



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 03:05 am GMT

PDB ID : 5B04
Title : Crystal structure of the eukaryotic translation initiation factor 2B from *Schizosaccharomyces pombe*
Authors : Kashiwagi, K.; Ito, T.; Yokoyama, S.
Deposited on : 2015-10-27
Resolution : 2.99 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

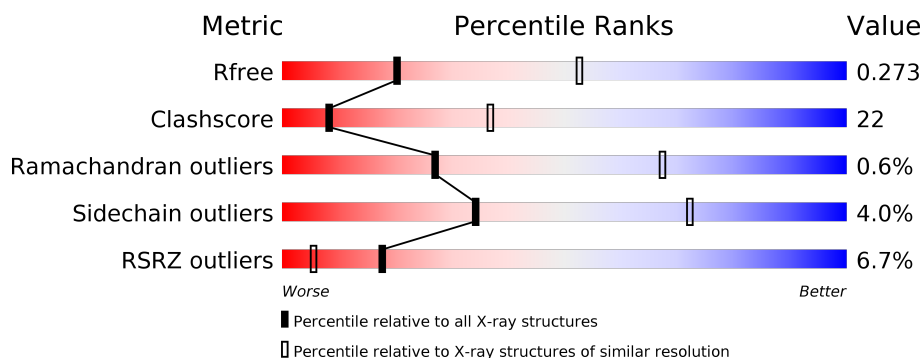
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	341	<div> <div>9%</div> <div> <div></div> <div>59%</div> <div>29%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	341	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>•</div> <div>6%</div> </div> </div>
2	C	399	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>
2	D	399	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>13%</div> </div> </div>
3	E	458	<div> <div>9%</div> <div> <div></div> <div>45%</div> <div>30%</div> <div>7%</div> <div>•</div> <div>16%</div> </div> </div>
3	F	458	<div> <div>12%</div> <div> <div></div> <div>38%</div> <div>36%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	467	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>58%</div><div>15%</div><div>•</div><div>25%</div></div></div>
4	H	467	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>62%</div><div>12%</div><div>•</div><div>25%</div></div></div>
5	I	678	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>47%</div><div>13%</div><div>••</div><div>37%</div></div></div>
5	J	678	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>44%</div><div>17%</div><div>•</div><div>37%</div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28584 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2472	1571	430	458	13			
1	B	319	Total	C	N	O	S	0	0	0
			2489	1582	434	460	13			

- Molecule 2 is a protein called Probable translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	349	Total	C	N	O	S	0	0	0
			2702	1714	459	515	14			
2	D	346	Total	C	N	O	S	0	0	0
			2674	1697	453	511	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q9UT76
C	-4	PRO	-	expression tag	UNP Q9UT76
C	-3	ILE	-	expression tag	UNP Q9UT76
C	-2	SER	-	expression tag	UNP Q9UT76
C	-1	GLU	-	expression tag	UNP Q9UT76
C	0	PHE	-	expression tag	UNP Q9UT76
D	-5	GLY	-	expression tag	UNP Q9UT76
D	-4	PRO	-	expression tag	UNP Q9UT76
D	-3	ILE	-	expression tag	UNP Q9UT76
D	-2	SER	-	expression tag	UNP Q9UT76
D	-1	GLU	-	expression tag	UNP Q9UT76
D	0	PHE	-	expression tag	UNP Q9UT76

- Molecule 3 is a protein called Probable translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	384	Total	C	N	O	S	0	0	0
			2976	1895	511	553	17			
3	F	383	Total	C	N	O	S	0	0	0
			2967	1890	509	551	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	157	TYR	ILE	engineered mutation	UNP P56288
E	158	THR	TYR	engineered mutation	UNP P56288
E	159	VAL	GLY	engineered mutation	UNP P56288
F	157	TYR	ILE	engineered mutation	UNP P56288
F	158	THR	TYR	engineered mutation	UNP P56288
F	159	VAL	GLY	engineered mutation	UNP P56288

- Molecule 4 is a protein called Probable translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			
4	H	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			

- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	428	Total	C	N	O	S	0	0	0
			3377	2123	592	647	15			
5	J	428	Total	C	N	O	S	0	0	0
			3372	2119	591	647	15			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

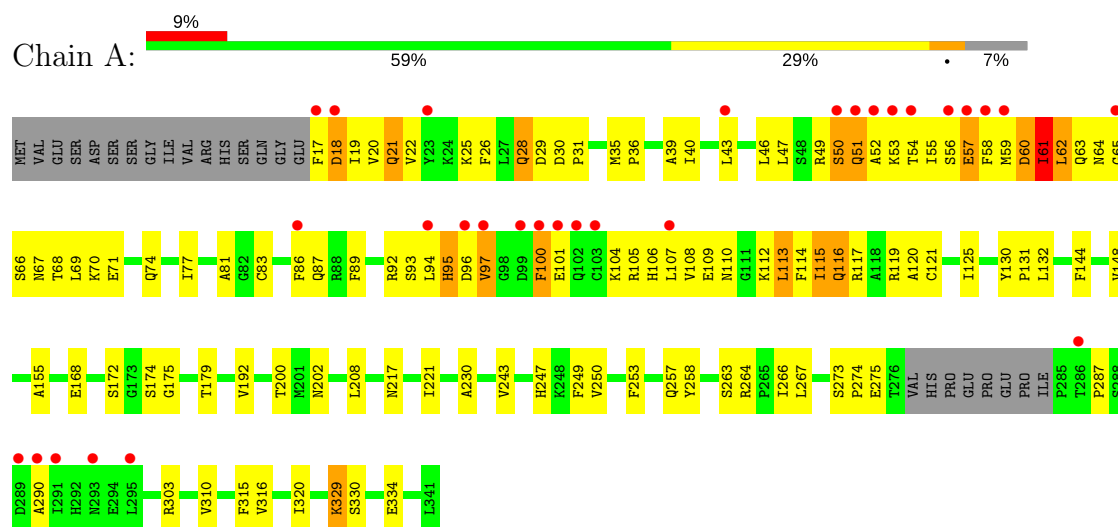


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		

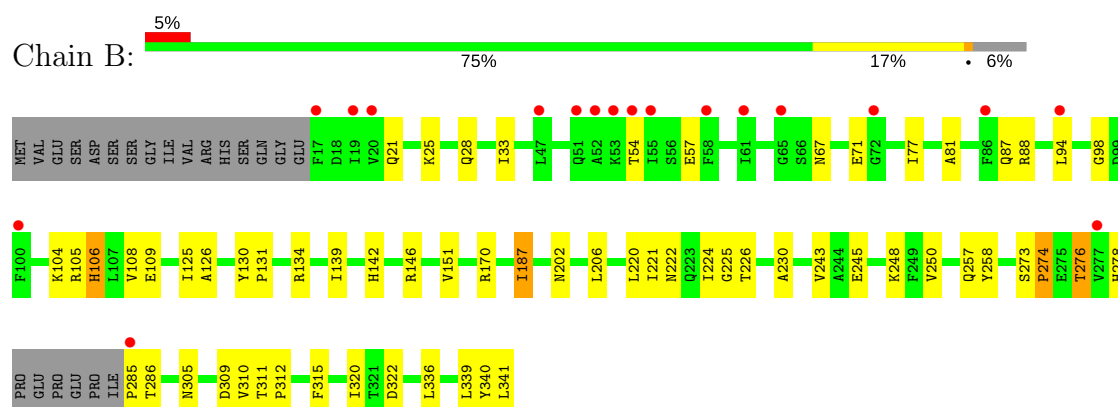
3 Residue-property plots

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

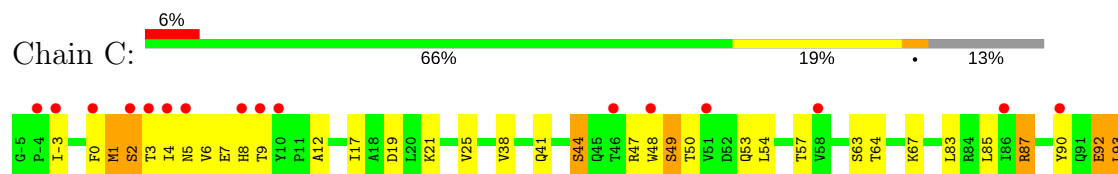
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

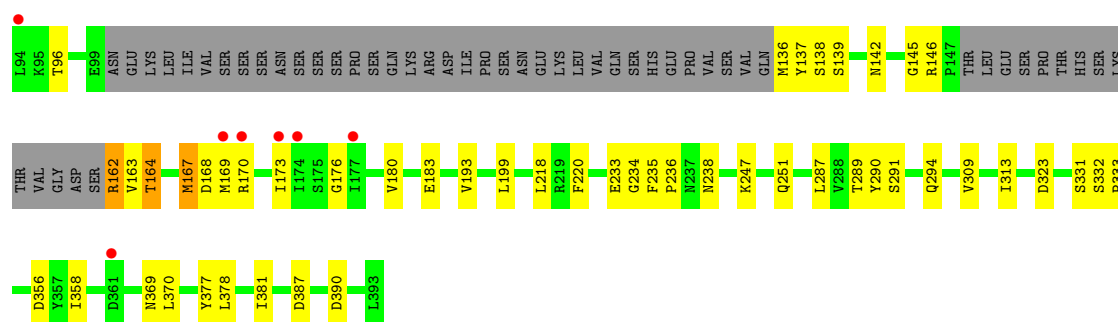


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

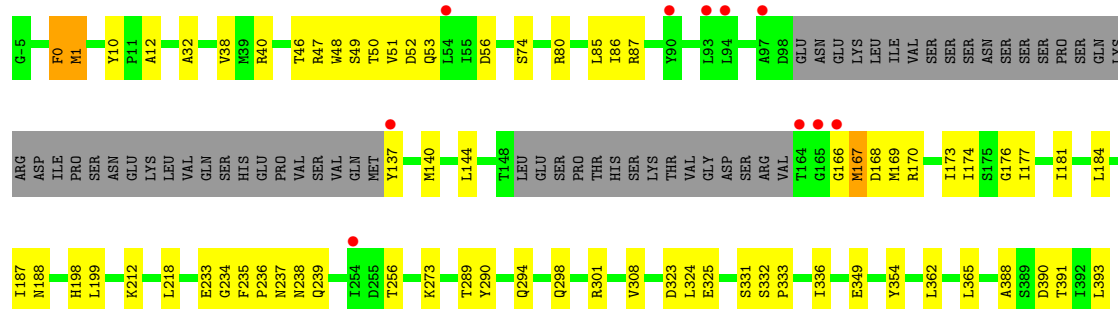


- Molecule 2: Probable translation initiation factor eIF-2B subunit beta

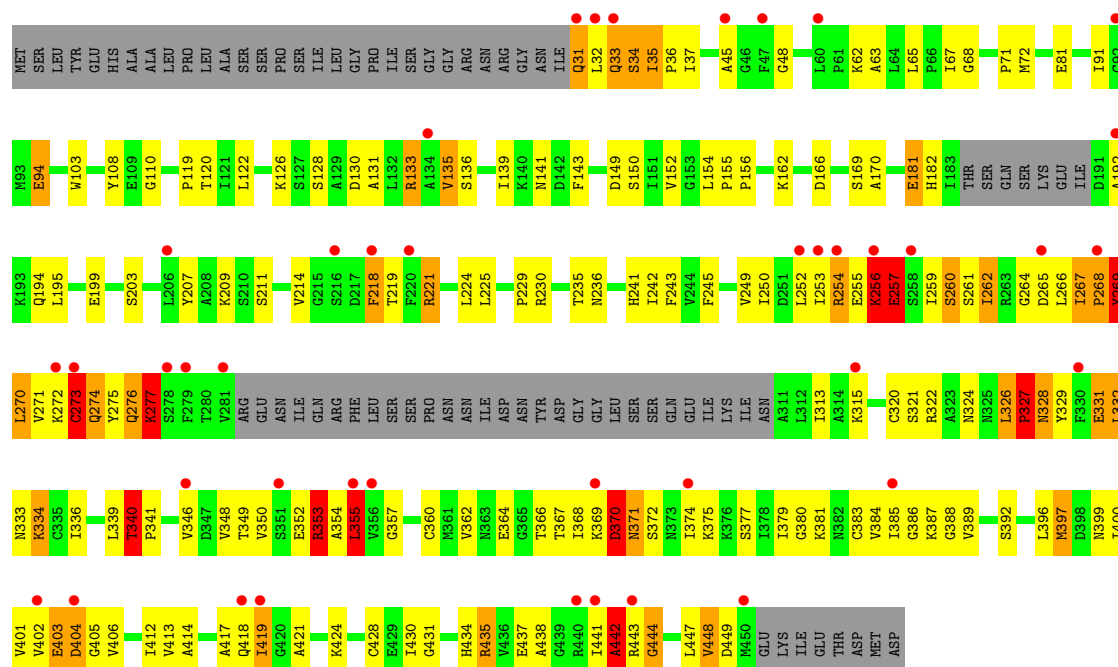
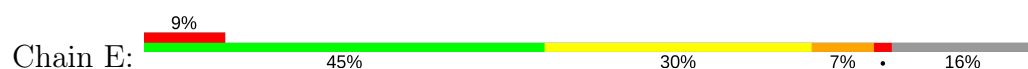




