ILE:HD11	2:P:93:ALA:HB3	2.03	0.41
1:N:501:ARG:O	1:N:505:GLN:HG3	2.20	0.41
1:J:321:LYS:HG2	1:J:322:ARG:HG2	2.03	0.41
1:I:190:VAL:HG11	1:I:194:GLN:HB3	2.03	0.41
1:L:420:ILE:HG23	1:L:470:LYS:HG2	2.03	0.41
1:F:195:PHE:HE1	1:F:197:ARG:HH11	1.69	0.40
1:F:252:GLU:HA	1:F:278:ALA:HB2	2.02	0.40
1:F:265:ASN:OD1	2:P:26:VAL:HA	2.21	0.40
1:I:372:LEU:HB2	1:I:373:ALA:H	1.68	0.40
1:E:197:ARG:O	1:E:330:THR:HG22	2.21	0.40
1:F:74:VAL:O	1:F:77:VAL:HG23	2.22	0.40
1:K:311:LYS:NZ	1:L:268:ARG:HH22	2.19	0.40
2:U:3:ILE:HG22	2:U:4:ARG:H	1.85	0.40
1:N:194:GLN:O	1:N:371:LYS:NZ	2.36	0.40
1:F:27:VAL:O	1:F:30:THR:HG22	2.21	0.40
1:G:248:LEU:HD12	1:G:274:ALA:O	2.21	0.40
1:A:418:ALA:O	1:A:422:VAL:HG22	2.20	0.40
1:E:284:ARG:O	1:E:288:MET:HG2	2.21	0.40
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.51	0.40
1:D:95:LEU:O	1:D:99:ILE:HG13	2.20	0.40
1:A:466:ALA:O	1:A:470:LYS:HG3	2.21	0.40
1:L:124:VAL:HG21	1:L:508:ALA:CB	2.51	0.40
1:J:515:ILE:HG12	1:J:515:ILE:O	2.21	0.40
1:D:215:LEU:HD13	1:D:323:VAL:HG13	2.03	0.40
1:I:161:LEU:HD11	1:I:187:LEU:HB2	2.04	0.40
2:P:91:ILE:HG22	2:Q:6:LEU:HD13	2.03	0.40
2:X:78:ILE:HD13	2:X:78:ILE:HA	1.88	0.40
2:Q:94:ILE:HD11	2:R:6:LEU:HD11	2.02	0.40
1:N:409:GLU:CD	1:N:501:ARG:HH21	2.22	0.40
1:E:417:VAL:O	1:E:421:ARG:HG2	2.21	0.40
1:D:348:GLN:N	1:D:348:GLN:OE1	2.49	0.40
1:G:31:LEU:HG	1:G:454:ILE:HG12	2.03	0.40
1:F:25:ASP:HA	1:F:28:LYS:CD	2.52	0.40
1:L:419:LEU:HB3	1:L:447:MET:HB3	2.02	0.40
1:N:234:LEU:N	1:N:235:PRO:HD2	2.36	0.40
1:L:285:ARG:HG3	1:L:286:LYS:N	2.36	0.40
1:A:264:VAL:HG22	1:G:306:GLY:H	1.87	0.40
1:L:199:TYR:HE1	1:L:202:PRO:HG3	1.86	0.40
1:G:51:LYS:NZ	3:G:601:ATP:O1A	2.54	0.40
1:K:42:LYS:HA	1:K:42:LYS:HD2	1.96	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASN:OD1	2:S:26:VAL:HG13	2.21	0.40
1:I:361:ASP:O	1:I:365:LEU:HD13	2.21	0.40
1:L:237:LEU:HD23	2:V:26:VAL:HG21	2.03	0.40
2:R:6:LEU:O	2:R:7:HIS:CG	2.75	0.40
1:H:222:LEU:CD1	1:H:301:ILE:H	2.32	0.40
1:C:326:ASN:ND2	1:C:329:THR:HG22	2.33	0.40
1:N:372:LEU:HB2	1:N:373:ALA:H	1.58	0.40
1:I:342:ILE:HG13	1:I:343:GLN:N	2.35	0.40
1:L:301:ILE:HD13	1:L:307:MET:SD	2.62	0.40
1:K:242:LYS:HB3	1:K:242:LYS:HE3	1.80	0.40
1:E:258:ALA:O	1:E:262:LEU:HD13	2.21	0.40
2:Y:92:LEU:HD22	2:Z:9:ARG:HD3	2.03	0.40
2:O:37:ARG:HD3	2:O:66:ILE:CD1	2.51	0.40
1:K:367:GLU:O	1:K:371:LYS:HG3	2.21	0.40
1:L:364:LYS:O	1:L:367:GLU:HB3	2.22	0.40
1:C:372:LEU:HB2	1:C:373:ALA:H	1.65	0.40
1:A:451:LEU:O	1:A:455:VAL:HG23	2.20	0.40
2:T:22:ALA:O	2:T:26:VAL:HB	2.21	0.40
1:A:285:ARG:HG3	1:A:286:LYS:N	2.37	0.40
1:J:147:VAL:O	1:J:150:ILE:HG22	2.22	0.40
1:A:441:LYS:HD3	1:A:441:LYS:HA	1.88	0.40
1:J:421:ARG:HD3	1:J:421:ARG:HA	1.89	0.40
1:J:70:GLY:O	1:J:74:VAL:HG23	2.21	0.40
1:J:221:LEU:HD13	1:J:317:LEU:HD21	2.04	0.40
1:N:237:LEU:O	1:N:241:ALA:N	2.51	0.40
1:B:90:THR:O	1:B:94:VAL:HG23	2.22	0.40
1:H:455:VAL:HG21	1:H:462:PRO:HA	2.04	0.40
1:K:369:VAL:O	1:K:372:LEU:HG	2.21	0.40
1:A:305:ILE:HG22	1:A:306:GLY:H	1.86	0.40
1:N:418:ALA:O	1:N:422:VAL:HG22	2.21	0.40
2:U:48:ILE:HG13	2:U:48:ILE:H	1.73	0.40
1:E:23:LEU:HD11	1:E:57:ALA:HA	2.02	0.40
1:B:405:ALA:HB1	1:B:498:LYS:HD3	2.03	0.40
1:J:76:GLU:OE2	1:K:386:GLU:N	2.54	0.40
2:V:75:SER:HB2	2:V:82:GLU:OE2	2.21	0.40
1:B:178:GLU:HA	1:B:393:LYS:NZ	2.35	0.40
1:N:31:LEU:HD23	1:N:453:GLN:HB3	2.03	0.40
2:T:37:ARG:HG3	2:T:66:ILE:HG12	2.02	0.40
1:G:34:LYS:NZ	1:G:483:GLU:OE2	2.35	0.40
1:F:252:GLU:HA	1:F:278:ALA:CB	2.52	0.40
1:H:510:VAL:O	1:H:514:MET:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:510:VAL:O	1:M:514:MET:HG3	2.21	0.40
1:I:314:LEU:HA	1:I:317:LEU:HD12	2.02	0.40
1:K:215:LEU:O	1:K:322:ARG:HA	2.22	0.40
1:I:226:LYS:HZ3	1:I:255:GLU:H	1.70	0.40
1:M:281:PHE:HE2	1:M:284:ARG:NH2	2.19	0.40
1:C:225:LYS:HZ3	1:C:309:LEU:HB3	1.86	0.40
1:J:270:ILE:HG13	1:J:271:VAL:HG22	2.02	0.40
1:M:226:LYS:HE2	1:M:227:ILE:H	1.87	0.40
2:W:45:ASN:O	2:W:56:PRO:HA	2.22	0.40
2:U:4:ARG:HA	2:U:5:PRO:HD2	1.92	0.40
2:V:6:LEU:O	2:V:7:HIS:CG	2.74	0.40
1:N:58:ARG:HA	1:N:75:LYS:HD3	2.03	0.40
1:F:232:GLU:OE1	1:F:232:GLU:N	2.52	0.40
1:E:299:THR:N	1:E:316:ASP:O	2.53	0.40
1:E:350:ARG:O	1:E:353:ILE:HB	2.21	0.40
1:A:288:MET:HA	1:A:291:ASP:OD2	2.21	0.40
2:O:4:ARG:HA	2:O:5:PRO:HD2	1.96	0.40
1:H:414:GLY:HA3	1:H:493:ILE:HG22	2.04	0.40
1:N:152:ALA:O	1:N:395:ARG:NH1	2.55	0.40
1:J:488:MET:CE	1:J:493:ILE:HD13	2.52	0.40
1:F:287:ALA:O	1:F:368:ARG:NH2	2.55	0.40
1:N:461:GLU:HA	1:N:462:PRO:HD3	1.91	0.40
2:O:20:LYS:HG2	2:O:27:LEU:CD1	2.52	0.40
1:D:489:ILE:HD12	1:D:489:ILE:H	1.87	0.40
1:A:255:GLU:OE1	1:A:255:GLU:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	522/548 (95%)	503 (96%)	17 (3%)	2 (0%)	39 80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	522/548 (95%)	504 (97%)	16 (3%)	2 (0%)	39	80
1	C	522/548 (95%)	503 (96%)	15 (3%)	4 (1%)	24	70
1	D	522/548 (95%)	500 (96%)	18 (3%)	4 (1%)	24	70
1	E	522/548 (95%)	500 (96%)	19 (4%)	3 (1%)	30	74
1	F	522/548 (95%)	498 (95%)	19 (4%)	5 (1%)	19	66
1	G	522/548 (95%)	500 (96%)	18 (3%)	4 (1%)	24	70
1	H	522/548 (95%)	502 (96%)	17 (3%)	3 (1%)	30	74
1	I	522/548 (95%)	502 (96%)	17 (3%)	3 (1%)	30	74
1	J	522/548 (95%)	497 (95%)	20 (4%)	5 (1%)	19	66
1	K	522/548 (95%)	503 (96%)	16 (3%)	3 (1%)	30	74
1	L	522/548 (95%)	501 (96%)	18 (3%)	3 (1%)	30	74
1	M	522/548 (95%)	501 (96%)	19 (4%)	2 (0%)	39	80
1	N	522/548 (95%)	500 (96%)	18 (3%)	4 (1%)	24	70
2	O	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	9	53
2	P	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	9	53
2	Q	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	9	53
2	R	95/97 (98%)	82 (86%)	10 (10%)	3 (3%)	5	44
2	S	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	9	53
2	T	95/97 (98%)	81 (85%)	12 (13%)	2 (2%)	9	53
2	U	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	5	44
2	V	95/97 (98%)	82 (86%)	11 (12%)	2 (2%)	9	53
2	W	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	9	53
2	X	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	9	53
2	Y	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	9	53
2	Z	95/97 (98%)	82 (86%)	10 (10%)	3 (3%)	5	44
2	a	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	5	44
2	b	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	9	53
All	All	8638/9030 (96%)	8172 (95%)	387 (4%)	79 (1%)	21	68

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	193	MET
1	C	356	ALA
1	D	360	TYR
1	G	193	MET
1	I	360	TYR
1	J	193	MET
1	J	360	TYR
1	N	360	TYR
2	O	7	HIS
2	O	52	GLY
2	P	7	HIS
2	Q	7	HIS
2	R	7	HIS
2	S	7	HIS
2	T	52	GLY
2	W	7	HIS
2	X	7	HIS
2	Y	7	HIS
2	a	7	HIS
2	a	52	GLY
2	b	7	HIS
1	E	357	THR
1	E	358	SER
1	F	360	TYR
1	H	360	TYR
1	K	205	ILE
1	L	360	TYR
1	N	358	SER
2	P	52	GLY
2	Q	52	GLY
2	R	52	GLY
2	S	52	GLY
2	T	7	HIS
2	U	7	HIS
2	V	7	HIS
2	V	52	GLY
2	X	52	GLY
2	Y	52	GLY
2	Z	7	HIS
2	Z	52	GLY
2	b	52	GLY
1	A	197	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	193	MET
1	E	197	ARG
1	F	358	SER
1	I	357	THR
2	U	52	GLY
1	D	197	ARG
1	F	356	ALA
1	G	197	ARG
1	I	197	ARG
1	K	197	ARG
1	M	197	ARG
1	M	360	TYR
1	N	197	ARG
1	N	357	THR
1	B	197	ARG
1	C	197	ARG
1	D	357	THR
1	F	197	ARG
1	H	197	ARG
1	J	197	ARG
1	J	356	ALA
1	K	206	ASN
1	L	197	ARG
2	a	15	LYS