- Molecule 2: Probable translation initiation factor eIF-2B subunit beta

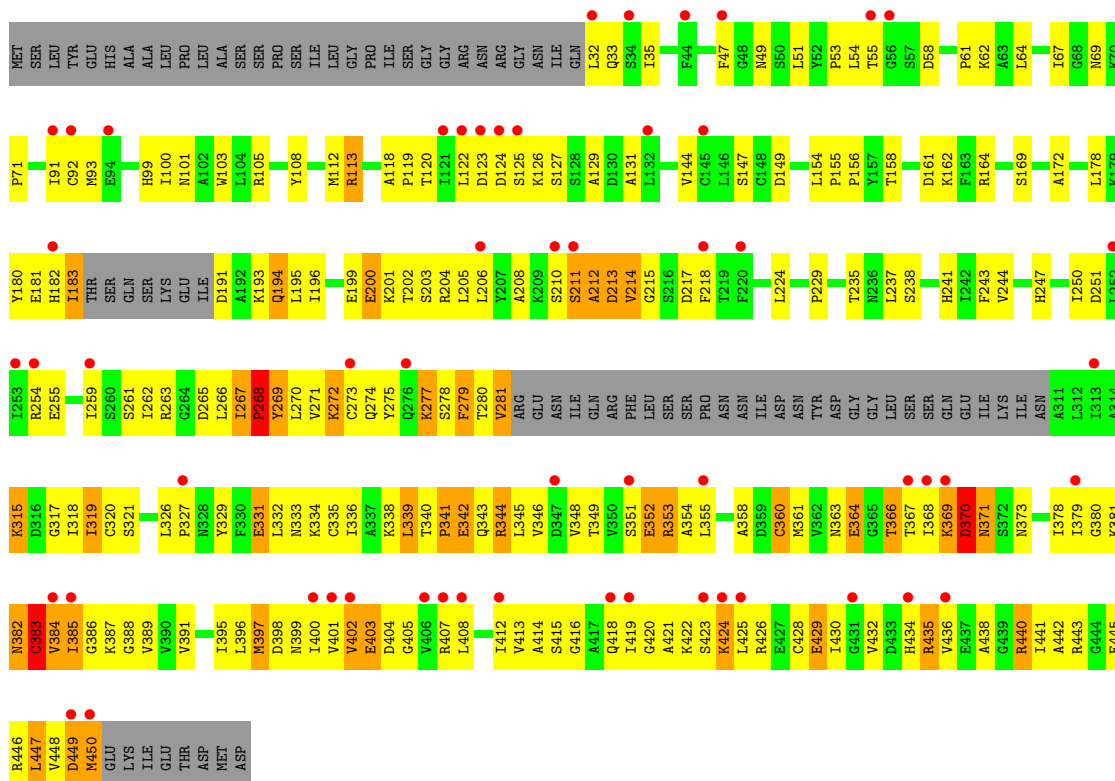


- Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

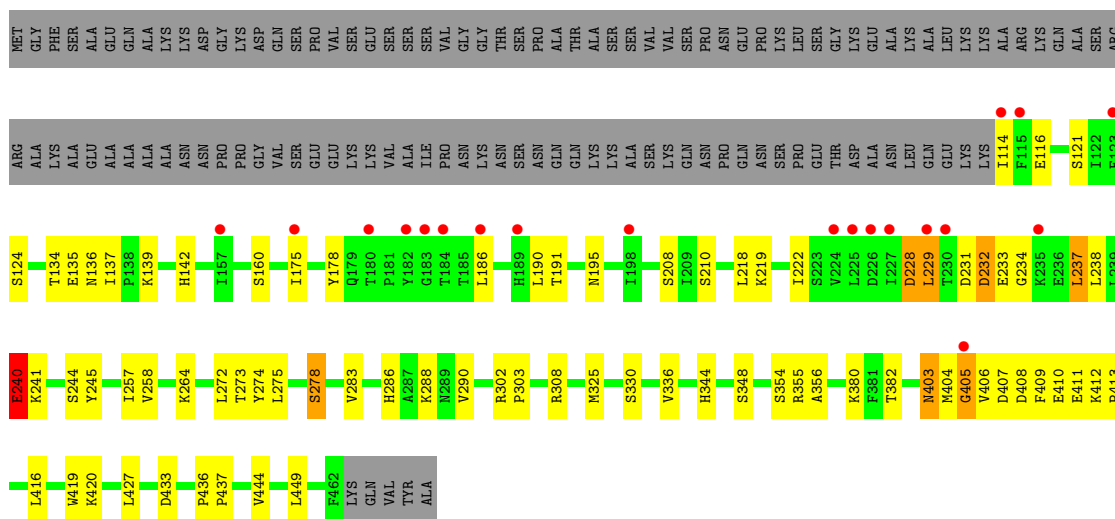


- Molecule 3: Probable translation initiation factor eIF-2B subunit gamma





- Molecule 4: Probable translation initiation factor eIF-2B subunit delta



- Molecule 4: Probable translation initiation factor eIF-2B subunit delta



GLU	ASN	PRO	GLY	SER	V388	N269
ASN	LYS	LYS	ASP	ASP	ASP	Y270
ALA	GLU	ALA	PHE	ASP	G391	R273
ILE	ALA	ILE	ASN	GLU	N392	V274
GLN	LEU	LEU	LYS	GLY	N393	
TRP	ALA	ALA	ALA	GLU	C394	K285
TYR	VAL	VAL	ALA	PHE	S395	
SER	MET	MET	GLN	MET	I396	R290
ASP	THR	THR	SER	ALA	E397	
PRO	ARG	PRO	LEU	SER	D398	Y293
ARG	TRP	TRP	GLU	GLY	G399	P294
SER	GLY	GLY	ARG	LEU	A400	
SER	PRO	PRO	ALA	ILE	I401	D298
GLU	LEU	LEU	PHE	GLU	V402	
GLU	LEU	LEU	GLU	SER	A403	
GLU	ALA	ALA	GLU	THR	V406	Q304
LEU	LYS	LYS	ASN	ASN	V407	T305
ALA	LEU	LEU	HIS	GLU	I408	Q309
ALA	THR	THR	GLN	LEU	G409	R310
ALA	PHE	PHE	ILE	HIS	D410	H311
ARG	ASP	ASP	ILE	LEU	N411	Q312
ALA	ASP	HIS	ILE	SER	I414	I313
ALA	GLU	GLU	ALA	ASP	E415	
GLY	GLU	GLN	ALA	SER	K416	E317
GLY	GLN	VAL	LEU	GLU	N417	
LYS	VAL	VAL	GLU	SER	K418	V320
GLN	ASP	ASN	LEU	SER	R419	L321
PHE	PHE	VAL	ASN	GLU	I420	A322
VAL	VAL	VAL	THR	THR		R323
ASP	ASP	LEU	LEU	SER	F423	S324
TRP	TRP	THR	ARG	SER	E424	C325
LEU	LEU	LEU	MET	SER	S425	I326
ASN	ASN	GLN	ALA	SER	H426	I327
ALA	ALA	LYS	MET	GLU	S427	K328
GLU	ALA	TYR	ASN	GLU	Q428	A329
SER	GLU	CYS	ALA	ASP	G429	R330
GLU	SER	VAL	ASN	MET	T430	
GLU	GLU	ARG	TYR	GLU	I431	V339
SER	SER	LEU	HIS	PHE	N432	A346
GLU	SER	THR	GLU	ILE	D433	
GLY	SER	MET	VAL	PRO	P434	I356
GLU	GLU	THR	ARG	PHE	S435	
SER	SER	ARG	SER	ALA	L436	
SER	HIS	HIS	ILE	ALA		I362
SER	PHE	PHE	ILE	ARG	W437	F366
GLU	LEU	LEU	VAL	ARG	G438	L367
GLN	LEU	GLN	LEU	ASP	I439	
LEU	LEU	LEU	ALA	SER	G440	
LEU	LEU	LEU	LEU	ALA	G441	G374
GLY	GLY	GLY	LEU	ASN	R442	
TYR	TYR	TYR	ARG	THR	G443	I379
PHE	PHE	TYR	ARG	ILE		G380
TYR	TYR	TYR	ILE	ASN		K381
GLN	GLN	GLN	MET	SER		A382
LEU	LEU	LEU	HIS	SER		I383
GLU	GLU	LEU	LEU	GLU		L384
ILE	ILE	ILE	ASP	ASP		A385
ALA	ALA	ALA	PHE	PHE		N386
VAL	VAL	VAL	VAL	GLU		
GLU	GLU	GLU	SER	GLU		S387

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	144.50Å 209.23Å 223.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.99 49.29 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.29-2.99) 99.6 (49.29-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.222 , 0.271 0.227 , 0.273	Depositor DCC
R_{free} test set	6815 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	0/2519	0.63	5/3409 (0.1%)
1	B	0.29	0/2537	0.48	2/3434 (0.1%)
2	C	0.31	0/2747	0.49	1/3726 (0.0%)
2	D	0.26	0/2719	0.46	2/3690 (0.1%)
3	E	0.57	2/3029 (0.1%)	0.91	21/4100 (0.5%)
3	F	0.51	3/3020 (0.1%)	1.08	30/4088 (0.7%)
4	G	0.38	1/2802 (0.0%)	0.58	3/3797 (0.1%)
4	H	0.27	0/2802	0.43	0/3797
5	I	0.46	1/3437 (0.0%)	0.77	14/4658 (0.3%)
5	J	0.45	2/3432 (0.1%)	0.63	5/4652 (0.1%)
All	All	0.40	9/29044 (0.0%)	0.69	83/39351 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	E	0	5
3	F	0	6
4	H	0	1
5	I	0	1
5	J	0	1
All	All	0	16

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	268	PRO	N-CD	-13.76	1.28	1.47
5	J	434	PRO	N-CD	-9.39	1.34	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	33	PRO	N-CD	8.86	1.60	1.47
5	I	434	PRO	N-CD	7.20	1.57	1.47
3	E	257	GLU	CG-CD	-6.17	1.42	1.51
3	F	382	ASN	CA-C	5.67	1.67	1.52
3	F	211	SER	CA-C	5.63	1.67	1.52
4	G	413	PRO	N-CD	5.42	1.55	1.47
3	F	268	PRO	N-CD	5.25	1.55	1.47

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	429	GLY	N-CA-C	16.66	154.74	113.10
3	F	370	ASP	N-CA-C	16.40	155.28	111.00
3	F	370	ASP	CB-CA-C	-15.86	78.69	110.40
5	I	432	ASN	CB-CA-C	-14.98	80.44	110.40
3	F	212	ALA	CB-CA-C	13.37	130.15	110.10
3	F	213	ASP	CB-CA-C	-12.36	85.68	110.40
3	F	213	ASP	N-CA-C	11.85	142.99	111.00
5	J	434	PRO	N-CA-CB	-11.58	89.41	103.30
3	F	384	VAL	N-CA-C	11.32	141.57	111.00
3	E	353	ARG	CB-CA-C	-11.28	87.84	110.40
5	I	431	LEU	N-CA-C	11.23	141.31	111.00
5	I	433	ASP	N-CA-CB	-10.64	91.44	110.60
3	F	371	ASN	N-CA-C	10.54	139.45	111.00
5	I	433	ASP	N-CA-C	10.26	138.70	111.00
3	F	212	ALA	N-CA-CB	9.87	123.92	110.10
1	A	95	HIS	CB-CA-C	9.40	129.21	110.40
5	I	432	ASN	N-CA-C	9.33	136.19	111.00
1	A	115	ILE	CB-CA-C	-9.32	92.95	111.60
3	F	383	CYS	N-CA-CB	9.08	126.95	110.60
3	F	211	SER	CB-CA-C	-8.72	93.53	110.10
5	J	434	PRO	N-CD-CG	-8.70	90.16	103.20
3	F	382	ASN	N-CA-C	8.53	134.02	111.00
3	E	435	ARG	CG-CD-NE	8.39	129.41	111.80
3	E	435	ARG	NE-CZ-NH1	8.30	124.45	120.30
3	E	435	ARG	N-CA-CB	-8.02	96.16	110.60
1	A	116	GLN	N-CA-CB	-7.89	96.39	110.60
3	E	355	LEU	CA-CB-CG	7.75	133.12	115.30
5	I	433	ASP	CB-CA-C	-7.34	95.71	110.40
3	F	385	ILE	N-CA-CB	7.31	127.62	110.80
3	E	403	GLU	CB-CA-C	6.89	124.18	110.40
3	F	364	GLU	N-CA-CB	-6.88	98.21	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLN	N-CA-C	6.71	129.12	111.00
3	F	382	ASN	CB-CA-C	-6.68	97.03	110.40
4	G	229	LEU	CA-CB-CG	6.62	130.53	115.30
4	G	405	GLY	N-CA-C	6.60	129.59	113.10
3	E	444	GLY	N-CA-C	6.47	129.26	113.10
3	E	370	ASP	N-CA-C	6.46	128.43	111.00
3	E	435	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	D	0	PHE	CB-CA-C	-6.36	97.68	110.40
3	F	194	GLN	N-CA-CB	-6.35	99.17	110.60
1	B	273	SER	C-N-CD	6.26	141.55	128.40
3	F	353	ARG	N-CA-C	-6.26	94.10	111.00
3	E	35	ILE	C-N-CD	6.23	141.49	128.40
3	F	210	SER	N-CA-C	-6.22	94.19	111.00
3	F	382	ASN	CA-C-O	6.16	133.03	120.10
3	E	257	GLU	N-CA-C	6.07	127.39	111.00
3	E	419	ILE	CB-CA-C	-6.04	99.52	111.60
3	F	449	ASP	N-CA-CB	-6.02	99.76	110.60
3	E	326	LEU	C-N-CD	6.01	141.02	128.40
3	F	382	ASN	CA-C-N	-5.95	104.11	117.20
3	F	118	ALA	C-N-CD	5.91	140.82	128.40
5	J	163	SER	C-N-CD	5.91	140.81	128.40
3	F	267	ILE	C-N-CD	5.88	140.75	128.40
3	E	404	ASP	CB-CA-C	-5.83	98.73	110.40
5	J	268	GLU	CB-CA-C	5.83	122.07	110.40
3	F	424	LYS	CA-CB-CG	5.81	126.19	113.40
5	I	202	ASP	C-N-CD	5.76	140.50	128.40
3	F	214	VAL	N-CA-C	-5.70	95.60	111.00
3	F	384	VAL	CB-CA-C	-5.66	100.65	111.40
5	I	440	GLY	N-CA-C	-5.63	99.02	113.10
3	F	366	THR	N-CA-C	5.63	126.21	111.00
3	E	355	LEU	CB-CG-CD2	5.49	120.33	111.00
3	F	397	MET	CB-CA-C	-5.48	99.44	110.40
3	E	371	ASN	CA-C-N	-5.44	105.24	117.20
3	E	435	ARG	CD-NE-CZ	5.43	131.21	123.60
2	C	167	MET	CB-CA-C	-5.43	99.54	110.40
5	J	415	GLU	N-CA-C	5.42	125.64	111.00
5	I	211	GLU	CB-CA-C	5.41	121.22	110.40
1	A	95	HIS	N-CA-C	-5.39	96.44	111.00
5	I	211	GLU	N-CA-C	-5.37	96.49	111.00
3	E	268	PRO	N-CD-CG	5.37	111.26	103.20
1	B	274	PRO	CA-N-CD	-5.28	104.11	111.50
5	I	210	GLU	CB-CA-C	-5.26	99.89	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	352	GLU	N-CA-C	5.25	125.16	111.00
5	I	29	TYR	CB-CA-C	-5.22	99.95	110.40
3	F	397	MET	N-CA-C	5.18	124.99	111.00
3	E	371	ASN	N-CA-CB	-5.18	101.28	110.60
3	E	256	LYS	C-N-CA	-5.12	108.89	121.70
3	E	435	ARG	N-CA-C	5.12	124.82	111.00
4	G	240	GLU	OE1-CD-OE2	-5.08	117.20	123.30
5	I	211	GLU	N-CA-CB	5.05	119.69	110.60
3	F	422	LYS	N-CA-C	5.05	124.62	111.00
2	D	1	MET	N-CA-CB	5.04	119.67	110.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	LYS	Peptide
1	A	60	ASP	Peptide
3	E	257	GLU	Peptide
3	E	260	SER	Peptide
3	E	269	TYR	Peptide
3	E	340	THR	Peptide
3	E	442	ALA	Peptide
3	F	269	TYR	Peptide
3	F	369	LYS	Peptide
3	F	370	ASP	Peptide
3	F	383	CYS	Peptide
3	F	403	GLU	Peptide
3	F	447	LEU	Peptide
4	H	355	ARG	Peptide
5	I	31	PHE	Peptide
5	J	432	ASN	Peptide

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	2472	0	2492	150	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2489	0	2512	52	0
2	C	2702	0	2744	95	0
2	D	2674	0	2714	52	1
3	E	2976	0	3032	265	0
3	F	2967	0	3022	325	7
4	G	2755	0	2841	91	0
4	H	2755	0	2841	45	0
5	I	3377	0	3361	140	1
5	J	3372	0	3351	134	7
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
6	G	10	0	0	1	0
6	H	10	0	0	0	0
6	I	5	0	0	1	0
All	All	28584	0	28910	1287	8

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 22.