2	R	51	ASN
2	U	51	ASN
2	W	52	GLY
2	Z	15	LYS
1	J	192	GLY
1	L	279	PRO
1	C	279	PRO
1	G	192	GLY
1	G	279	PRO
1	F	279	PRO
1	H	279	PRO
1	B	279	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/413 (97%)	393 (98%)	9 (2%)	60	85
1	B	402/413 (97%)	381 (95%)	21 (5%)	29	69
1	C	402/413 (97%)	381 (95%)	21 (5%)	29	69
1	D	402/413 (97%)	372 (92%)	30 (8%)	17	57
1	E	402/413 (97%)	375 (93%)	27 (7%)	20	62
1	F	402/413 (97%)	382 (95%)	20 (5%)	30	70
1	G	402/413 (97%)	388 (96%)	14 (4%)	43	78
1	H	402/413 (97%)	386 (96%)	16 (4%)	38	75
1	I	402/413 (97%)	378 (94%)	24 (6%)	24	65
1	J	402/413 (97%)	379 (94%)	23 (6%)	25	67
1	K	402/413 (97%)	378 (94%)	24 (6%)	24	65
1	L	402/413 (97%)	377 (94%)	25 (6%)	23	64
1	M	402/413 (97%)	384 (96%)	18 (4%)	34	73
1	N	402/413 (97%)	377 (94%)	25 (6%)	23	64
2	O	80/80 (100%)	77 (96%)	3 (4%)	40	76
2	P	80/80 (100%)	75 (94%)	5 (6%)	22	64
2	Q	80/80 (100%)	68 (85%)	12 (15%)	3	26
2	R	80/80 (100%)	73 (91%)	7 (9%)	12	50
2	S	80/80 (100%)	71 (89%)	9 (11%)	7	38
2	T	80/80 (100%)	70 (88%)	10 (12%)	6	33
2	U	80/80 (100%)	68 (85%)	12 (15%)	3	26
2	V	80/80 (100%)	67 (84%)	13 (16%)	3	21
2	W	80/80 (100%)	71 (89%)	9 (11%)	7	38
2	X	80/80 (100%)	71 (89%)	9 (11%)	7	38
2	Y	80/80 (100%)	67 (84%)	13 (16%)	3	21
2	Z	80/80 (100%)	75 (94%)	5 (6%)	22	64
2	a	80/80 (100%)	76 (95%)	4 (5%)	30	70
2	b	80/80 (100%)	72 (90%)	8 (10%)	9	43
All	All	6748/6902 (98%)	6332 (94%)	416 (6%)	23	64

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	A	230	ILE
1	A	261	THR
1	A	271	VAL
1	A	310	GLU
1	A	313	THR
1	A	329	THR
1	A	387	VAL
1	A	494	LEU
1	B	40	LEU
1	B	140	ASP
1	B	200	LEU
1	B	219	PHE
1	B	220	ILE
1	B	226	LYS
1	B	227	ILE
1	B	230	ILE
1	B	236	VAL
1	B	237	LEU
1	B	238	GLU
1	B	291	ASP
1	B	301	ILE
1	B	313	THR
1	B	328	ASP
1	B	330	THR
1	B	372	LEU
1	B	376	VAL
1	B	387	VAL
1	B	432	GLN
1	B	494	LEU
1	C	101	THR
1	C	176	THR
1	C	177	VAL
1	C	196	ASP
1	C	209	GLU
1	C	210	THR
1	C	222	LEU
1	C	230	ILE
1	C	232	GLU
1	C	250	ILE
1	C	264	VAL
1	C	284	ARG
1	C	291	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	310	GLU
1	C	317	LEU
1	C	329	THR
1	C	351	GLN
1	C	372	LEU
1	C	386	GLU
1	C	387	VAL
1	C	453	GLN
1	D	17	LEU
1	D	38	VAL
1	D	89	THR
1	D	97	GLN
1	D	177	VAL
1	D	203	TYR
1	D	222	LEU
1	D	226	LYS
1	D	230	ILE
1	D	259	LEU
1	D	281	PHE
1	D	284	ARG
1	D	289	LEU
1	D	291	ASP
1	D	301	ILE
1	D	310	GLU
1	D	311	LYS
1	D	313	THR
1	D	315	GLU
1	D	330	THR
1	D	345	ARG
1	D	355	GLU
1	D	360	TYR
1	D	361	ASP
1	D	366	GLN
1	D	372	LEU
1	D	387	VAL
1	D	493	ILE
1	D	494	LEU
1	D	521	VAL
1	E	80	LYS
1	E	104	LEU
1	E	153	ASN
1	E	172	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	175	ILE
1	E	183	LEU
1	E	187	LEU
1	E	196	ASP
1	E	209	GLU
1	E	230	ILE
1	E	254	VAL
1	E	257	GLU
1	E	259	LEU
1	E	283	ASP
1	E	301	ILE
1	E	309	LEU
1	E	313	THR
1	E	325	ILE
1	E	330	THR
1	E	342	ILE
1	E	345	ARG
1	E	372	LEU
1	E	379	ILE
1	E	417	VAL
1	E	453	GLN
1	E	463	SER
1	E	494	LEU
1	F	175	ILE
1	F	179	ASP
1	F	197	ARG
1	F	209	GLU
1	F	214	GLU
1	F	220	ILE
1	F	240	VAL
1	F	257	GLU
1	F	259	LEU
1	F	301	ILE
1	F	309	LEU
1	F	310	GLU
1	F	317	LEU
1	F	324	VAL
1	F	329	THR
1	F	387	VAL
1	F	426	LEU
1	F	494	LEU
1	F	521	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	524	LEU
1	G	14	VAL
1	G	54	VAL
1	G	177	VAL
1	G	190	VAL
1	G	195	PHE
1	G	199	TYR
1	G	222	LEU
1	G	230	ILE
1	G	254	VAL
1	G	259	LEU
1	G	313	THR
1	G	372	LEU
1	G	380	LYS
1	G	387	VAL
1	H	94	VAL
1	H	105	LYS
1	H	160	LYS
1	H	183	LEU
1	H	204	PHE
1	H	205	ILE
1	H	240	VAL
1	H	273	VAL
1	H	301	ILE
1	H	305	ILE
1	H	310	GLU
1	H	313	THR
1	H	319	GLN
1	H	372	LEU
1	H	379	ILE
1	H	387	VAL