All (1287) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:218:PHE:CE2	5:I:203:PRO:HB3	1.37	1.58
3:F:368:ILE:HA	3:F:385:ILE:O	1.17	1.24
3:E:355:LEU:HD21	3:E:369:LYS:O	1.05	1.23
3:F:218:PHE:HE2	5:I:203:PRO:CB	1.54	1.21
3:F:265:ASP:O	3:F:268:PRO:HD2	1.35	1.21
1:A:62:LEU:O	1:A:65:GLY:N	1.72	1.20
3:E:355:LEU:CD2	3:E:369:LYS:O	1.89	1.20
3:E:371:ASN:O	3:E:388:GLY:HA2	1.42	1.19
3:F:212:ALA:O	3:F:213:ASP:CG	1.81	1.18
1:A:18:ASP:HB3	1:A:21:GLN:HG3	1.25	1.18
3:E:276:GLN:O	3:E:277:LYS:CG	1.92	1.18
3:E:276:GLN:O	3:E:277:LYS:HG2	1.02	1.17
3:E:37:ILE:HD11	3:E:141:ASN:CG	1.66	1.16
3:F:368:ILE:CA	3:F:385:ILE:O	1.94	1.14
3:F:348:VAL:CG1	3:F:364:GLU:HG2	1.78	1.13
1:A:52:ALA:O	1:A:57:GLU:OE1	1.67	1.13
3:E:355:LEU:HD23	3:E:370:ASP:HA	1.31	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:238:LEU:O	4:G:240:GLU:OE1	1.66	1.12
5:J:399:GLY:O	5:J:417:ASN:HA	1.49	1.12
1:B:106:HIS:CE1	2:C:146:ARG:HG2	1.86	1.10
5:I:18:LEU:CD2	5:I:63:VAL:HA	1.82	1.10
3:F:201:LYS:HE3	4:G:409:PHE:HE1	1.01	1.10
2:D:48:TRP:NE1	2:D:166:GLY:O	1.83	1.10
5:J:439:ILE:HG22	5:J:441:GLY:H	1.14	1.09
3:E:276:GLN:C	3:E:277:LYS:HG2	1.66	1.09
1:A:53:LYS:CE	1:A:104:LYS:NZ	2.15	1.09
3:F:201:LYS:CE	4:G:409:PHE:HE1	1.63	1.08
3:E:269:TYR:CE1	3:E:270:LEU:HD23	1.88	1.08
3:F:351:SER:OG	3:F:355:LEU:HD11	1.51	1.08
5:I:439:ILE:HD12	5:I:440:GLY:N	1.66	1.08
5:I:431:LEU:HD23	5:I:432:ASN:H	1.17	1.08
1:A:53:LYS:NZ	1:A:104:LYS:CE	2.15	1.08
3:F:397:MET:O	3:F:398:ASP:OD1	1.72	1.06
3:E:149:ASP:HB2	3:E:327:PRO:HD2	1.38	1.06
5:I:33:PRO:HG2	5:I:419:ARG:HG2	1.37	1.06
4:G:403:ASN:ND2	4:G:404:MET:O	1.88	1.06
3:F:218:PHE:CE2	5:I:203:PRO:CB	2.31	1.06
3:F:218:PHE:CD2	5:I:203:PRO:HB3	1.90	1.06
5:J:439:ILE:HD12	5:J:439:ILE:H	1.19	1.06
3:F:385:ILE:HG12	3:F:402:VAL:HB	1.35	1.03
3:E:355:LEU:CD2	3:E:370:ASP:HA	1.88	1.03
3:F:348:VAL:HG11	3:F:364:GLU:HG2	1.08	1.02
3:E:211:SER:HA	3:E:214:VAL:CG1	1.90	1.02
3:F:201:LYS:HE3	4:G:409:PHE:CE1	1.93	1.02
5:I:187:VAL:HG11	5:I:205:ILE:CG2	1.90	1.02
3:E:418:GLN:OE1	3:E:435:ARG:NH1	1.92	1.01
3:F:343:GLN:HG3	3:F:344:ARG:H	1.21	1.01
1:A:115:ILE:O	1:A:115:ILE:HG22	1.59	1.00
3:F:385:ILE:HG12	3:F:402:VAL:CB	1.91	1.00
3:F:343:GLN:HG3	3:F:344:ARG:HG3	1.43	0.99
3:F:421:ALA:O	3:F:438:ALA:HA	1.61	0.99
3:F:446:ARG:HG2	3:F:447:LEU:HB2	1.44	0.99
1:A:62:LEU:C	1:A:65:GLY:H	1.66	0.99
2:D:239:GLN:NE2	4:H:404:MET:HB2	1.76	0.98
3:F:123:ASP:OD1	3:F:124:ASP:N	1.95	0.98
3:F:265:ASP:C	3:F:268:PRO:HD2	1.82	0.98
3:F:447:LEU:O	3:F:448:VAL:HG23	1.64	0.98
3:E:355:LEU:HD21	3:E:369:LYS:C	1.83	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:430:THR:O	5:I:439:ILE:HD13	1.63	0.97
3:E:37:ILE:HD11	3:E:141:ASN:OD1	1.61	0.97
5:I:18:LEU:HD21	5:I:63:VAL:HA	1.43	0.97
3:E:355:LEU:HD23	3:E:370:ASP:CA	1.96	0.96
3:F:363:ASN:OD1	3:F:364:GLU:N	1.99	0.95
5:I:407:VAL:O	5:I:431:LEU:O	1.83	0.95
3:E:274:GLN:HB3	3:E:276:GLN:HE22	1.27	0.95
5:I:32:ARG:O	5:I:33:PRO:C	2.01	0.94
5:I:439:ILE:HD12	5:I:440:GLY:C	1.87	0.94
3:F:193:LYS:O	3:F:211:SER:HB3	1.65	0.94
3:F:352:GLU:O	3:F:355:LEU:HG	1.65	0.94
3:F:201:LYS:NZ	4:G:409:PHE:CE1	2.34	0.94
3:F:363:ASN:OD1	3:F:381:LYS:HG3	1.67	0.94
3:E:91:ILE:HG21	3:E:131:ALA:HB1	1.49	0.94
5:I:431:LEU:HD23	5:I:432:ASN:N	1.83	0.94
3:E:355:LEU:HD23	3:E:370:ASP:C	1.88	0.94
3:F:191:ASP:N	3:F:329:TYR:CZ	2.36	0.94
3:E:269:TYR:CD1	3:E:270:LEU:HA	2.02	0.93
5:J:418:LYS:HZ1	5:J:420:LEU:HA	1.31	0.93
3:F:336:ILE:HD12	3:F:395:ILE:HD13	1.50	0.93
2:C:47:ARG:CG	2:C:167:MET:HE1	1.99	0.92
5:J:418:LYS:NZ	5:J:420:LEU:HD23	1.83	0.92
3:E:355:LEU:HB3	3:E:372:SER:O	1.70	0.92
3:F:348:VAL:HG11	3:F:364:GLU:CG	2.00	0.92
1:A:46:LEU:O	1:A:50:SER:OG	1.87	0.92
3:F:367:THR:O	3:F:385:ILE:N	2.02	0.92
3:E:37:ILE:HD11	3:E:141:ASN:ND2	1.85	0.92
3:F:446:ARG:CG	3:F:447:LEU:HB2	1.99	0.91
3:F:201:LYS:CE	4:G:409:PHE:CE1	2.50	0.91
3:F:351:SER:OG	3:F:355:LEU:CD1	2.19	0.91
3:F:191:ASP:N	3:F:329:TYR:CE2	2.38	0.90
2:C:167:MET:HG2	2:C:168:ASP:H	1.33	0.90
5:J:409:GLY:HA3	5:J:433:ASP:O	1.70	0.90
3:F:349:THR:OG1	3:F:366:THR:O	1.90	0.90
3:E:37:ILE:CD1	3:E:141:ASN:CG	2.41	0.89
3:F:424:LYS:C	3:F:425:LEU:HD12	1.92	0.89
5:I:430:THR:OG1	5:I:441:GLY:HA2	1.71	0.89
5:J:397:GLU:HG3	5:J:398:ASP:H	1.34	0.89
1:A:52:ALA:C	1:A:57:GLU:OE1	2.10	0.88
1:A:62:LEU:O	1:A:65:GLY:CA	2.20	0.88
3:F:193:LYS:O	3:F:211:SER:CB	2.22	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:402:VAL:O	4:H:404:MET:HE2	1.73	0.88
3:F:199:GLU:OE1	3:F:202:THR:OG1	1.91	0.88
5:I:431:LEU:CD2	5:I:432:ASN:H	1.86	0.88
5:I:18:LEU:HD21	5:I:63:VAL:CA	2.04	0.88
3:F:426:ARG:HE	3:F:442:ALA:HB1	1.37	0.88
3:F:385:ILE:CG1	3:F:402:VAL:HB	2.04	0.87
2:C:87:ARG:HH11	2:C:87:ARG:HG3	1.36	0.87
4:G:238:LEU:C	4:G:240:GLU:OE1	2.11	0.87
5:J:439:ILE:CG2	5:J:442:ARG:H	1.86	0.87
5:J:418:LYS:HE2	5:J:420:LEU:HG	1.56	0.87
3:E:320:CYS:SG	3:E:321:SER:N	2.47	0.87
1:A:62:LEU:O	1:A:66:SER:N	2.08	0.86
3:F:366:THR:HG22	3:F:383:CYS:H	1.38	0.86
1:A:60:ASP:C	1:A:61:ILE:HD12	1.95	0.86
1:A:62:LEU:HD12	1:A:63:GLN:N	1.90	0.86
3:F:434:HIS:CD2	3:F:448:VAL:HG23	2.10	0.86
3:F:212:ALA:O	3:F:213:ASP:OD1	1.93	0.86
3:F:366:THR:HB	3:F:383:CYS:O	1.76	0.85
5:I:28:ASN:O	5:I:29:TYR:HD1	1.58	0.85
5:I:33:PRO:CG	5:I:419:ARG:HG2	2.06	0.85
1:B:105:ARG:HH11	1:B:105:ARG:HG3	1.40	0.85
5:J:33:PRO:CG	5:J:419:ARG:HB3	2.06	0.85
1:A:55:ILE:HA	1:A:58:PHE:HB3	1.59	0.85
1:A:18:ASP:CB	1:A:21:GLN:HG3	2.05	0.85
3:F:366:THR:HG21	3:F:380:GLY:O	1.77	0.85
3:F:396:LEU:HD23	3:F:413:VAL:HG22	1.58	0.85
3:F:354:ALA:HB3	3:F:370:ASP:OD1	1.77	0.84
2:C:93:LEU:O	2:C:96:THR:OG1	1.93	0.84
5:J:418:LYS:HZ1	5:J:420:LEU:HD23	1.41	0.84
3:E:368:ILE:HG22	3:E:385:ILE:HB	1.59	0.84
1:A:47:LEU:HA	1:A:50:SER:OG	1.78	0.84
3:F:396:LEU:HD22	3:F:413:VAL:HG21	1.60	0.83
2:C:136:MET:HG3	2:C:138:SER:O	1.78	0.83
3:F:265:ASP:O	3:F:268:PRO:CD	2.25	0.83
3:F:434:HIS:CD2	3:F:448:VAL:CG2	2.62	0.83
1:A:61:ILE:HD13	1:A:62:LEU:HD12	1.60	0.82
1:B:105:ARG:O	1:B:109:GLU:HG3	1.79	0.82
5:I:187:VAL:HG11	5:I:205:ILE:HG22	1.60	0.82
3:F:367:THR:HB	3:F:384:VAL:HG12	1.58	0.82
3:E:348:VAL:HG21	3:E:364:GLU:HG2	1.62	0.82
2:C:47:ARG:HG2	2:C:167:MET:HE1	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:187:VAL:CG1	5:I:205:ILE:CG2	2.58	0.81
2:C:47:ARG:HG3	2:C:167:MET:SD	2.20	0.81
4:H:402:VAL:O	4:H:404:MET:CE	2.27	0.81
1:A:55:ILE:HG13	1:A:56:SER:H	1.46	0.81
5:I:187:VAL:HG11	5:I:205:ILE:HG21	1.63	0.81
3:E:274:GLN:HB3	3:E:276:GLN:NE2	1.96	0.81
3:F:446:ARG:CB	3:F:447:LEU:HB2	2.10	0.81
3:F:396:LEU:CD2	3:F:413:VAL:CG2	2.58	0.81
3:E:211:SER:HA	3:E:214:VAL:HG11	1.60	0.81
3:E:329:TYR:HB2	3:E:331:GLU:OE1	1.79	0.81
1:A:113:LEU:HA	1:A:116:GLN:HG3	1.62	0.80
3:E:130:ASP:HA	3:E:133:ARG:CZ	2.13	0.79
4:G:228:ASP:CB	4:G:229:LEU:HD12	2.13	0.79
3:E:385:ILE:HG23	3:E:389:VAL:HG21	1.64	0.79
5:I:18:LEU:HD23	5:I:63:VAL:HA	1.62	0.79
3:E:352:GLU:O	3:E:353:ARG:CG	2.29	0.79
5:I:202:ASP:OD1	5:I:205:ILE:HD11	1.82	0.79
1:A:53:LYS:HZ3	1:A:104:LYS:CE	1.83	0.79
3:E:396:LEU:HD22	3:E:400:ILE:HD11	1.64	0.79
5:I:187:VAL:CG1	5:I:205:ILE:HG21	2.13	0.79
5:I:429:GLY:HA3	5:I:436:LEU:HD23	1.64	0.79
1:A:25:LYS:HA	1:A:28:GLN:OE1	1.83	0.78
3:F:434:HIS:CG	3:F:448:VAL:HG23	2.19	0.78
5:J:397:GLU:HG3	5:J:398:ASP:N	1.94	0.78
5:J:409:GLY:CA	5:J:433:ASP:O	2.32	0.78
3:F:367:THR:O	3:F:384:VAL:CA	2.32	0.78
2:D:50:THR:HB	2:D:53:GLN:HG3	1.65	0.78
3:F:421:ALA:O	3:F:438:ALA:CA	2.30	0.78
5:J:33:PRO:HG3	5:J:419:ARG:HB3	1.64	0.78
5:J:381:LYS:HB3	5:J:398:ASP:HA	1.66	0.78
3:E:267:ILE:N	3:E:267:ILE:HD13	1.98	0.78
3:E:352:GLU:O	3:E:353:ARG:CB	2.32	0.77
5:I:439:ILE:CD1	5:I:441:GLY:N	2.47	0.77
3:F:366:THR:CB	3:F:383:CYS:O	2.32	0.77
1:B:106:HIS:NE2	2:C:146:ARG:CG	2.46	0.77
2:C:167:MET:HG2	2:C:168:ASP:N	1.98	0.77
3:E:211:SER:CA	3:E:214:VAL:CG1	2.63	0.77
4:G:228:ASP:HB2	4:G:229:LEU:CD1	2.13	0.77
2:C:48:TRP:CD1	2:C:54:LEU:HB2	2.18	0.77
3:F:358:ALA:N	3:F:360:CYS:SG	2.58	0.77
4:G:278:SER:OG	6:G:501:PO4:O4	2.02	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:0:PHE:O	2:D:1:MET:HG3	1.86	0.76
1:B:106:HIS:CE1	2:C:146:ARG:CG	2.68	0.76
2:C:162:ARG:NE	2:C:162:ARG:HA	1.97	0.76
2:C:93:LEU:HA	2:C:96:THR:CG2	2.16	0.76
5:I:205:ILE:H	5:I:205:ILE:HD13	1.50	0.76
3:F:341:PRO:C	3:F:342:GLU:HG2	2.05	0.76
3:E:182:HIS:CD2	3:E:334:LYS:HE3	2.21	0.76
3:F:343:GLN:HA	3:F:343:GLN:HE21	1.50	0.76
1:A:63:GLN:O	1:A:67:ASN:OD1	2.02	0.75
3:F:343:GLN:CG	3:F:344:ARG:H	1.99	0.75
1:A:61:ILE:HD13	1:A:62:LEU:N	2.00	0.75
3:E:369:LYS:HB2	3:E:386:GLY:CA	2.17	0.75
3:F:385:ILE:HG12	3:F:402:VAL:CG2	2.16	0.75
3:F:181:GLU:H	3:F:334:LYS:HE3	1.52	0.75
3:E:369:LYS:HB2	3:E:386:GLY:HA3	1.68	0.75
5:J:386:ASN:H	5:J:386:ASN:ND2	1.84	0.75
3:E:269:TYR:CD1	3:E:270:LEU:CA	2.70	0.75
5:J:431:LEU:O	5:J:432:ASN:HB2	1.86	0.75
3:F:320:CYS:SG	3:F:321:SER:N	2.60	0.75
3:F:343:GLN:HA	3:F:343:GLN:NE2	2.03	0.74
5:I:32:ARG:O	5:I:34:LEU:N	2.19	0.74
5:I:205:ILE:HD13	5:I:205:ILE:N	2.03	0.74
1:A:62:LEU:HD12	1:A:63:GLN:H	1.51	0.74
3:F:269:TYR:CD1	3:F:270:LEU:HA	2.21	0.74
3:F:396:LEU:HD22	3:F:413:VAL:CG2	2.16	0.74
3:F:426:ARG:HE	3:F:442:ALA:CB	2.00	0.74
3:E:211:SER:C	3:E:214:VAL:HG13	2.06	0.74
3:F:361:MET:HB2	3:F:378:ILE:HD13	1.70	0.74
1:A:22:VAL:O	1:A:25:LYS:HB2	1.88	0.74
4:G:241:LYS:HA	4:G:244:SER:HB2	1.68	0.74
5:I:188:HIS:HD2	5:I:201:MET:HB3	1.52	0.74
5:I:439:ILE:CD1	5:I:440:GLY:C	2.56	0.74
3:F:363:ASN:CG	3:F:381:LYS:HG3	2.07	0.74
3:F:447:LEU:O	3:F:448:VAL:CG2	2.36	0.74
3:E:252:LEU:HD12	3:E:256:LYS:HE3	1.70	0.73
1:A:18:ASP:HB3	1:A:21:GLN:CG	2.14	0.73
3:E:269:TYR:HD1	3:E:270:LEU:CA	2.01	0.73
1:A:94:LEU:C	1:A:95:HIS:O	2.22	0.73
3:F:266:LEU:O	3:F:269:TYR:HD2	1.71	0.73
3:F:371:ASN:O	3:F:388:GLY:HA2	1.88	0.73
2:C:50:THR:OG1	2:C:53:GLN:OE1	2.06	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:430:THR:OG1	5:I:439:ILE:HD11	1.88	0.73
3:F:119:PRO:HG2	3:F:122:LEU:HG	1.70	0.73
3:F:430:ILE:HA	3:F:446:ARG:O	1.89	0.73
5:I:28:ASN:O	5:I:29:TYR:CD1	2.40	0.73
5:J:399:GLY:C	5:J:417:ASN:HA	2.09	0.73
3:F:265:ASP:C	3:F:268:PRO:CD	2.57	0.73
5:I:437:VAL:HG22	5:I:438:GLY:H	1.54	0.73
5:I:430:THR:O	5:I:439:ILE:CD1	2.35	0.73
2:C:47:ARG:HG3	2:C:167:MET:HE1	1.70	0.73
2:C:87:ARG:NH1	2:C:87:ARG:HG3	1.98	0.72
3:F:366:THR:CA	3:F:383:CYS:O	2.36	0.72
1:A:115:ILE:CG2	1:A:115:ILE:O	2.31	0.72
1:A:25:LYS:O	1:A:28:GLN:OE1	2.06	0.72
1:A:26:PHE:O	1:A:29:ASP:N	2.22	0.72
3:E:182:HIS:CD2	3:E:334:LYS:CE	2.72	0.72
3:F:418:GLN:O	3:F:435:ARG:HA	1.89	0.72
5:I:439:ILE:HD12	5:I:441:GLY:N	2.05	0.72
3:E:81:GLU:OE2	3:E:110:GLY:O	2.07	0.72
3:E:269:TYR:CE1	3:E:270:LEU:HA	2.24	0.72
1:A:61:ILE:HD13	1:A:62:LEU:CD1	2.19	0.72
2:D:48:TRP:HE1	2:D:166:GLY:C	1.92	0.72
3:F:267:ILE:N	3:F:267:ILE:HD13	2.05	0.72
5:J:418:LYS:NZ	5:J:420:LEU:HA	2.03	0.72
3:F:124:ASP:OD1	3:F:125:SER:N	2.23	0.72
2:C:377:TYR:OH	4:H:460:ASN:ND2	2.23	0.72
5:J:385:ALA:O	5:J:388:VAL:HG23	1.90	0.72
3:E:274:GLN:CB	3:E:276:GLN:HE22	2.02	0.71
1:A:57:GLU:O	1:A:61:ILE:HG23	1.91	0.71
1:B:104:LYS:O	1:B:108:VAL:HG23	1.90	0.71
3:F:446:ARG:HG2	3:F:447:LEU:CB	2.19	0.71
1:B:106:HIS:NE2	2:C:146:ARG:HG2	2.06	0.71
3:E:349:THR:OG1	3:E:366:THR:O	2.04	0.71
5:J:418:LYS:HE2	5:J:420:LEU:CG	2.21	0.71
2:C:235:PHE:HE1	4:G:405:GLY:HA3	1.55	0.71
2:D:51:VAL:HG13	2:D:52:ASP:OD1	1.91	0.71
4:G:228:ASP:HB3	4:G:229:LEU:HD12	1.71	0.71
3:E:355:LEU:HD23	3:E:371:ASN:N	2.05	0.71
4:G:240:GLU:CD	4:G:241:LYS:H	1.93	0.71
1:A:59:MET:C	1:A:61:ILE:HG13	2.11	0.71
3:F:426:ARG:NE	3:F:442:ALA:HB1	2.04	0.71
5:J:439:ILE:HG22	5:J:441:GLY:N	1.99	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:170:ALA:HB3	3:E:315:LYS:HG2	1.74	0.70
3:F:387:LYS:HB2	3:F:404:ASP:HB3	1.73	0.70
5:I:130:VAL:HG12	5:I:273:ARG:HG2	1.73	0.70
5:I:437:VAL:HG22	5:I:438:GLY:N	2.04	0.70
3:E:269:TYR:CD1	3:E:270:LEU:N	2.58	0.70
1:A:63:GLN:O	1:A:67:ASN:CG	2.29	0.70
2:C:167:MET:CG	2:C:168:ASP:H	2.04	0.70
3:E:387:LYS:HD3	3:E:404:ASP:HA	1.73	0.70
3:F:122:LEU:HD11	3:F:131:ALA:HA	1.74	0.70
3:F:169:SER:HB2	3:F:315:LYS:HZ3	1.56	0.70
3:E:371:ASN:O	3:E:388:GLY:CA	2.33	0.70
3:E:403:GLU:O	3:E:406:VAL:HG13	1.90	0.70
3:F:212:ALA:O	3:F:213:ASP:CB	2.39	0.70
2:C:47:ARG:CG	2:C:167:MET:CE	2.68	0.70
5:J:418:LYS:HE3	5:J:420:LEU:N	2.05	0.70
3:F:373:ASN:N	3:F:389:VAL:O	2.23	0.69
1:A:59:MET:CA	1:A:61:ILE:HG13	2.22	0.69
5:J:439:ILE:HG21	5:J:442:ARG:H	1.55	0.69
3:F:127:SER:HB3	3:F:261:SER:HB2	1.74	0.69
3:F:396:LEU:CD2	3:F:413:VAL:HG21	2.20	0.69
5:I:188:HIS:CD2	5:I:201:MET:HB3	2.27	0.69
5:J:418:LYS:CE	5:J:420:LEU:HG	2.22	0.69
1:A:64:ASN:O	1:A:68:THR:OG1	2.01	0.69
5:I:439:ILE:HD11	5:I:441:GLY:CA	2.22	0.69
5:J:418:LYS:HE2	5:J:420:LEU:CD2	2.23	0.69
5:J:409:GLY:N	5:J:433:ASP:O	2.25	0.69
3:E:352:GLU:C	3:E:353:ARG:HG2	2.13	0.69
3:E:37:ILE:CD1	3:E:141:ASN:ND2	2.56	0.69
3:F:368:ILE:HG22	3:F:385:ILE:HB	1.74	0.69
5:J:433:ASP:HB2	5:J:434:PRO:HD3	1.73	0.69
2:C:48:TRP:HH2	2:C:170:ARG:HG2	1.56	0.69
2:C:47:ARG:HG3	2:C:167:MET:CE	2.22	0.69
3:F:180:TYR:OH	3:F:331:GLU:OE2	2.09	0.69
5:I:433:ASP:O	5:I:433:ASP:OD2	2.11	0.69
4:G:229:LEU:HD23	4:G:233:GLU:CB	2.23	0.69
2:C:333:PRO:HD3	5:I:290:ARG:HB2	1.75	0.69
3:F:407:ARG:HD2	3:F:424:LYS:HE3	1.75	0.69
4:G:410:GLU:C	4:G:411:GLU:HG3	2.14	0.68
5:J:400:ALA:O	5:J:401:ILE:HG13	1.92	0.68
3:E:37:ILE:CD1	3:E:141:ASN:OD1	2.40	0.68
5:I:18:LEU:HD21	5:I:63:VAL:N	2.07	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PHE:HA	1:A:29:ASP:CG	2.13	0.68
3:E:387:LYS:CD	3:E:404:ASP:HA	2.24	0.68
3:F:397:MET:O	3:F:398:ASP:CG	2.31	0.68
3:F:403:GLU:CB	3:F:420:GLY:HA2	2.23	0.68
1:B:105:ARG:NH1	1:B:105:ARG:HG3	2.09	0.68
3:E:355:LEU:HD11	3:E:368:ILE:HG13	1.75	0.68
5:I:257:LEU:O	5:I:259:LYS:HG2	1.93	0.68
5:J:111:ARG:NH2	5:J:240:TYR:O	2.27	0.68
2:C:291:SER:HA	2:C:356:ASP:HB2	1.75	0.68
1:A:53:LYS:CE	1:A:104:LYS:HZ1	1.92	0.68
3:F:343:GLN:HG3	3:F:344:ARG:N	2.03	0.68
4:H:411:GLU:OE1	4:H:411:GLU:N	2.27	0.68
5:J:290:ARG:NH1	5:J:298:ASP:OD1	2.27	0.67
5:J:439:ILE:CD1	5:J:439:ILE:H	1.94	0.67
3:E:255:GLU:HG2	3:E:256:LYS:HD3	1.75	0.67
4:G:228:ASP:CB	4:G:229:LEU:CD1	2.72	0.67
3:E:133:ARG:NE	3:E:257:GLU:OE1	2.27	0.67
3:E:355:LEU:HD22	3:E:372:SER:HB2	1.77	0.67
5:J:406:VAL:HG11	5:J:420:LEU:HD13	1.76	0.67
5:I:433:ASP:HA	5:I:434:PRO:C	2.15	0.67
5:J:418:LYS:HZ1	5:J:420:LEU:CA	2.07	0.67
3:E:68:GLY:HA3	3:E:339:LEU:HD22	1.75	0.67
3:F:407:ARG:HB2	3:F:424:LYS:HD3	1.76	0.67
2:D:50:THR:HG22	2:D:52:ASP:H	1.60	0.67
5:J:391:GLY:C	5:J:394:CYS:SG	2.73	0.67
5:J:414:ILE:C	5:J:415:GLU:HG2	2.15	0.67
3:E:249:VAL:O	3:E:253:ILE:HG13	1.94	0.67
5:J:169:ARG:NH1	5:J:218:LEU:O	2.27	0.67
3:E:274:GLN:OE1	3:E:274:GLN:N	2.27	0.67
3:E:385:ILE:HA	3:E:402:VAL:O	1.94	0.67
5:I:209:HIS:O	5:I:210:GLU:HB2	1.95	0.67
1:A:53:LYS:NZ	1:A:104:LYS:NZ	0.69	0.66
5:I:436:LEU:HD12	5:I:436:LEU:C	2.16	0.66
5:I:290:ARG:NH1	5:I:298:ASP:OD1	2.24	0.66
5:J:416:LYS:C	5:J:417:ASN:ND2	2.48	0.66
2:C:93:LEU:HA	2:C:96:THR:HG21	1.76	0.66
3:E:352:GLU:C	3:E:353:ARG:CG	2.63	0.66
5:J:383:ILE:C	5:J:384:LEU:HD23	2.15	0.66
1:A:55:ILE:O	1:A:59:MET:N	2.27	0.66
3:F:403:GLU:HB3	3:F:420:GLY:HA2	1.76	0.66
3:F:161:ASP:OD1	4:G:134:THR:CG2	2.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:397:MET:SD	3:F:414:ALA:HA	2.36	0.66
4:H:117:GLU:O	4:H:119:GLN:NE2	2.29	0.66
5:J:33:PRO:HG2	5:J:419:ARG:HB3	1.77	0.66
3:E:413:VAL:HG22	3:E:430:ILE:HD12	1.78	0.66
3:F:91:ILE:HG21	3:F:131:ALA:HB1	1.78	0.66
5:I:439:ILE:HG13	5:I:441:GLY:HA3	1.78	0.66
1:B:339:LEU:HD23	1:B:340:TYR:CE2	2.29	0.65
3:E:211:SER:HA	3:E:214:VAL:HG12	1.75	0.65
3:F:144:VAL:HG22	3:F:244:VAL:HG12	1.77	0.65
1:A:55:ILE:HG13	1:A:56:SER:N	2.07	0.65
1:A:59:MET:HA	1:A:61:ILE:HG13	1.79	0.65
3:F:391:VAL:HG12	3:F:408:LEU:HB2	1.78	0.65
5:I:18:LEU:CD2	5:I:62:GLY:O	2.45	0.65
1:A:53:LYS:CE	1:A:104:LYS:HZ2	1.94	0.65
3:E:352:GLU:O	3:E:353:ARG:HB2	1.97	0.65
4:H:405:GLY:O	4:H:406:VAL:HG12	1.96	0.65
3:E:385:ILE:HG12	3:E:402:VAL:HB	1.79	0.65
4:H:408:ASP:OD1	4:H:408:ASP:N	2.27	0.65
5:I:18:LEU:CD2	5:I:63:VAL:CA	2.64	0.65
3:E:211:SER:C	3:E:214:VAL:CG1	2.65	0.64
3:E:348:VAL:HG21	3:E:364:GLU:CG	2.27	0.64
3:F:262:ILE:HG23	3:F:266:LEU:HD13	1.79	0.64
3:F:420:GLY:N	3:F:436:VAL:O	2.26	0.64
4:G:407:ASP:OD1	4:G:408:ASP:N	2.30	0.64
3:E:339:LEU:C	3:E:341:PRO:HD2	2.18	0.64
3:E:355:LEU:CD2	3:E:370:ASP:CA	2.64	0.64
3:F:169:SER:CB	3:F:315:LYS:HZ3	2.10	0.64
4:G:237:LEU:HD12	4:G:238:LEU:N	2.12	0.64
3:E:221:ARG:NH1	5:J:198:TYR:OH	2.30	0.64
3:E:418:GLN:OE1	3:E:435:ARG:HD3	1.96	0.64
1:A:47:LEU:CA	1:A:50:SER:OG	2.44	0.64
3:F:396:LEU:CD2	3:F:413:VAL:HG22	2.18	0.64
1:A:58:PHE:O	1:A:61:ILE:HG21	1.97	0.64