1	I	40	LEU
1	I	44	PHE
1	I	91	THR
1	I	95	LEU
1	I	101	THR
1	I	175	ILE
1	I	177	VAL
1	I	213	VAL
1	I	215	LEU
1	I	219	PHE
1	I	230	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	236	VAL
1	I	249	ILE
1	I	254	VAL
1	I	301	ILE
1	I	303	GLU
1	I	310	GLU
1	I	313	THR
1	I	332	ILE
1	I	333	ILE
1	I	372	LEU
1	I	387	VAL
1	I	463	SER
1	I	494	LEU
1	J	34	LYS
1	J	95	LEU
1	J	177	VAL
1	J	181	THR
1	J	183	LEU
1	J	196	ASP
1	J	204	PHE
1	J	210	THR
1	J	230	ILE
1	J	236	VAL
1	J	240	VAL
1	J	257	GLU
1	J	281	PHE
1	J	305	ILE
1	J	309	LEU
1	J	310	GLU
1	J	313	THR
1	J	372	LEU
1	J	387	VAL
1	J	453	GLN
1	J	467	ASN
1	J	494	LEU
1	J	515	ILE
1	K	44	PHE
1	K	200	LEU
1	K	219	PHE
1	K	221	LEU
1	K	222	LEU
1	K	230	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	236	VAL
1	K	240	VAL
1	K	242	LYS
1	K	259	LEU
1	K	283	ASP
1	K	301	ILE
1	K	308	GLU
1	K	309	LEU
1	K	313	THR
1	K	317	LEU
1	K	324	VAL
1	K	330	THR
1	K	336	VAL
1	K	343	GLN
1	K	345	ARG
1	K	348	GLN
1	K	372	LEU
1	K	379	ILE
1	L	62	LEU
1	L	175	ILE
1	L	183	LEU
1	L	204	PHE
1	L	227	ILE
1	L	230	ILE
1	L	240	VAL
1	L	247	LEU
1	L	259	LEU
1	L	291	ASP
1	L	305	ILE
1	L	309	LEU
1	L	311	LYS
1	L	313	THR
1	L	314	LEU
1	L	316	ASP
1	L	325	ILE
1	L	329	THR
1	L	330	THR
1	L	333	ILE
1	L	357	THR
1	L	372	LEU
1	L	387	VAL
1	L	515	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	521	VAL
1	M	181	THR
1	M	183	LEU
1	M	196	ASP
1	M	209	GLU
1	M	210	THR
1	M	226	LYS
1	M	230	ILE
1	M	240	VAL
1	M	254	VAL
1	M	270	ILE
1	M	296	THR
1	M	301	ILE
1	M	313	THR
1	M	331	THR
1	M	365	LEU
1	M	378	VAL
1	M	387	VAL
1	M	440	ILE
1	N	4	LYS
1	N	75	LYS
1	N	177	VAL
1	N	179	ASP
1	N	183	LEU
1	N	190	VAL
1	N	194	GLN
1	N	196	ASP
1	N	204	PHE
1	N	230	ILE
1	N	237	LEU
1	N	277	LYS
1	N	289	LEU
1	N	304	GLU
1	N	313	THR
1	N	314	LEU
1	N	319	GLN
1	N	329	THR
1	N	330	THR
1	N	348	GLN
1	N	357	THR
1	N	372	LEU
1	N	387	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	420	ILE
1	N	463	SER
2	O	28	THR
2	O	59	VAL
2	O	64	ILE
2	P	20	LYS
2	P	25	ILE
2	P	54	VAL
2	P	57	LEU
2	P	60	LYS
2	Q	1	MET
2	Q	3	ILE
2	Q	4	ARG
2	Q	6	LEU
2	Q	12	VAL
2	Q	13	LYS
2	Q	26	VAL
2	Q	28	THR
2	Q	37	ARG
2	Q	59	VAL
2	Q	64	ILE
2	Q	66	ILE
2	R	18	GLU
2	R	25	ILE
2	R	28	THR
2	R	48	ILE
2	R	57	LEU
2	R	64	ILE
2	R	80	ASN
2	S	3	ILE
2	S	10	VAL
2	S	11	ILE
2	S	20	LYS
2	S	25	ILE
2	S	59	VAL
2	S	64	ILE
2	S	67	PHE
2	S	77	LYS
2	T	4	ARG
2	T	16	GLU
2	T	19	THR
2	T	27	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	28	THR
2	T	49	LEU
2	T	59	VAL
2	T	64	ILE
2	T	67	PHE
2	T	95	VAL
2	U	6	LEU
2	U	8	ASP
2	U	12	VAL
2	U	15	LYS
2	U	17	VAL
2	U	20	LYS
2	U	26	VAL
2	U	36	THR
2	U	57	LEU
2	U	59	VAL
2	U	80	ASN
2	U	81	GLU
2	V	3	ILE
2	V	6	LEU
2	V	8	ASP
2	V	14	ARG
2	V	16	GLU
2	V	25	ILE
2	V	27	LEU
2	V	28	THR
2	V	54	VAL
2	V	57	LEU
2	V	60	LYS
2	V	67	PHE
2	V	85	ILE
2	W	3	ILE
2	W	8	ASP
2	W	11	ILE
2	W	20	LYS
2	W	27	LEU
2	W	57	LEU
2	W	64	ILE
2	W	66	ILE
2	W	88	GLU
2	X	11	ILE
2	X	17	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	19	THR
2	X	20	LYS
2	X	27	LEU
2	X	28	THR
2	X	66	ILE
2	X	85	ILE
2	X	95	VAL
2	Y	1	MET
2	Y	9	ARG
2	Y	11	ILE
2	Y	12	VAL
2	Y	20	LYS
2	Y	25	ILE
2	Y	26	VAL
2	Y	28	THR
2	Y	54	VAL
2	Y	57	LEU
2	Y	59	VAL
2	Y	71	TYR
2	Y	95	VAL
2	Z	28	THR
2	Z	43	VAL
2	Z	57	LEU
2	Z	64	ILE
2	Z	82	GLU
2	a	26	VAL
2	a	28	THR
2	a	59	VAL
2	a	67	PHE
2	b	6	LEU
2	b	8	ASP
2	b	25	ILE
2	b	34	LYS
2	b	50	GLU
2	b	59	VAL
2	b	64	ILE
2	b	67	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	10	ASN
1	D	290	GLN
1	F	206	ASN
1	F	326	ASN
1	F	479	ASN
1	G	10	ASN
1	H	10	ASN
1	H	505	GLN
1	I	343	GLN
1	I	432	GLN
1	J	352	GLN
1	K	206	ASN