3:F:446:ARG:CA	3:F:447:LEU:HB2	2.28	0.64
3:F:202:THR:O	3:F:203:SER:HB2	1.97	0.64
5:I:348:THR:HG21	5:I:362:ILE:HG22	1.79	0.64
2:C:87:ARG:NH1	2:C:387:ASP:OD2	2.31	0.64
4:G:241:LYS:O	4:G:245:TYR:HB2	1.96	0.64
5:J:226:CYS:HB3	5:J:230:VAL:HG21	1.78	0.64
5:I:50:LEU:HD11	5:I:274:VAL:HG21	1.80	0.64
3:F:202:THR:HB	3:F:204:ARG:HG2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:29:TYR:O	5:I:29:TYR:CD2	2.51	0.63
3:E:352:GLU:HG3	3:E:370:ASP:N	2.13	0.63
3:F:339:LEU:HD13	3:F:339:LEU:O	1.99	0.63
3:F:368:ILE:C	3:F:385:ILE:O	2.37	0.63
2:C:-3:ILE:HG22	2:C:64:THR:HG21	1.80	0.63
1:A:53:LYS:HD3	1:A:53:LYS:N	2.13	0.63
2:C:92:GLU:O	2:C:96:THR:HG23	1.99	0.63
5:I:439:ILE:C	5:I:439:ILE:HD12	2.18	0.63
4:G:444:VAL:HG22	4:G:449:LEU:HG	1.80	0.63
2:C:93:LEU:HA	2:C:96:THR:HG23	1.80	0.63
3:F:367:THR:CB	3:F:384:VAL:HG12	2.29	0.63
3:E:385:ILE:CG2	3:E:389:VAL:HG21	2.29	0.62
5:I:154:ILE:HD11	5:I:259:LYS:HE3	1.80	0.62
1:A:28:GLN:CD	1:A:28:GLN:H	2.02	0.62
1:B:106:HIS:NE2	2:C:146:ARG:HG3	2.13	0.62
5:J:386:ASN:HD22	5:J:386:ASN:H	1.46	0.62
1:A:117:ARG:O	1:A:120:ALA:N	2.32	0.62
3:F:423:SER:OG	3:F:438:ALA:O	2.18	0.62
5:I:420:LEU:HA	5:I:428:GLN:O	1.98	0.62
2:C:47:ARG:HG2	2:C:167:MET:CE	2.27	0.62
3:E:276:GLN:CD	3:E:276:GLN:H	2.01	0.62
4:G:228:ASP:HB2	4:G:229:LEU:HD13	1.81	0.62
2:C:163:VAL:HG12	2:C:164:THR:OG1	1.99	0.62
2:D:50:THR:HB	2:D:53:GLN:CG	2.30	0.62
3:F:194:GLN:HB2	3:F:237:LEU:O	2.00	0.62
5:J:430:THR:HG22	5:J:431:LEU:H	1.64	0.62
1:A:25:LYS:CA	1:A:28:GLN:OE1	2.47	0.62
2:C:136:MET:O	2:C:137:TYR:HB2	2.00	0.62
3:E:352:GLU:HG3	3:E:369:LYS:HA	1.81	0.62
3:E:48:GLY:HA2	3:E:62:LYS:HD2	1.80	0.62
3:F:363:ASN:OD1	3:F:381:LYS:CG	2.43	0.61
2:C:294:GLN:HG2	4:G:330:SER:HB2	1.81	0.61
5:J:391:GLY:O	5:J:394:CYS:SG	2.58	0.61
5:I:439:ILE:CD1	5:I:441:GLY:CA	2.78	0.61
3:E:261:SER:O	3:E:262:ILE:HB	1.99	0.61
3:E:355:LEU:HD22	3:E:372:SER:N	2.15	0.61
1:B:336:LEU:O	1:B:340:TYR:HD2	1.82	0.61
1:A:117:ARG:O	1:A:121:CYS:N	2.26	0.61
1:A:168:GLU:OE2	1:B:170:ARG:NH1	2.32	0.61
1:B:25:LYS:HA	1:B:28:GLN:NE2	2.15	0.61
3:E:354:ALA:HB3	3:E:370:ASP:HB3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:396:LEU:HD22	3:E:400:ILE:CD1	2.30	0.61
3:F:273:CYS:O	3:F:275:TYR:HD2	1.83	0.61
5:I:439:ILE:HD12	5:I:440:GLY:CA	2.31	0.61
5:J:439:ILE:HD12	5:J:439:ILE:N	2.04	0.61
3:E:119:PRO:HG2	3:E:122:LEU:HG	1.82	0.61
5:J:156:THR:HG22	5:J:262:HIS:HB2	1.82	0.61
3:E:182:HIS:CD2	3:E:334:LYS:HE2	2.35	0.61
3:E:389:VAL:HG12	3:E:406:VAL:N	2.16	0.61
3:F:426:ARG:O	3:F:426:ARG:HG3	2.01	0.61
4:G:114:ILE:HG22	4:G:116:GLU:H	1.65	0.61
3:E:418:GLN:OE1	3:E:435:ARG:CD	2.49	0.61
1:A:101:GLU:O	1:A:105:ARG:HG2	2.01	0.60
4:G:356:ALA:HA	4:G:433:ASP:HB2	1.83	0.60
1:A:113:LEU:O	1:A:113:LEU:HD12	2.01	0.60
1:A:51:GLN:O	1:A:53:LYS:HG2	2.01	0.60
3:F:218:PHE:CD2	5:I:203:PRO:CB	2.76	0.60
1:A:172:SER:HB2	1:B:286:THR:HG21	1.83	0.60
3:F:269:TYR:CE1	3:F:270:LEU:HA	2.35	0.60
4:G:272:LEU:HD12	4:G:336:VAL:HG21	1.82	0.60
3:F:366:THR:HG22	3:F:383:CYS:N	2.12	0.60
5:J:407:VAL:HB	5:J:431:LEU:HG	1.83	0.60
1:A:113:LEU:HA	1:A:116:GLN:CG	2.30	0.60
3:E:32:LEU:O	3:E:32:LEU:HD23	2.02	0.60
1:A:95:HIS:CD2	1:A:96:ASP:H	2.20	0.60
3:F:161:ASP:OD1	4:G:134:THR:HG23	2.01	0.60
3:F:213:ASP:OD1	3:F:214:VAL:N	2.35	0.60
2:D:198:HIS:O	2:D:273:LYS:NZ	2.32	0.60
2:C:93:LEU:CA	2:C:96:THR:HG23	2.32	0.60
3:E:404:ASP:OD2	3:E:421:ALA:N	2.28	0.60
3:F:403:GLU:HG2	3:F:421:ALA:H	1.67	0.60
3:F:270:LEU:HD23	3:F:270:LEU:N	2.17	0.60
3:E:154:LEU:HD12	3:E:155:PRO:HD2	1.84	0.59
3:E:380:GLY:N	3:E:396:LEU:O	2.35	0.59
3:F:183:ILE:HG22	3:F:183:ILE:O	2.01	0.59
1:A:249:PHE:HB2	2:D:140:MET:HE1	1.85	0.59
1:A:53:LYS:HZ3	1:A:104:LYS:NZ	0.74	0.59
3:E:182:HIS:HD2	3:E:334:LYS:HE2	1.67	0.59
3:E:269:TYR:HD1	3:E:270:LEU:HA	1.53	0.59
3:F:336:ILE:CD1	3:F:395:ILE:HD13	2.30	0.59
3:F:346:VAL:HG12	3:F:348:VAL:H	1.67	0.59
3:F:419:ILE:HB	3:F:436:VAL:HB	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:449:ASP:OD1	3:F:450:MET:N	2.35	0.59
3:F:251:ASP:HA	3:F:254:ARG:HB2	1.82	0.59
3:F:154:LEU:HD12	3:F:155:PRO:HD2	1.83	0.59
3:F:214:VAL:HG23	3:F:218:PHE:CD1	2.38	0.59
2:C:0:PHE:C	2:C:1:MET:HG3	2.23	0.59
2:C:136:MET:HG2	2:C:137:TYR:H	1.68	0.59
3:E:387:LYS:HB2	3:E:404:ASP:H	1.68	0.59
5:J:398:ASP:N	5:J:398:ASP:OD1	2.32	0.59
3:E:441:ILE:HG13	3:E:443:ARG:HH21	1.66	0.58
3:E:224:LEU:HD23	3:E:225:LEU:HD12	1.84	0.58
2:D:10:TYR:OH	2:D:46:THR:OG1	1.79	0.58
3:E:256:LYS:O	3:E:259:ILE:CG1	2.51	0.58
3:F:367:THR:O	3:F:384:VAL:HA	2.01	0.58
4:G:240:GLU:OE1	4:G:241:LYS:N	2.28	0.58
3:F:194:GLN:HG3	3:F:238:SER:HA	1.86	0.58
4:G:237:LEU:HD12	4:G:238:LEU:H	1.69	0.58
5:I:436:LEU:HA	5:I:437:VAL:C	2.23	0.58
2:C:19:ASP:HB3	2:C:25:VAL:HG12	1.85	0.58
5:I:409:GLY:HA3	5:I:434:PRO:HA	1.86	0.58
1:A:61:ILE:CD1	1:A:62:LEU:HD12	2.32	0.58
3:E:434:HIS:CG	3:E:447:LEU:HA	2.39	0.58
3:F:424:LYS:O	3:F:425:LEU:HD12	2.03	0.58
3:F:446:ARG:HG2	3:F:447:LEU:HD22	1.85	0.58
5:J:285:LYS:HE2	5:J:330:ARG:HH21	1.69	0.58
5:J:33:PRO:HG2	5:J:419:ARG:HG2	1.85	0.58
5:J:418:LYS:CE	5:J:420:LEU:HD23	2.32	0.58
1:A:113:LEU:CD1	1:A:116:GLN:HG3	2.34	0.58
2:D:46:THR:O	2:D:170:ARG:NH2	2.36	0.58
3:E:260:SER:OG	3:E:264:GLY:HA3	2.03	0.58
3:E:328:ASN:N	3:E:328:ASN:OD1	2.30	0.58
3:E:274:GLN:CD	3:E:274:GLN:H	2.07	0.57
4:H:258:VAL:HA	4:H:283:VAL:HG22	1.86	0.57
2:C:41:GLN:HA	2:C:44:SER:HB3	1.85	0.57
2:C:5:ASN:O	2:C:9:THR:OG1	2.16	0.57
3:E:211:SER:CA	3:E:214:VAL:HG11	2.29	0.57
3:E:195:LEU:HD23	3:E:218:PHE:CE2	2.39	0.57
3:F:122:LEU:HD11	3:F:131:ALA:CB	2.34	0.57
1:A:74:GLN:HB3	1:A:263:SER:HB2	1.86	0.57
3:F:122:LEU:CD1	3:F:131:ALA:CB	2.82	0.57
4:G:160:SER:HB3	4:G:344:HIS:HD2	1.70	0.57
5:I:226:CYS:HB3	5:I:230:VAL:HG21	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:418:LYS:HE3	5:J:419:ARG:C	2.24	0.57
5:J:429:GLY:HA2	5:J:436:LEU:HD21	1.85	0.57
1:A:61:ILE:HD13	1:A:62:LEU:H	1.68	0.57
1:A:67:ASN:O	1:A:71:GLU:HG3	2.03	0.57
4:H:411:GLU:O	4:H:412:LYS:HG2	2.04	0.57
2:D:12:ALA:HB1	2:D:38:VAL:HG22	1.85	0.57
2:D:236:PRO:HG3	2:D:336:ILE:HG22	1.87	0.57
3:E:136:SER:HB2	3:E:254:ARG:HH11	1.70	0.57
3:E:256:LYS:O	3:E:259:ILE:HG13	2.05	0.57
3:E:357:GLY:HA3	3:E:374:ILE:HG13	1.87	0.57
3:E:369:LYS:HB2	3:E:386:GLY:HA2	1.86	0.57
3:F:122:LEU:HD13	3:F:131:ALA:HB2	1.85	0.57
3:F:430:ILE:HD12	3:F:430:ILE:O	2.04	0.57
3:F:447:LEU:HG	3:F:448:VAL:N	2.19	0.57
5:I:431:LEU:CD2	5:I:432:ASN:N	2.57	0.57
3:F:401:VAL:O	3:F:401:VAL:HG23	2.05	0.57
4:G:231:ASP:O	4:G:234:GLY:N	2.37	0.57
2:D:325:GLU:OE2	5:J:310:ARG:NE	2.37	0.56
3:F:413:VAL:HA	3:F:430:ILE:HG13	1.87	0.56
4:H:213:ASN:OD1	4:H:216:ARG:NH1	2.37	0.56
5:I:24:SER:O	5:I:25:ASP:HB3	2.04	0.56
2:C:21:LYS:HE3	5:I:301:LEU:HA	1.86	0.56
5:J:416:LYS:C	5:J:417:ASN:HD22	2.09	0.56
3:E:182:HIS:H	3:E:334:LYS:HE3	1.70	0.56
3:F:380:GLY:HA3	3:F:397:MET:O	2.06	0.56
4:G:234:GLY:O	4:G:237:LEU:HD12	2.05	0.56
5:I:186:CYS:HB3	5:I:261:ILE:HG23	1.88	0.56
3:E:437:GLU:H	3:E:437:GLU:CD	2.08	0.56
3:F:229:PRO:HB3	5:I:164:PRO:HG3	1.88	0.56
3:F:343:GLN:CA	3:F:343:GLN:HE21	2.16	0.56
2:D:239:GLN:CD	4:H:404:MET:HB2	2.25	0.56
3:E:255:GLU:OE1	3:E:255:GLU:N	2.31	0.56
3:F:385:ILE:HG12	3:F:402:VAL:HG21	1.86	0.56
3:F:398:ASP:O	3:F:399:ASN:HB2	2.04	0.56
1:A:117:ARG:HA	1:A:120:ALA:HB3	1.86	0.56
4:G:232:ASP:N	4:G:232:ASP:OD1	2.39	0.56
5:I:409:GLY:HA3	5:I:433:ASP:HB2	1.88	0.56
5:J:415:GLU:HB3	5:J:416:LYS:HG2	1.88	0.56
3:F:369:LYS:N	3:F:385:ILE:O	2.38	0.56
3:F:363:ASN:CG	3:F:364:GLU:H	2.02	0.56
5:I:348:THR:HG22	5:I:365:ALA:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:127:SER:O	5:J:273:ARG:NH1	2.37	0.56
1:A:266:ILE:HG12	1:A:267:LEU:HG	1.87	0.55
4:G:229:LEU:HD23	4:G:233:GLU:HB2	1.86	0.55
3:F:69:ASN:HB3	3:F:363:ASN:HD22	1.71	0.55
3:E:152:VAL:HG11	3:E:242:ILE:HD11	1.89	0.55
3:F:367:THR:CA	3:F:384:VAL:HG12	2.37	0.55
3:F:447:LEU:HD12	3:F:448:VAL:H	1.72	0.55
3:F:342:GLU:OE1	3:F:361:MET:CE	2.55	0.55
3:F:387:LYS:CG	3:F:404:ASP:HB3	2.36	0.55
5:J:433:ASP:CB	5:J:434:PRO:HD3	2.36	0.55
2:C:2:SER:HB3	2:C:4:ILE:HG22	1.89	0.55
5:I:403:ALA:HB3	5:I:421:THR:HA	1.88	0.55
1:A:53:LYS:NZ	1:A:104:LYS:HZ2	0.69	0.55
3:E:236:ASN:N	5:J:210:GLU:OE1	2.40	0.55
3:F:367:THR:O	3:F:384:VAL:C	2.45	0.55
5:I:35:THR:HA	5:I:38:LYS:O	2.07	0.55
5:I:416:LYS:HB3	5:I:417:ASN:ND2	2.22	0.55
1:A:287:PRO:HG2	1:A:290:ALA:HB2	1.89	0.55
3:E:386:GLY:O	3:E:389:VAL:HG13	2.06	0.55
1:A:25:LYS:C	1:A:28:GLN:OE1	2.45	0.55
1:A:51:GLN:O	1:A:53:LYS:HE2	2.07	0.55
2:C:234:GLY:HA3	2:C:238:ASN:HB2	1.88	0.55
3:E:108:TYR:CZ	3:E:110:GLY:HA3	2.41	0.55
5:J:434:PRO:HD2	5:J:434:PRO:O	2.06	0.55
5:I:17:ALA:HA	5:I:64:GLN:HG3	1.88	0.55
3:E:352:GLU:O	3:E:353:ARG:HG3	2.08	0.54
1:A:58:PHE:CE2	1:A:94:LEU:HD21	2.43	0.54
3:F:385:ILE:CG1	3:F:402:VAL:CG2	2.83	0.54
3:F:401:VAL:O	3:F:403:GLU:N	2.40	0.54
3:F:366:THR:CG2	3:F:380:GLY:O	2.52	0.54
4:G:229:LEU:HD23	4:G:233:GLU:HB3	1.89	0.54
5:J:178:VAL:HB	5:J:188:HIS:HB3	1.89	0.54
5:J:39:PRO:HG2	5:J:42:LEU:HB2	1.89	0.54
5:J:418:LYS:CE	5:J:420:LEU:CD2	2.86	0.54
1:A:83:CYS:HB3	1:A:87:GLN:HE22	1.72	0.54
1:B:222:ASN:HB3	1:B:226:THR:HG21	1.90	0.54
3:F:149:ASP:O	3:F:327:PRO:HD2	2.07	0.54
3:F:432:VAL:O	3:F:434:HIS:CD2	2.60	0.54
3:F:161:ASP:OD1	4:G:134:THR:HG21	2.07	0.54
2:D:237:ASN:ND2	2:D:354:TYR:HA	2.21	0.54
3:F:92:CYS:SG	3:F:93:MET:N	2.80	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:TRP:CD2	2:C:54:LEU:HD13	2.43	0.54
3:E:91:ILE:HG12	3:E:135:VAL:HG21	1.89	0.54
3:E:275:TYR:HD1	3:E:275:TYR:O	1.91	0.54
3:E:352:GLU:HG2	3:E:368:ILE:O	2.07	0.54
3:F:32:LEU:HD12	3:F:33:GLN:N	2.23	0.54
3:F:161:ASP:OD2	4:G:134:THR:HG23	2.07	0.54
1:B:224:ILE:HA	1:B:309:ASP:HB2	1.90	0.54
2:D:86:ILE:HG12	2:D:173:ILE:HD12	1.89	0.54
3:E:253:ILE:HG22	3:E:253:ILE:O	2.08	0.54
5:J:397:GLU:CG	5:J:398:ASP:H	2.14	0.54
1:A:61:ILE:HD13	1:A:63:GLN:H	1.73	0.54
2:C:142:ASN:O	2:C:145:GLY:N	2.30	0.54
5:I:187:VAL:HG12	5:I:205:ILE:HG21	1.90	0.54
3:F:193:LYS:O	3:F:211:SER:HB2	2.05	0.54
3:F:366:THR:HA	3:F:383:CYS:O	2.08	0.54
3:F:53:PRO:HG2	3:F:429:GLU:HG3	1.90	0.54
5:I:431:LEU:CG	5:I:432:ASN:N	2.67	0.54
1:A:113:LEU:HD13	1:A:116:GLN:HG3	1.90	0.53
1:A:26:PHE:CA	1:A:29:ASP:CG	2.74	0.53
5:I:439:ILE:CG1	5:I:441:GLY:HA3	2.37	0.53
5:I:18:LEU:CD2	5:I:62:GLY:C	2.77	0.53
3:F:446:ARG:HA	3:F:447:LEU:HB2	1.90	0.53
1:A:273:SER:O	1:A:275:GLU:N	2.41	0.53
1:B:312:PRO:HG2	1:B:315:PHE:CD2	2.44	0.53
3:E:276:GLN:C	3:E:277:LYS:CG	2.53	0.53
3:E:355:LEU:HD22	3:E:372:SER:H	1.72	0.53
3:E:396:LEU:HB3	3:E:400:ILE:HD11	1.91	0.53
3:F:353:ARG:O	3:F:354:ALA:HB3	2.07	0.53
3:F:368:ILE:HA	3:F:385:ILE:C	2.17	0.53
3:F:429:GLU:HG3	3:F:445:GLU:CB	2.38	0.53
3:F:429:GLU:O	3:F:445:GLU:HA	2.09	0.53
3:F:67:ILE:HA	3:F:336:ILE:HG12	1.90	0.53
3:F:161:ASP:CG	4:G:134:THR:HG23	2.28	0.53
5:I:202:ASP:O	5:I:205:ILE:HG12	2.08	0.53
5:I:202:ASP:CG	5:I:205:ILE:HD11	2.28	0.53
3:E:162:LYS:NZ	3:E:166:ASP:OD2	2.35	0.53
3:E:260:SER:O	3:E:261:SER:OG	2.27	0.53
4:G:191:THR:HB	4:G:222:ILE:HG21	1.90	0.53
5:I:205:ILE:H	5:I:205:ILE:CD1	2.15	0.53
4:G:240:GLU:CD	4:G:241:LYS:N	2.61	0.53
3:E:389:VAL:HG12	3:E:406:VAL:H	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:204:ARG:HH11	3:F:204:ARG:HB3	1.73	0.53
3:F:425:LEU:N	3:F:425:LEU:HD12	2.22	0.53
5:I:29:TYR:CG	5:I:29:TYR:O	2.57	0.53
3:E:133:ARG:NE	3:E:257:GLU:CD	2.62	0.53
3:E:149:ASP:O	3:E:327:PRO:HD2	2.08	0.53
3:E:355:LEU:HD22	3:E:372:SER:CB	2.39	0.53
1:A:60:ASP:O	1:A:61:ILE:HD12	2.08	0.53
2:C:93:LEU:C	2:C:96:THR:HG23	2.28	0.53
3:F:181:GLU:H	3:F:334:LYS:CE	2.22	0.53
5:I:34:LEU:O	5:I:35:THR:OG1	2.26	0.53
5:I:436:LEU:HD12	5:I:437:VAL:N	2.24	0.53
5:J:439:ILE:HG22	5:J:442:ARG:H	1.69	0.53
2:D:301:ARG:HH21	2:D:362:LEU:HA	1.74	0.53
5:J:267:LYS:C	5:J:268:GLU:HG3	2.30	0.53
1:A:61:ILE:CD1	1:A:62:LEU:CD1	2.85	0.52
1:A:40:ILE:HG23	1:A:86:PHE:HD2	1.73	0.52
3:E:434:HIS:HB2	3:E:448:VAL:HG23	1.91	0.52
3:F:379:ILE:HA	3:F:396:LEU:HB2	1.91	0.52
3:F:403:GLU:HG3	3:F:404:ASP:H	1.74	0.52
3:F:419:ILE:HG22	3:F:436:VAL:CG2	2.39	0.52
3:E:182:HIS:HD2	3:E:334:LYS:CE	2.16	0.52
3:E:355:LEU:CD2	3:E:370:ASP:C	2.71	0.52
3:E:45:ALA:HB1	3:E:63:ALA:HB2	1.92	0.52
3:F:119:PRO:CG	3:F:122:LEU:HG	2.38	0.52
4:G:195:ASN:OD1	4:G:219:LYS:NZ	2.43	0.52
1:A:192:VAL:HG11	1:A:200:THR:HG21	1.92	0.52
3:E:340:THR:N	3:E:341:PRO:HD2	2.25	0.52
3:F:413:VAL:HB	3:F:430:ILE:HD11	1.91	0.52
4:H:117:GLU:C	4:H:119:GLN:HE21	2.12	0.52
5:I:431:LEU:CG	5:I:432:ASN:H	2.19	0.52
5:J:384:LEU:HD23	5:J:384:LEU:N	2.24	0.52
1:B:257:GLN:HA	1:B:310:VAL:HB	1.90	0.52
2:C:87:ARG:NH2	2:C:390:ASP:OD1	2.43	0.52
5:I:437:VAL:CG2	5:I:438:GLY:H	2.22	0.52
5:I:437:VAL:CG2	5:I:438:GLY:N	2.73	0.52
2:D:333:PRO:HD3	5:J:290:ARG:HB2	1.92	0.52
1:A:55:ILE:CG1	1:A:56:SER:N	2.73	0.52
3:E:269:TYR:HE1	3:E:270:LEU:HD23	1.62	0.52
3:F:429:GLU:CG	3:F:445:GLU:HB3	2.40	0.52
4:G:237:LEU:CD1	4:G:238:LEU:N	2.73	0.52
2:D:234:GLY:HA3	2:D:238:ASN:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:447:LEU:CG	3:F:448:VAL:N	2.72	0.52
4:G:228:ASP:OD1	4:G:228:ASP:N	2.43	0.52
5:J:418:LYS:CE	5:J:420:LEU:CG	2.85	0.52
3:E:384:VAL:O	3:E:402:VAL:N	2.43	0.52
3:F:122:LEU:HD11	3:F:131:ALA:CA	2.39	0.52
3:F:162:LYS:HE3	3:F:318:ILE:HD13	1.92	0.52
1:B:245:GLU:H	1:B:248:LYS:HE3	1.75	0.51
1:B:312:PRO:HG2	1:B:315:PHE:HD2	1.75	0.51
5:J:396:ILE:HG22	5:J:397:GLU:N	2.26	0.51
3:E:126:LYS:HD2	3:E:130:ASP:HB3	1.92	0.51
3:E:348:VAL:CG2	3:E:364:GLU:HG2	2.36	0.51
3:F:212:ALA:C	3:F:213:ASP:OD1	2.49	0.51
3:F:446:ARG:CB	3:F:447:LEU:CB	2.85	0.51
5:I:16:HIS:ND1	5:I:16:HIS:O	2.43	0.51
1:A:81:ALA:HB2	1:A:250:VAL:HB	1.92	0.51
3:E:257:GLU:HA	3:E:259:ILE:H	1.75	0.51
4:H:168:LEU:HD21	4:H:214:ALA:HB1	1.92	0.51
2:C:136:MET:CG	2:C:137:TYR:N	2.73	0.51
3:F:108:TYR:OH	3:F:112:MET:HB3	2.10	0.51
3:F:32:LEU:HD12	3:F:33:GLN:H	1.75	0.51
5:J:418:LYS:CE	5:J:420:LEU:N	2.73	0.51
1:A:202:ASN:HB3	1:B:258:TYR:CE2	2.45	0.51
2:D:308:VAL:HG22	2:D:365:LEU:HB3	1.92	0.51
3:E:385:ILE:CG2	3:E:389:VAL:CG2	2.89	0.51
3:F:212:ALA:C	3:F:213:ASP:CG	2.66	0.51
4:G:137:ILE:O	4:G:137:ILE:HG23	2.10	0.51
2:D:48:TRP:CE2	2:D:166:GLY:O	2.63	0.51
2:D:323:ASP:OD1	2:D:324:LEU:N	2.44	0.51
3:E:199:GLU:O	3:E:203:SER:N	2.43	0.51
3:F:379:ILE:HG12	3:F:396:LEU:HD12	1.92	0.51
3:E:255:GLU:HG2	3:E:256:LYS:N	2.25	0.51
3:E:434:HIS:HB2	3:E:448:VAL:N	2.25	0.51
3:F:263:ARG:O	3:F:267:ILE:HD11	2.10	0.51
3:F:378:ILE:O	3:F:396:LEU:N	2.37	0.51
5:I:107:GLY:HA2	5:I:110:LEU:HB2	1.93	0.51
3:E:428:CYS:SG	3:E:442:ALA:O	2.69	0.51
1:A:17:PHE:CD2	1:A:46:LEU:HD12	2.46	0.51
1:A:95:HIS:O	1:A:96:ASP:OD1	2.29	0.51
3:E:194:GLN:O	3:E:235:THR:HA	2.11	0.51
3:F:224:LEU:O	3:F:224:LEU:HG	2.11	0.51
3:F:363:ASN:HB3	3:F:380:GLY:C	2.30	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:410:GLU:O	4:G:411:GLU:HG3	2.10	0.51
5:J:381:LYS:HB3	5:J:398:ASP:CA	2.39	0.51
4:H:444:VAL:HG22	4:H:449:LEU:HG	1.93	0.51
2:C:85:LEU:HD11	2:C:176:GLY:HA3	1.92	0.50
3:E:126:LYS:HB3	3:E:130:ASP:HB2	1.93	0.50
3:F:215:GLY:HA2	3:F:218:PHE:CZ	2.46	0.50
3:F:385:ILE:HG23	3:F:389:VAL:HG21	1.93	0.50
5:J:305:THR:HB	5:J:317:GLU:HG3	1.92	0.50
3:F:35:ILE:HG22	4:G:142:HIS:HA	1.92	0.50
1:A:53:LYS:HZ1	1:A:104:LYS:NZ	0.92	0.50
1:A:62:LEU:O	1:A:65:GLY:C	2.50	0.50
3:F:195:LEU:O	3:F:196:ILE:HD13	2.11	0.50
3:F:387:LYS:CB	3:F:404:ASP:HB3	2.40	0.50
5:I:435:SER:OG	5:I:436:LEU:N	2.44	0.50
3:F:169:SER:HB2	3:F:315:LYS:NZ	2.27	0.50
3:F:202:THR:CB	3:F:204:ARG:HG2	2.41	0.50
1:B:125:ILE:HG21	1:B:243:VAL:HG13	1.93	0.50
2:D:199:LEU:HD11	2:D:218:LEU:HD23	1.94	0.50
3:F:446:ARG:HG2	3:F:447:LEU:CD2	2.42	0.50
5:J:439:ILE:HG21	5:J:442:ARG:N	2.26	0.50
1:A:29:ASP:OD1	1:A:30:ASP:N	2.45	0.50
2:C:313:ILE:HG21	2:C:370:LEU:HD22	1.92	0.50
3:E:37:ILE:O	3:E:37:ILE:HG13	2.11	0.50
3:F:269:TYR:C	3:F:269:TYR:CD1	2.85	0.50
3:F:386:GLY:O	3:F:404:ASP:HA	2.11	0.50
5:J:328:LYS:HD3	5:J:346:ALA:HB2	1.94	0.50
1:B:67:ASN:O	1:B:71:GLU:HG3	2.12	0.50
2:D:48:TRP:NE1	2:D:166:GLY:C	2.59	0.50
3:E:130:ASP:HA	3:E:133:ARG:NH2	2.26	0.50
3:F:123:ASP:CG	3:F:124:ASP:N	2.63	0.50
4:G:228:ASP:HB2	4:G:229:LEU:HD12	1.77	0.50
5:J:116:LYS:HD2	5:J:116:LYS:N	2.27	0.50
1:B:134:ARG:NH1	2:C:323:ASP:OD2	2.45	0.50
3:F:419:ILE:HG22	3:F:436:VAL:HG23	1.94	0.50
1:A:63:GLN:O	1:A:67:ASN:CB	2.59	0.50
3:F:251:ASP:O	3:F:255:GLU:HG3	2.11	0.50
3:F:218:PHE:HE2	5:I:203:PRO:HB3	0.78	0.50
2:C:287:LEU:HD11	2:C:309:VAL:HG21	1.94	0.49
4:H:271:ILE:HG21	4:H:284:LEU:HD21	1.93	0.49
5:J:133:ASN:OD1	5:J:269:ASN:HB3	2.11	0.49
3:E:276:GLN:NE2	3:E:276:GLN:N	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:MET:HG2	2:C:137:TYR:N	2.27	0.49
3:E:255:GLU:CD	3:E:255:GLU:H	2.16	0.49