2	R	51	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 28 are monoatomic - leaving 14 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	$\# Z > 2$
3	ATP	A	601	5,4	24,33,33	0.96	1 (4%)	31,52,52	1.85	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	601	5,4	24,33,33	0.97	1 (4%)	31,52,52	1.81	5 (16%)
3	ATP	C	601	5,4	24,33,33	0.96	1 (4%)	31,52,52	1.89	5 (16%)
3	ATP	D	601	5,4	24,33,33	0.93	1 (4%)	31,52,52	1.91	5 (16%)
3	ATP	E	601	5,4	24,33,33	0.96	1 (4%)	31,52,52	1.99	5 (16%)
3	ATP	F	601	5,4	24,33,33	0.94	1 (4%)	31,52,52	1.85	5 (16%)
3	ATP	G	601	5,4	24,33,33	0.93	1 (4%)	31,52,52	1.96	6 (19%)
3	ATP	H	601	5,4	24,33,33	0.97	1 (4%)	31,52,52	1.81	5 (16%)
3	ATP	I	601	5,4	24,33,33	0.96	1 (4%)	31,52,52	1.89	5 (16%)
3	ATP	J	601	5,4	24,33,33	0.98	1 (4%)	31,52,52	2.00	5 (16%)
3	ATP	K	601	5,4	24,33,33	0.94	1 (4%)	31,52,52	1.89	5 (16%)
3	ATP	L	601	5,4	24,33,33	0.94	1 (4%)	31,52,52	1.98	6 (19%)
3	ATP	M	601	5,4	24,33,33	0.94	1 (4%)	31,52,52	1.90	6 (19%)
3	ATP	N	601	5,4	24,33,33	0.95	1 (4%)	31,52,52	1.84	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	B	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	C	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	D	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	E	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	F	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	G	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	H	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	I	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	J	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	K	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	L	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	M	601	5,4	-	0/18/38/38	0/3/3/3
3	ATP	N	601	5,4	-	0/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	ATP	C5-C4	2.97	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	601	ATP	C5-C4	2.99	1.47	1.40
3	F	601	ATP	C5-C4	3.02	1.47	1.40
3	E	601	ATP	C5-C4	3.02	1.47	1.40
3	G	601	ATP	C5-C4	3.04	1.47	1.40
3	K	601	ATP	C5-C4	3.05	1.47	1.40
3	L	601	ATP	C5-C4	3.06	1.47	1.40
3	H	601	ATP	C5-C4	3.09	1.47	1.40
3	N	601	ATP	C5-C4	3.09	1.47	1.40
3	A	601	ATP	C5-C4	3.10	1.47	1.40
3	C	601	ATP	C5-C4	3.12	1.47	1.40
3	B	601	ATP	C5-C4	3.12	1.47	1.40
3	I	601	ATP	C5-C4	3.14	1.47	1.40
3	J	601	ATP	C5-C4	3.21	1.47	1.40

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	ATP	N3-C2-N1	-7.02	123.52	128.89
3	L	601	ATP	N3-C2-N1	-6.96	123.57	128.89
3	M	601	ATP	N3-C2-N1	-6.88	123.62	128.89
3	E	601	ATP	N3-C2-N1	-6.85	123.65	128.89
3	K	601	ATP	N3-C2-N1	-6.68	123.78	128.89
3	B	601	ATP	N3-C2-N1	-6.66	123.79	128.89
3	I	601	ATP	N3-C2-N1	-6.65	123.80	128.89
3	J	601	ATP	N3-C2-N1	-6.65	123.81	128.89
3	C	601	ATP	N3-C2-N1	-6.63	123.82	128.89
3	G	601	ATP	N3-C2-N1	-6.61	123.83	128.89
3	F	601	ATP	N3-C2-N1	-6.51	123.91	128.89
3	N	601	ATP	N3-C2-N1	-6.51	123.91	128.89
3	A	601	ATP	N3-C2-N1	-6.47	123.94	128.89
3	H	601	ATP	N3-C2-N1	-6.45	123.96	128.89
3	J	601	ATP	C2'-C1'-N9	-4.21	107.86	114.29
3	E	601	ATP	PA-O3A-PB	-4.20	120.94	132.73
3	G	601	ATP	PA-O3A-PB	-4.08	121.26	132.73
3	C	601	ATP	PA-O3A-PB	-4.02	121.45	132.73
3	J	601	ATP	PA-O3A-PB	-4.02	121.45	132.73
3	L	601	ATP	PA-O3A-PB	-3.92	121.73	132.73
3	D	601	ATP	PB-O3B-PG	-3.89	119.62	132.67
3	G	601	ATP	C2'-C1'-N9	-3.84	108.42	114.29
3	A	601	ATP	PA-O3A-PB	-3.74	122.22	132.73
3	F	601	ATP	PA-O3A-PB	-3.72	122.29	132.73
3	I	601	ATP	PA-O3A-PB	-3.71	122.31	132.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	601	ATP	PB-O3B-PG	-3.66	120.39	132.67