3:E:269:TYR:C	3:E:269:TYR:CD1	2.85	0.49
3:E:271:VAL:O	3:E:272:LYS:HD3	2.12	0.49
3:E:437:GLU:OE1	3:E:437:GLU:N	2.45	0.49
4:H:406:VAL:HG13	4:H:406:VAL:O	2.10	0.49
5:I:140:LEU:O	5:I:144:ARG:HG3	2.12	0.49
5:I:433:ASP:CG	5:I:433:ASP:O	2.48	0.49
5:J:147:ARG:NH1	5:J:153:ALA:O	2.44	0.49
2:D:167:MET:HG3	2:D:168:ASP:N	2.28	0.49
3:F:280:THR:OG1	3:F:281:VAL:N	2.45	0.49
3:F:47:PHE:CE2	3:F:93:MET:HE2	2.47	0.49
5:J:414:ILE:O	5:J:415:GLU:HG2	2.12	0.49
1:A:115:ILE:O	1:A:119:ARG:HG3	2.12	0.49
1:A:96:ASP:O	1:A:97:VAL:HG22	2.12	0.49
3:E:262:ILE:HA	3:E:265:ASP:HB3	1.94	0.49
1:A:257:GLN:HA	1:A:310:VAL:HB	1.95	0.49
1:B:54:THR:HG22	1:B:57:GLU:CD	2.33	0.49
2:D:51:VAL:HG13	2:D:52:ASP:N	2.28	0.49
3:E:218:PHE:C	3:E:218:PHE:CD1	2.85	0.49
3:F:279:PHE:C	3:F:279:PHE:CD1	2.85	0.49
3:F:61:PRO:HD2	3:F:64:LEU:HD12	1.95	0.49
3:E:352:GLU:CG	3:E:369:LYS:HA	2.43	0.49
3:E:421:ALA:HB1	3:E:438:ALA:HB2	1.93	0.49
3:F:367:THR:HB	3:F:384:VAL:CG1	2.36	0.49
3:E:384:VAL:HB	3:E:401:VAL:HG13	1.94	0.49
3:F:400:ILE:HD13	3:F:413:VAL:HG23	1.95	0.49
5:I:202:ASP:N	5:I:202:ASP:OD1	2.40	0.49
5:J:293:TYR:CG	5:J:294:PRO:HA	2.48	0.49
2:C:12:ALA:HB1	2:C:38:VAL:HG22	1.94	0.49
2:D:169:MET:O	2:D:173:ILE:HG12	2.12	0.49
2:D:85:LEU:HD21	2:D:176:GLY:HA3	1.95	0.49
3:E:400:ILE:HG22	3:E:417:ALA:H	1.77	0.49
3:F:275:TYR:O	3:F:275:TYR:HD1	1.96	0.49
1:A:104:LYS:O	1:A:108:VAL:HG23	2.13	0.48
2:C:48:TRP:CH2	2:C:170:ARG:HG2	2.44	0.48
3:E:260:SER:O	3:E:264:GLY:CA	2.61	0.48
3:E:269:TYR:HD1	3:E:270:LEU:N	2.03	0.48
3:F:385:ILE:CD1	3:F:402:VAL:HG21	2.43	0.48
3:F:58:ASP:O	3:F:99:HIS:NE2	2.46	0.48
4:H:406:VAL:HG22	4:H:406:VAL:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:431:LEU:HD23	5:I:432:ASN:CA	2.43	0.48
1:A:39:ALA:O	1:A:43:LEU:HG	2.13	0.48
3:F:182:HIS:ND1	3:F:183:ILE:N	2.60	0.48
5:I:33:PRO:HG2	5:I:419:ARG:CG	2.26	0.48
5:J:194:ARG:HD3	5:J:195:GLY:N	2.28	0.48
3:E:218:PHE:HD1	3:E:219:THR:N	2.11	0.48
3:E:414:ALA:HB3	3:E:431:GLY:C	2.33	0.48
1:A:112:LYS:O	1:A:116:GLN:HG2	2.14	0.48
1:B:106:HIS:CD2	2:C:146:ARG:HD3	2.48	0.48
3:E:252:LEU:HD12	3:E:256:LYS:CE	2.43	0.48
3:F:269:TYR:HD1	3:F:271:VAL:HG13	1.79	0.48
1:B:77:ILE:HG21	1:B:221:ILE:HD12	1.95	0.48
3:F:321:SER:OG	3:F:321:SER:O	2.28	0.48
3:F:368:ILE:HA	3:F:385:ILE:H	1.78	0.48
3:F:71:PRO:HG2	3:F:103:TRP:CE2	2.49	0.48
4:G:121:SER:HB3	4:G:124:SER:HB3	1.94	0.48
4:G:210:SER:HB3	4:G:380:LYS:HG2	1.96	0.48
1:A:230:ALA:HB1	1:A:315:PHE:HB3	1.96	0.48
1:B:94:LEU:HA	1:B:98:GLY:HA2	1.95	0.48
3:E:149:ASP:O	3:E:327:PRO:CD	2.61	0.48
3:E:149:ASP:CB	3:E:327:PRO:HD2	2.25	0.48
4:G:286:HIS:O	4:G:290:VAL:HG23	2.13	0.48
1:A:61:ILE:CD1	1:A:62:LEU:N	2.73	0.48
2:C:87:ARG:HH11	2:C:87:ARG:CG	2.12	0.48
4:G:416:LEU:HD13	4:G:427:LEU:HD11	1.96	0.48
4:H:312:LYS:NZ	4:H:316:GLU:OE2	2.44	0.48
5:I:327:ILE:HG22	5:I:345:VAL:HB	1.96	0.48
1:A:17:PHE:HE2	1:A:46:LEU:HB2	1.79	0.48
3:E:130:ASP:HA	3:E:133:ARG:NH1	2.28	0.48
3:E:349:THR:OG1	3:E:350:VAL:N	2.47	0.48
1:A:106:HIS:ND1	1:A:110:ASN:OD1	2.45	0.48
2:C:53:GLN:O	2:C:57:THR:OG1	2.22	0.48
3:E:441:ILE:HG13	3:E:443:ARG:NH2	2.28	0.48
3:E:149:ASP:HB2	3:E:327:PRO:CD	2.26	0.48
3:F:383:CYS:CB	3:F:400:ILE:O	2.62	0.48
4:G:240:GLU:N	4:G:240:GLU:OE1	2.47	0.48
5:J:21:ILE:HG12	5:J:113:LEU:HD11	1.94	0.48
2:D:388:ALA:HA	2:D:391:THR:HG23	1.96	0.47
3:E:81:GLU:CD	3:E:110:GLY:O	2.52	0.47
3:E:269:TYR:CE1	3:E:270:LEU:CD2	2.80	0.47
3:F:340:THR:N	3:F:341:PRO:HD3	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HA	1:A:61:ILE:CG1	2.43	0.47
3:E:276:GLN:O	3:E:277:LYS:CD	2.58	0.47
3:E:379:ILE:HA	3:E:396:LEU:HB2	1.96	0.47
3:F:269:TYR:CD1	3:F:271:VAL:HG13	2.49	0.47
5:J:169:ARG:NH2	5:J:216:ASN:OD1	2.47	0.47
1:A:89:PHE:HE2	1:A:107:LEU:HD21	1.79	0.47
2:C:83:LEU:O	2:C:87:ARG:HG3	2.14	0.47
3:F:241:HIS:HB2	3:F:326:LEU:HD21	1.95	0.47
3:F:419:ILE:CB	3:F:436:VAL:HB	2.43	0.47
4:G:308:ARG:NH2	4:G:406:VAL:O	2.47	0.47
5:J:29:TYR:CE2	5:J:30:ARG:CD	2.97	0.47
1:A:54:THR:H	1:A:57:GLU:HB3	1.80	0.47
2:C:199:LEU:HD11	2:C:218:LEU:HD23	1.95	0.47
3:E:370:ASP:OD1	3:E:370:ASP:N	2.36	0.47
5:I:18:LEU:HD21	5:I:62:GLY:C	2.34	0.47
5:J:105:SER:OG	5:J:108:ASP:OD2	2.32	0.47
1:A:130:TYR:HB2	1:A:155:ALA:HB2	1.95	0.47
2:C:169:MET:O	2:C:173:ILE:HG12	2.14	0.47
2:C:3:THR:O	2:C:6:VAL:HG12	2.14	0.47
2:C:4:ILE:O	2:C:7:GLU:HB2	2.15	0.47
2:C:7:GLU:OE2	5:I:90:SER:OG	2.24	0.47
1:A:316:VAL:HB	1:A:329:LYS:HE3	1.96	0.47
2:D:233:GLU:OE1	4:H:302:ARG:HD3	2.15	0.47
3:F:440:ARG:O	3:F:441:ILE:HG13	2.14	0.47
5:I:421:THR:OG1	5:I:422:THR:N	2.47	0.47
3:E:230:ARG:NH2	5:J:213:GLU:OE2	2.41	0.47
3:F:243:PHE:CE2	3:F:262:ILE:HG21	2.49	0.47
3:F:336:ILE:HD12	3:F:395:ILE:CD1	2.35	0.47
5:I:435:SER:O	5:I:436:LEU:C	2.53	0.47
3:E:245:PHE:HB3	3:E:249:VAL:HG21	1.97	0.47
3:E:256:LYS:O	3:E:259:ILE:HG12	2.15	0.47
3:E:346:VAL:HG13	3:E:348:VAL:HG22	1.97	0.47
4:H:220:LEU:O	4:H:224:VAL:HG23	2.15	0.47
5:I:178:VAL:HB	5:I:188:HIS:HB3	1.96	0.47
3:E:218:PHE:O	5:J:200:SER:HA	2.14	0.47
1:A:53:LYS:N	1:A:53:LYS:CD	2.73	0.47
3:F:329:TYR:HB2	3:F:331:GLU:HG3	1.95	0.47
3:F:399:ASN:HB2	3:F:416:GLY:H	1.80	0.47
1:A:100:PHE:N	1:A:100:PHE:CD1	2.78	0.47
1:B:125:ILE:HG23	1:B:320:ILE:HG22	1.96	0.47
3:E:218:PHE:CD1	3:E:219:THR:N	2.83	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:241:HIS:HA	3:E:243:PHE:CE2	2.50	0.47
3:F:413:VAL:HG12	3:F:430:ILE:HG12	1.97	0.47
4:G:274:TYR:CD1	4:G:275:LEU:HG	2.49	0.47
2:D:349:GLU:OE2	5:J:311:HIS:HA	2.15	0.46
3:E:355:LEU:CD2	3:E:372:SER:H	2.27	0.46
3:F:155:PRO:HA	3:F:156:PRO:HD3	1.80	0.46
3:F:206:LEU:HB3	3:F:224:LEU:HD11	1.98	0.46
3:F:235:THR:HG21	5:I:206:PHE:HB3	1.97	0.46
5:I:30:ARG:NH2	6:I:701:PO4:O3	2.48	0.46
5:I:332:LEU:HD22	5:I:349:ILE:HG23	1.97	0.46
3:E:260:SER:O	3:E:264:GLY:HA3	2.16	0.46
3:F:267:ILE:O	3:F:270:LEU:HD21	2.14	0.46
2:C:167:MET:CG	2:C:168:ASP:N	2.67	0.46
3:F:344:ARG:HG3	3:F:344:ARG:H	1.43	0.46
4:G:175:ILE:HG12	4:G:190:LEU:HD11	1.98	0.46
2:C:87:ARG:HH22	2:C:390:ASP:CG	2.19	0.46
1:A:114:PHE:CE1	2:D:144:LEU:HA	2.50	0.46
3:E:128:SER:N	3:E:261:SER:HA	2.30	0.46
3:F:224:LEU:HD12	3:F:272:LYS:HD2	1.97	0.46
5:I:439:ILE:CD1	5:I:440:GLY:N	2.57	0.46
5:J:115:SER:C	5:J:116:LYS:HD2	2.35	0.46
1:A:19:ILE:HD12	1:A:46:LEU:HD13	1.97	0.46
2:C:313:ILE:HG12	2:C:370:LEU:HD13	1.96	0.46
3:E:397:MET:HG3	3:E:413:VAL:O	2.16	0.46
1:A:61:ILE:HD13	1:A:62:LEU:CG	2.46	0.46
3:E:320:CYS:SG	3:E:322:ARG:N	2.89	0.46
3:E:34:SER:C	3:E:35:ILE:HG13	2.36	0.46
3:F:127:SER:CB	3:F:261:SER:HB2	2.43	0.46
4:G:218:LEU:O	4:G:222:ILE:HG12	2.16	0.46
4:H:411:GLU:CD	4:H:411:GLU:H	2.18	0.46
4:H:416:LEU:HD22	4:H:425:LEU:HD21	1.98	0.46
3:E:369:LYS:N	3:E:385:ILE:O	2.34	0.46
4:G:240:GLU:O	4:G:244:SER:OG	2.20	0.46
5:J:19:GLN:OE1	5:J:119:ILE:HA	2.15	0.46
1:A:92:ARG:CZ	2:D:137:TYR:HD2	2.29	0.46
2:C:162:ARG:HE	2:C:162:ARG:HA	1.74	0.46
3:E:257:GLU:HG3	3:E:259:ILE:HB	1.96	0.46
3:E:362:VAL:O	3:E:362:VAL:HG13	2.15	0.46
3:F:381:LYS:O	3:F:382:ASN:HB2	2.16	0.46
2:C:63:SER:OG	2:C:67:LYS:NZ	2.48	0.46
3:F:241:HIS:HA	3:F:243:PHE:CZ	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:274:GLN:O	3:F:275:TYR:CG	2.69	0.46
3:F:382:ASN:ND2	3:F:399:ASN:OD1	2.45	0.46
1:B:187:ILE:HA	1:B:187:ILE:HD12	1.88	0.45
3:E:34:SER:O	3:E:35:ILE:HG13	2.16	0.45
3:E:448:VAL:HG12	3:E:449:ASP:N	2.31	0.45
1:A:125:ILE:HG21	1:A:243:VAL:HG13	1.98	0.45
2:C:48:TRP:O	2:C:48:TRP:CD1	2.69	0.45
5:J:33:PRO:HG2	5:J:419:ARG:CB	2.46	0.45
3:E:346:VAL:CG1	3:E:348:VAL:HG22	2.46	0.45
3:F:164:ARG:NH1	4:G:134:THR:HG21	2.31	0.45
5:I:416:LYS:CB	5:I:417:ASN:ND2	2.79	0.45
1:A:66:SER:O	1:A:70:LYS:N	2.39	0.45
1:A:202:ASN:HB3	1:B:258:TYR:CZ	2.51	0.45
5:I:323:ARG:O	5:I:324:SER:OG	2.32	0.45
5:I:418:LYS:HD2	5:I:418:LYS:HA	1.90	0.45
1:A:192:VAL:HA	1:B:305:ASN:HD21	1.82	0.45
1:A:22:VAL:O	1:A:25:LYS:N	2.50	0.45
2:C:180:VAL:HA	2:C:183:GLU:HG3	1.99	0.45
3:E:181:GLU:OE1	3:E:182:HIS:CG	2.69	0.45
3:E:218:PHE:C	3:E:218:PHE:HD1	2.20	0.45
3:F:122:LEU:HD13	3:F:131:ALA:CB	2.46	0.45
3:F:125:SER:O	3:F:126:LYS:HG2	2.17	0.45
5:I:401:ILE:HB	5:I:419:ARG:HG3	1.97	0.45
5:J:402:VAL:HG22	5:J:420:LEU:HD12	1.97	0.45
1:A:18:ASP:CG	1:A:21:GLN:CG	2.85	0.45
2:C:162:ARG:NE	2:C:162:ARG:CA	2.75	0.45
2:C:247:LYS:NZ	2:C:251:GLN:OE1	2.45	0.45
4:H:409:PHE:CD1	4:H:409:PHE:O	2.70	0.45
5:J:146:ARG:HD2	5:J:262:HIS:CE1	2.51	0.45