3	I	601	ATP	PB-O3B-PG	-3.66	120.41	132.67
3	B	601	ATP	PA-O3A-PB	-3.66	122.47	132.73
3	L	601	ATP	PB-O3B-PG	-3.65	120.43	132.67
3	K	601	ATP	PB-O3B-PG	-3.63	120.49	132.67
3	M	601	ATP	PA-O3A-PB	-3.63	122.54	132.73
3	K	601	ATP	PA-O3A-PB	-3.58	122.69	132.73
3	J	601	ATP	PB-O3B-PG	-3.56	120.72	132.67
3	E	601	ATP	PB-O3B-PG	-3.51	120.90	132.67
3	M	601	ATP	PB-O3B-PG	-3.45	121.09	132.67
3	H	601	ATP	PB-O3B-PG	-3.39	121.31	132.67
3	H	601	ATP	PA-O3A-PB	-3.37	123.27	132.73
3	K	601	ATP	C4-C5-N7	-3.37	106.38	109.48
3	G	601	ATP	PB-O3B-PG	-3.34	121.46	132.67
3	D	601	ATP	C4-C5-N7	-3.27	106.47	109.48
3	N	601	ATP	C4-C5-N7	-3.27	106.47	109.48
3	C	601	ATP	PB-O3B-PG	-3.25	121.76	132.67
3	D	601	ATP	PA-O3A-PB	-3.24	123.62	132.73
3	H	601	ATP	C4-C5-N7	-3.24	106.50	109.48
3	M	601	ATP	C4-C5-N7	-3.22	106.52	109.48
3	L	601	ATP	C2'-C1'-N9	-3.22	109.37	114.29
3	N	601	ATP	PA-O3A-PB	-3.19	123.78	132.73
3	A	601	ATP	C4-C5-N7	-3.18	106.55	109.48
3	F	601	ATP	PB-O3B-PG	-3.17	122.03	132.67
3	E	601	ATP	C4-C5-N7	-3.12	106.61	109.48
3	C	601	ATP	C4-C5-N7	-3.12	106.61	109.48
3	L	601	ATP	C4-C5-N7	-3.10	106.63	109.48
3	I	601	ATP	C4-C5-N7	-3.04	106.68	109.48
3	A	601	ATP	PB-O3B-PG	-3.03	122.51	132.67
3	E	601	ATP	C2'-C1'-N9	-3.03	109.67	114.29
3	G	601	ATP	C4-C5-N7	-3.00	106.72	109.48
3	B	601	ATP	C4-C5-N7	-2.98	106.74	109.48
3	J	601	ATP	C4-C5-N7	-2.88	106.83	109.48
3	F	601	ATP	C4-C5-N7	-2.88	106.83	109.48
3	F	601	ATP	C2'-C1'-N9	-2.77	110.05	114.29
3	A	601	ATP	C2'-C1'-N9	-2.72	110.14	114.29
3	C	601	ATP	C2'-C1'-N9	-2.70	110.16	114.29
3	B	601	ATP	PB-O3B-PG	-2.66	123.74	132.67
3	K	601	ATP	C2'-C1'-N9	-2.51	110.45	114.29
3	N	601	ATP	C2'-C1'-N9	-2.47	110.52	114.29
3	H	601	ATP	C2'-C1'-N9	-2.25	110.85	114.29
3	I	601	ATP	C2'-C1'-N9	-2.20	110.93	114.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	601	ATP	C2'-C1'-N9	-2.13	111.03	114.29
3	B	601	ATP	C2'-C1'-N9	-2.00	111.23	114.29
3	D	601	ATP	O3G-PG-O2G	2.00	115.01	107.38
3	G	601	ATP	O3G-PG-O2G	2.01	115.04	107.38
3	L	601	ATP	O3G-PG-O2G	2.02	115.06	107.38
3	M	601	ATP	O3G-PG-O2G	2.17	115.65	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ATP	1	0
3	B	601	ATP	3	0
3	D	601	ATP	1	0
3	F	601	ATP	1	0
3	G	601	ATP	1	0
3	H	601	ATP	1	0
3	I	601	ATP	4	0
3	J	601	ATP	1	0
3	K	601	ATP	1	0
3	L	601	ATP	1	0
3	N	601	ATP	1	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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/548 (95%)	-0.22	9 (1%) 73 58	68, 134, 281, 335	0
1	B	524/548 (95%)	-0.23	6 (1%) 82 69	71, 134, 286, 336	0
1	C	524/548 (95%)	-0.29	7 (1%) 79 65	65, 132, 275, 331	0
1	D	524/548 (95%)	-0.30	8 (1%) 76 62	68, 130, 277, 327	0
1	E	524/548 (95%)	-0.29	4 (0%) 87 77	65, 133, 275, 330	0
1	F	524/548 (95%)	-0.35	6 (1%) 82 69	67, 133, 274, 324	0
1	G	524/548 (95%)	-0.25	8 (1%) 76 62	68, 135, 282, 344	0
1	H	524/548 (95%)	-0.23	7 (1%) 79 65	64, 134, 288, 342	0
1	I	524/548 (95%)	-0.20	8 (1%) 76 62	66, 135, 292, 349	0
1	J	524/548 (95%)	-0.31	6 (1%) 82 69	66, 132, 274, 332	0
1	K	524/548 (95%)	-0.30	6 (1%) 82 69	64, 130, 275, 326	0
1	L	524/548 (95%)	-0.29	6 (1%) 82 69	69, 132, 276, 328	0
1	M	524/548 (95%)	-0.33	4 (0%) 87 77	63, 134, 276, 334	0
1	N	524/548 (95%)	-0.25	8 (1%) 76 62	73, 132, 297, 355	0
2	O	97/97 (100%)	0.31	9 (9%) 11 7	183, 233, 312, 338	0
2	P	97/97 (100%)	0.17	1 (1%) 84 72	189, 233, 313, 346	0
2	Q	97/97 (100%)	0.94	14 (14%) 3 3	194, 240, 324, 352	0
2	R	97/97 (100%)	0.76	16 (16%) 2 2	205, 243, 313, 341	0
2	S	97/97 (100%)	0.71	14 (14%) 3 3	207, 246, 314, 354	0
2	T	97/97 (100%)	1.15	22 (22%) 1 1	205, 244, 315, 346	0
2	U	97/97 (100%)	0.77	10 (10%) 9 6	188, 234, 314, 348	0
2	V	97/97 (100%)	0.33	7 (7%) 18 11	190, 236, 312, 348	0
2	W	97/97 (100%)	0.25	1 (1%) 84 72	195, 237, 315, 347	0
2	X	97/97 (100%)	0.79	13 (13%) 4 4	186, 232, 316, 346	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
2	Y	97/97 (100%)	0.98	19 (19%)	1 1	191, 232, 313, 344	0
2	Z	97/97 (100%)	0.61	10 (10%)	9 6	197, 236, 316, 355	0
2	a	97/97 (100%)	0.80	13 (13%)	4 4	189, 233, 316, 342	0
2	b	97/97 (100%)	0.80	13 (13%)	4 4	193, 237, 315, 344	0
All	All	8694/9030 (96%)	-0.13	255 (2%)	55 38	63, 157, 291, 355	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	32	ALA	9.3
2	Z	31	ALA	8.4
2	X	32	ALA	7.9
2	Y	32	ALA	7.5
2	R	32	ALA	7.5
1	G	339	GLU	7.2
2	X	97	ALA	5.6
2	Y	31	ALA	5.5
2	T	32	ALA	5.3
1	M	211	GLY	5.3
2	S	25	ILE	5.2
1	J	373	ALA	5.2
2	T	3	ILE	5.0
2	X	1	MET	4.9
1	N	339	GLU	4.7
2	R	1	MET	4.7
1	E	231	ARG	4.7
2	T	25	ILE	4.7
1	F	211	GLY	4.6
2	R	31	ALA	4.6
2	T	93	ALA	4.5
2	O	1	MET	4.4
2	Y	3	ILE	4.4
2	T	97	ALA	4.3
2	U	31	ALA	4.2
2	V	1	MET	4.1
2	Y	86	MET	4.0
2	Q	97	ALA	4.0
2	V	32	ALA	4.0
2	Z	33	ALA	3.9
1	N	343	GLN	3.8
2	b	48	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	78	ILE	3.7
1	N	374	GLY	3.7
1	N	373	ALA	3.7
2	a	32	ALA	3.7
1	E	208	PRO	3.7
2	S	33	ALA	3.7
2	Q	32	ALA	3.6
2	R	33	ALA	3.6
2	b	76	GLU	3.6
2	Q	34	LYS	3.6
2	Q	31	ALA	3.6
2	U	97	ALA	3.6
1	C	275	ALA	3.5
2	X	33	ALA	3.5
1	C	373	ALA	3.4
2	S	93	ALA	3.4
2	Q	37	ARG	3.4
2	T	47	ARG	3.4
1	I	245	LYS	3.4
2	P	53	GLU	3.3
2	Q	33	ALA	3.3
1	C	274	ALA	3.3
2	S	92	LEU	3.3
2	Y	85	ILE	3.2
1	N	251	ALA	3.2
1	H	223	ALA	3.1
1	H	322	ARG	3.1
1	J	374	GLY	3.1
2	b	3	ILE	3.1
2	Y	27	LEU	3.1
2	a	93	ALA	3.0
2	b	2	ASN	3.0
2	Q	68	ASN	3.0
2	U	50	GLU	3.0
1	J	357	THR	3.0
1	L	211	GLY	3.0
2	R	78	ILE	3.0
1	I	223	ALA	3.0
2	V	28	THR	3.0
1	B	272	LYS	3.0
1	E	203	TYR	3.0
2	a	94	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Y	34	LYS	2.9
2	b	1	MET	2.9
2	X	31	ALA	2.9
2	Z	29	GLY	2.9
2	a	25	ILE	2.9
2	T	59	VAL	2.9
2	O	54	VAL	2.9
2	R	90	ASP	2.9
2	Y	75	SER	2.9
2	Y	11	ILE	2.9
2	Y	97	ALA	2.8
1	A	268	ARG	2.8
1	A	351	GLN	2.8
1	J	207	LYS	2.8
2	T	50	GLU	2.7
2	Y	53	GLU	2.7
2	T	92	LEU	2.7
2	X	54	VAL	2.7
1	F	375	GLY	2.7
2	b	21	SER	2.7
2	T	94	ILE	2.7
2	T	29	GLY	2.7
2	V	25	ILE	2.7
1	B	375	GLY	2.7
1	D	208	PRO	2.6
2	Z	17	VAL	2.6
2	b	97	ALA	2.6
2	X	43	VAL	2.6
2	X	96	GLU	2.6
2	Z	18	GLU	2.6
1	D	272	LYS	2.6
2	Q	51	ASN	2.6
2	R	48	ILE	2.6
1	K	307	MET	2.6
2	Y	6	LEU	2.6
2	T	37	ARG	2.6
1	C	306	GLY	2.6
1	G	338	GLU	2.6
1	M	207	LYS	2.6
1	D	207	LYS	2.6
2	Z	28	THR	2.6
1	I	375	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	211	GLY	2.5
1	F	373	ALA	2.5
1	N	355	GLU	2.5
1	D	306	GLY	2.5
1	A	231	ARG	2.5
1	G	343	GLN	2.5
2	U	3	ILE	2.5
1	H	216	GLU	2.5
2	T	65	VAL	2.5
1	D	211	GLY	2.5
1	F	207	LYS	2.5
2	O	29	GLY	2.5
1	M	375	GLY	2.5
2	U	41	LEU	2.5
2	X	11	ILE	2.5
1	B	275	ALA	2.5
2	V	54	VAL	2.5
2	Y	10	VAL	2.5
2	W	24	GLY	2.5
2	V	42	ALA	2.5
2	S	32	ALA	2.4
2	a	18	GLU	2.4
2	X	17	VAL	2.4
2	a	33	ALA	2.4
2	Y	48	ILE	2.4
2	U	21	SER	2.4
1	I	208	PRO	2.4
2	V	19	THR	2.4
2	T	66	ILE	2.4
2	S	38	GLY	2.4
2	S	24	GLY	2.4
1	B	333	ILE	2.4
1	K	271	VAL	2.4
2	Q	6	LEU	2.4
2	T	41	LEU	2.4
2	Y	49	LEU	2.4
1	D	307	MET	2.3
1	L	275	ALA	2.3
2	Q	49	LEU	2.3
2	R	3	ILE	2.3
1	C	208	PRO	2.3
1	K	272	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	S	50	GLU	2.3
1	H	246	PRO	2.3
1	I	246	PRO	2.3
2	T	96	GLU	2.3
1	J	260	ALA	2.3
2	R	47	ARG	2.3
2	R	2	ASN	2.3
2	R	75	SER	2.3
2	T	85	ILE	2.3
1	B	373	ALA	2.3
2	Q	13	LYS	2.3
2	Q	95	VAL	2.3
2	S	30	SER	2.3
2	a	31	ALA	2.3
2	T	28	THR	2.3
2	Z	34	LYS	2.3
2	Z	30	SER	2.3
2	S	28	THR	2.3
2	S	53	GLU	2.3
1	H	211	GLY	2.3
1	B	215	LEU	2.2
1	L	251	ALA	2.2
1	K	275	ALA	2.2
2	S	66	ILE	2.2
1	D	245	LYS	2.2
1	C	374	GLY	2.2
2	U	2	ASN	2.2
2	R	84	LEU	2.2
2	X	42	ALA	2.2
1	K	306	GLY	2.2
1	L	207	LYS	2.2
1	L	373	ALA	2.2
2	O	18	GLU	2.2
2	Q	63	ASP	2.2
2	Y	41	LEU	2.2
1	I	219	PHE	2.2
1	G	373	ALA	2.2
2	U	42	ALA	2.2
2	a	17	VAL	2.2
2	O	30	SER	2.2
1	N	246	PRO	2.2
2	S	31	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	325	ILE	2.2
2	T	64	ILE	2.2
2	O	19	THR	2.2
1	A	247	LEU	2.2
2	O	27	LEU	2.2
2	S	91	ILE	2.2
2	R	67	PHE	2.2
2	a	95	VAL	2.2
2	R	68	ASN	2.1
2	a	34	LYS	2.1
1	A	273	VAL	2.1
1	H	245	LYS	2.1
2	Q	28	THR	2.1
2	R	11	ILE	2.1
2	T	55	LYS	2.1
1	I	241	ALA	2.1
1	N	245	LYS	2.1
1	I	315	GLU	2.1
2	Z	11	ILE	2.1
2	U	5	PRO	2.1
1	J	339	GLU	2.1
1	L	276	VAL	2.1
1	C	259	LEU	2.1
2	O	6	LEU	2.1
2	b	49	LEU	2.1
1	A	204	PHE	2.1
1	D	210	THR	2.1
2	b	6	LEU	2.1
1	G	207	LYS	2.1
1	F	212	ALA	2.1
2	b	41	LEU	2.1
2	T	95	VAL	2.1
1	G	251	ALA	2.1
2	U	11	ILE	2.1
2	b	83	VAL	2.1
2	T	31	ALA	2.1
2	a	97	ALA	2.1
2	Y	39	GLU	2.1
1	E	256	GLY	2.1
2	a	37	ARG	2.0
2	O	25	ILE	2.0
2	Y	13	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Y	80	ASN	2.0
1	H	247	LEU	2.0
2	a	92	LEU	2.0
1	G	278	ALA	2.0
1	M	373	ALA	2.0
1	A	221	LEU	2.0
1	G	351	GLN	2.0
2	X	94	ILE	2.0
2	b	33	ALA	2.0
2	R	27	LEU	2.0
2	X	13	LYS	2.0
1	A	338	GLU	2.0
1	F	210	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	K	M	603	1/1	0.92	0.20	1.00	192,192,192,192	0
3	ATP	I	601	31/31	0.96	0.20	0.51	58,120,159,197	0
3	ATP	A	601	31/31	0.95	0.23	0.42	74,112,169,195	0
3	ATP	C	601	31/31	0.94	0.22	0.39	65,116,176,192	0
5	K	I	603	1/1	0.89	0.20	0.39	138,138,138,138	0
3	ATP	N	601	31/31	0.95	0.23	0.37	75,110,162,207	0
3	ATP	J	601	31/31	0.95	0.20	0.34	76,112,176,190	0
3	ATP	E	601	31/31	0.94	0.23	0.33	61,95,148,174	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ATP	H	601	31/31	0.94	0.23	0.22	67,95,170,203	0
5	K	F	603	1/1	0.94	0.19	0.13	132,132,132,132	0
3	ATP	K	601	31/31	0.96	0.20	0.12	55,109,148,207	0
3	ATP	B	601	31/31	0.94	0.20	0.02	70,113,189,206	0
3	ATP	D	601	31/31	0.97	0.20	0.02	67,95,205,263	0
3	ATP	F	601	31/31	0.97	0.19	-0.01	76,101,160,203	0
3	ATP	M	601	31/31	0.97	0.17	-0.07	71,98,158,206	0
3	ATP	G	601	31/31	0.96	0.20	-0.11	68,99,162,188	0
3	ATP	L	601	31/31	0.96	0.20	-0.13	66,97,157,198	0
5	K	A	603	1/1	0.86	0.20	-0.35	200,200,200,200	0
5	K	D	603	1/1	0.88	0.14	-1.59	139,139,139,139	0
5	K	H	603	1/1	0.99	0.14	-3.04	168,168,168,168	0
4	MG	A	602	1/1	0.96	0.24	-	76,76,76,76	0
4	MG	M	602	1/1	1.00	0.19	-	81,81,81,81	0
5	K	G	603	1/1	0.95	0.25	-	197,197,197,197	0
4	MG	D	602	1/1	0.99	0.17	-	87,87,87,87	0
4	MG	C	602	1/1	0.97	0.25	-	71,71,71,71	0
4	MG	F	602	1/1	1.00	0.20	-	77,77,77,77	0
4	MG	E	602	1/1	0.99	0.26	-	94,94,94,94	0
4	MG	B	602	1/1	0.98	0.27	-	68,68,68,68	0
5	K	E	603	1/1	0.72	0.21	-	140,140,140,140	0
4	MG	L	602	1/1	0.98	0.20	-	87,87,87,87	0
4	MG	H	602	1/1	0.97	0.32	-	74,74,74,74	0
4	MG	J	602	1/1	0.99	0.24	-	112,112,112,112	0
5	K	K	603	1/1	0.93	0.17	-	149,149,149,149	0
5	K	J	603	1/1	0.98	0.23	-	251,251,251,251	0
4	MG	N	602	1/1	0.98	0.21	-	103,103,103,103	0
5	K	L	603	1/1	0.93	0.25	-	185,185,185,185	0
5	K	N	603	1/1	0.96	0.24	-	165,165,165,165	0
5	K	B	603	1/1	0.97	0.19	-	200,200,200,200	0
4	MG	K	602	1/1	1.00	0.21	-	71,71,71,71	0
4	MG	I	602	1/1	0.98	0.26	-	106,106,106,106	0
5	K	C	603	1/1	0.92	0.34	-	291,291,291,291	0
4	MG	G	602	1/1	0.99	0.24	-	88,88,88,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.