5:J:309:GLN:HB2	5:J:313:ILE:HG13	1.99	0.45
5:J:339:VAL:HA	5:J:356:ILE:HB	1.98	0.45
1:B:220:LEU:HB2	1:B:311:THR:HB	1.97	0.45
2:C:49:SER:N	2:C:167:MET:HE2	2.31	0.45
2:D:80:ARG:NH1	2:D:391:THR:O	2.50	0.45
3:E:192:ALA:HB3	3:E:329:TYR:OH	2.17	0.45
3:E:35:ILE:HD11	4:H:140:ASP:HA	1.97	0.45
3:E:397:MET:CE	3:E:414:ALA:HA	2.46	0.45
3:F:71:PRO:HG2	3:F:103:TRP:NE1	2.32	0.45
3:F:178:LEU:HD23	3:F:178:LEU:HA	1.79	0.45
4:G:240:GLU:HG2	4:G:241:LYS:HG2	1.99	0.45
4:G:436:PRO:HA	4:G:437:PRO:HD3	1.86	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:27:TYR:C	5:I:28:ASN:O	2.51	0.45
3:E:366:THR:HG23	3:E:383:CYS:HB2	1.99	0.45
3:E:71:PRO:HG2	3:E:103:TRP:NE1	2.32	0.45
3:F:275:TYR:O	3:F:275:TYR:CD1	2.70	0.45
4:G:408:ASP:O	4:G:409:PHE:CG	2.70	0.45
5:I:439:ILE:HG13	5:I:441:GLY:CA	2.44	0.45
1:A:19:ILE:HG23	1:A:20:VAL:N	2.32	0.44
1:A:28:GLN:CD	1:A:28:GLN:N	2.71	0.44
1:A:36:PRO:HG2	1:A:247:HIS:HD2	1.82	0.44
3:E:434:HIS:HA	3:E:448:VAL:HG23	1.99	0.44
3:F:181:GLU:CG	3:F:182:HIS:N	2.79	0.44
3:F:259:ILE:HD12	3:F:259:ILE:O	2.17	0.44
3:F:332:LEU:O	3:F:336:ILE:HG13	2.17	0.44
4:G:274:TYR:CE1	4:G:275:LEU:HG	2.53	0.44
4:G:408:ASP:O	4:G:409:PHE:CD2	2.70	0.44
5:J:23:LEU:HD21	5:J:106:VAL:HA	1.99	0.44
1:A:46:LEU:C	1:A:50:SER:HG	2.02	0.44
3:E:155:PRO:HA	3:E:156:PRO:HD3	1.76	0.44
3:E:262:ILE:HG22	3:E:262:ILE:O	2.16	0.44
3:E:273:CYS:O	3:E:275:TYR:CD2	2.70	0.44
3:E:275:TYR:O	3:E:275:TYR:CD1	2.70	0.44
3:E:352:GLU:C	3:E:354:ALA:H	2.20	0.44
3:F:181:GLU:HG3	3:F:182:HIS:N	2.32	0.44
3:F:318:ILE:C	3:F:319:ILE:HG13	2.38	0.44
4:G:257:ILE:HG23	4:G:444:VAL:HG12	2.00	0.44
4:G:348:SER:OG	4:G:382:THR:O	2.31	0.44
4:G:409:PHE:O	4:G:409:PHE:CD1	2.70	0.44
4:H:221:GLU:OE1	4:H:241:LYS:NZ	2.40	0.44
4:H:277:SER:OG	4:H:342:GLY:HA3	2.17	0.44
5:I:24:SER:O	5:I:25:ASP:CB	2.63	0.44
5:J:418:LYS:NZ	5:J:420:LEU:CA	2.73	0.44
2:C:17:ILE:HG22	2:C:21:LYS:HD2	1.99	0.44
3:E:181:GLU:OE1	3:E:182:HIS:CE1	2.70	0.44
3:E:229:PRO:HB2	5:J:217:ASP:HB3	1.99	0.44
3:E:402:VAL:HA	3:E:419:ILE:HG13	1.99	0.44
3:F:381:LYS:N	3:F:398:ASP:OD1	2.51	0.44
4:H:115:PHE:CE1	4:H:117:GLU:O	2.71	0.44
5:J:418:LYS:HZ2	5:J:419:ARG:C	2.21	0.44
5:J:430:THR:O	5:J:435:SER:OG	2.32	0.44
2:C:8:HIS:CD2	5:I:89:PRO:HG3	2.53	0.44
2:D:87:ARG:NH1	2:D:390:ASP:OD2	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:139:ILE:HB	3:E:250:ILE:HD13	1.98	0.44
3:F:92:CYS:SG	3:F:100:ILE:HD12	2.57	0.44
1:B:88:ARG:HH22	1:B:341:LEU:HD12	1.82	0.44
2:C:47:ARG:HB2	2:C:170:ARG:NH2	2.33	0.44
3:E:35:ILE:HG23	4:H:143:PRO:HD3	1.98	0.44
3:E:360:CYS:HB2	3:E:377:SER:O	2.18	0.44
3:F:182:HIS:CE1	3:F:183:ILE:O	2.71	0.44
3:F:214:VAL:CG2	3:F:218:PHE:CD1	3.01	0.44
3:F:267:ILE:N	3:F:268:PRO:CD	2.81	0.44
3:F:339:LEU:HD22	3:F:339:LEU:HA	1.76	0.44
3:F:333:ASN:HB2	3:F:412:ILE:HD11	1.99	0.44
4:G:354:SER:OG	4:G:355:ARG:N	2.50	0.44
5:J:418:LYS:CD	5:J:418:LYS:C	2.85	0.44
2:C:93:LEU:O	2:C:96:THR:HG23	2.17	0.44
3:E:274:GLN:O	3:E:275:TYR:CD1	2.70	0.44
3:F:183:ILE:N	3:F:183:ILE:CD1	2.81	0.44
3:F:397:MET:HB3	3:F:415:SER:OG	2.17	0.44
4:G:408:ASP:OD1	4:G:409:PHE:CD2	2.71	0.44
1:A:58:PHE:CD1	1:A:58:PHE:O	2.70	0.44
1:A:59:MET:C	1:A:61:ILE:CG1	2.85	0.44
1:A:59:MET:C	1:A:61:ILE:CD1	2.86	0.44
1:B:33:ILE:O	1:B:146:ARG:NH1	2.46	0.44
3:E:434:HIS:CG	3:E:435:ARG:N	2.86	0.44
3:E:434:HIS:CD2	3:E:447:LEU:HA	2.52	0.44
3:F:122:LEU:CD1	3:F:131:ALA:HB2	2.48	0.44
3:F:274:GLN:O	3:F:275:TYR:CD2	2.70	0.44
4:G:408:ASP:OD1	4:G:409:PHE:CE2	2.70	0.44
2:D:256:THR:N	4:H:424:ASN:O	2.49	0.44
5:J:418:LYS:CE	5:J:419:ARG:C	2.85	0.44
1:A:130:TYR:CD2	1:A:131:PRO:HD3	2.52	0.44
1:A:17:PHE:CD1	1:A:17:PHE:O	2.70	0.44
1:B:25:LYS:HA	1:B:28:GLN:HE22	1.81	0.44
3:E:181:GLU:OE1	3:E:182:HIS:CD2	2.70	0.44
3:E:396:LEU:HD23	3:E:413:VAL:HB	1.98	0.44
5:J:385:ALA:HB3	5:J:403:ALA:HA	2.00	0.44
1:A:59:MET:O	1:A:61:ILE:HD11	2.17	0.44
2:C:235:PHE:CE2	4:G:325:MET:HE2	2.53	0.44
2:D:184:LEU:O	2:D:187:ILE:HG12	2.18	0.44
2:D:331:SER:OG	2:D:332:SER:N	2.51	0.44
3:E:181:GLU:OE2	3:E:182:HIS:CE1	2.70	0.44
3:E:245:PHE:CD1	3:E:249:VAL:HG11	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:276:GLN:NE2	3:E:276:GLN:H	2.15	0.44
3:F:383:CYS:HB2	3:F:400:ILE:O	2.18	0.44
4:G:208:SER:HB2	4:G:344:HIS:NE2	2.33	0.44
5:J:418:LYS:HD2	5:J:418:LYS:C	2.39	0.44
3:F:354:ALA:CB	3:F:370:ASP:OD1	2.56	0.43
4:H:329:LEU:HD21	4:H:361:ILE:HA	2.00	0.43
5:I:18:LEU:HD23	5:I:62:GLY:O	2.15	0.43
5:J:322:ALA:O	5:J:325:CYS:HB3	2.18	0.43
1:A:52:ALA:CA	1:A:57:GLU:OE1	2.65	0.43
1:B:28:GLN:CD	1:B:28:GLN:H	2.22	0.43
2:C:313:ILE:HG13	2:C:313:ILE:H	1.60	0.43
3:F:204:ARG:NH1	3:F:204:ARG:HB3	2.33	0.43
4:G:258:VAL:HA	4:G:283:VAL:HG22	2.00	0.43
3:F:214:VAL:HG23	3:F:218:PHE:HD1	1.81	0.43
3:F:315:LYS:N	3:F:315:LYS:HD2	2.33	0.43
3:F:434:HIS:CG	3:F:447:LEU:O	2.71	0.43
4:G:186:LEU:HD11	4:G:190:LEU:HD22	2.01	0.43
5:J:366:PHE:N	5:J:382:ALA:O	2.45	0.43
2:D:289:THR:OG1	2:D:290:TYR:N	2.52	0.43
3:F:446:ARG:CA	3:F:447:LEU:CB	2.93	0.43
3:F:51:LEU:HD22	3:F:54:LEU:HD12	2.00	0.43
4:H:411:GLU:O	4:H:412:LYS:CG	2.66	0.43
5:I:178:VAL:HG22	5:I:214:VAL:HG22	2.00	0.43
2:C:136:MET:CG	2:C:137:TYR:H	2.28	0.43
2:C:48:TRP:CE2	2:C:54:LEU:HD22	2.53	0.43
3:E:260:SER:O	3:E:264:GLY:N	2.51	0.43
1:A:53:LYS:HZ1	1:A:104:LYS:HZ3	0.44	0.43
1:B:54:THR:O	1:B:57:GLU:HG2	2.18	0.43
3:E:255:GLU:CD	3:E:255:GLU:N	2.71	0.43
3:E:327:PRO:HG2	3:E:327:PRO:O	2.19	0.43
3:F:269:TYR:CD1	3:F:270:LEU:CA	2.96	0.43
5:I:203:PRO:O	5:I:205:ILE:N	2.52	0.43
5:J:362:ILE:HA	5:J:379:ILE:O	2.18	0.43
1:B:134:ARG:HA	1:B:134:ARG:HD3	1.69	0.43
3:E:355:LEU:CD1	3:E:368:ILE:HG13	2.44	0.43
5:I:242:ASP:O	5:I:246:ASP:HB2	2.19	0.43
5:J:29:TYR:CE2	5:J:30:ARG:HD3	2.54	0.43
5:J:426:HIS:C	5:J:426:HIS:ND1	2.72	0.43
1:A:113:LEU:HD12	1:A:116:GLN:HG3	2.01	0.43
3:E:274:GLN:CB	3:E:276:GLN:NE2	2.73	0.43
1:A:105:ARG:O	1:A:109:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HD12	1:B:206:LEU:HD22	2.00	0.43
3:E:355:LEU:CB	3:E:372:SER:O	2.56	0.43
3:E:375:LYS:O	3:E:392:SER:HA	2.18	0.43
3:F:213:ASP:OD1	3:F:214:VAL:HG22	2.19	0.43
3:F:247:HIS:O	3:F:250:ILE:HG22	2.19	0.43
4:H:348:SER:OG	4:H:383:GLU:HA	2.18	0.43
5:J:178:VAL:HG22	5:J:214:VAL:HG13	1.99	0.43
1:A:77:ILE:HG21	1:A:221:ILE:HD12	2.01	0.43
1:A:54:THR:O	1:A:57:GLU:N	2.51	0.43
1:A:60:ASP:N	1:A:61:ILE:HG13	2.34	0.43
3:E:211:SER:O	3:E:214:VAL:HG13	2.19	0.43
3:E:67:ILE:HA	3:E:336:ILE:HG12	2.01	0.43
3:F:101:ASN:O	3:F:105:ARG:HG2	2.18	0.43
3:F:155:PRO:O	3:F:158:THR:OG1	2.36	0.43
3:F:262:ILE:HA	3:F:265:ASP:HB3	2.01	0.42
2:C:233:GLU:OE2	4:G:302:ARG:HD3	2.19	0.42
5:J:209:HIS:HB3	5:J:212:LEU:HD21	2.01	0.42
5:J:423:PHE:HB3	5:J:424:GLU:H	1.58	0.42
1:B:130:TYR:CD2	1:B:131:PRO:HD3	2.54	0.42
2:D:187:ILE:HG13	2:D:188:ASN:H	1.84	0.42
3:E:143:PHE:CE1	3:E:250:ILE:HG23	2.54	0.42
3:F:401:VAL:HG22	3:F:418:GLN:HA	2.01	0.42
5:J:121:SER:OG	5:J:122:ASP:N	2.50	0.42
5:J:400:ALA:O	5:J:401:ILE:CG1	2.62	0.42
5:J:414:ILE:HG22	5:J:415:GLU:N	2.34	0.42
5:J:50:LEU:HD22	5:J:274:VAL:HG21	2.00	0.42
2:D:177:ILE:O	2:D:181:ILE:HG12	2.19	0.42
2:D:237:ASN:HD21	2:D:354:TYR:HA	1.84	0.42
3:E:334:LYS:HD2	3:E:334:LYS:HA	1.88	0.42
3:E:31:GLN:HB3	3:E:33:GLN:OE1	2.19	0.42
3:F:182:HIS:ND1	3:F:183:ILE:C	2.73	0.42
3:F:368:ILE:HG22	3:F:385:ILE:CB	2.46	0.42
3:F:429:GLU:HG3	3:F:445:GLU:HB3	1.98	0.42
5:I:416:LYS:C	5:I:417:ASN:ND2	2.73	0.42
5:J:116:LYS:HB2	5:J:118:LEU:HG	2.02	0.42
1:A:258:TYR:CE2	1:B:202:ASN:HB3	2.54	0.42
3:E:257:GLU:HA	3:E:259:ILE:HG12	2.01	0.42
3:E:381:LYS:O	3:E:399:ASN:N	2.41	0.42
3:E:389:VAL:HG12	3:E:405:GLY:CA	2.49	0.42
3:F:351:SER:OG	3:F:355:LEU:HD13	2.14	0.42
3:F:385:ILE:HD11	3:F:402:VAL:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:425:LEU:CD1	3:F:425:LEU:N	2.83	0.42
3:F:55:THR:HG21	3:F:62:LYS:HB2	2.00	0.42
4:G:419:TRP:CZ2	4:G:420:LYS:HD3	2.54	0.42
5:I:27:TYR:O	5:I:28:ASN:C	2.58	0.42
5:J:35:THR:HA	5:J:38:LYS:O	2.19	0.42
1:B:21:GLN:O	1:B:25:LYS:HB2	2.20	0.42
2:D:393:LEU:HA	2:D:393:LEU:HD12	1.88	0.42
3:F:205:LEU:HD21	3:F:208:ALA:HB2	2.01	0.42
5:I:53:TYR:CG	5:I:131:VAL:HG12	2.55	0.42
3:F:280:THR:O	3:F:281:VAL:HB	2.20	0.42
3:F:387:LYS:HB2	3:F:404:ASP:CB	2.45	0.42
3:F:382:ASN:HB2	3:F:399:ASN:H	1.84	0.42
4:G:135:GLU:O	4:G:136:ASN:HB2	2.20	0.42
4:G:241:LYS:HA	4:G:244:SER:CB	2.42	0.42
5:J:116:LYS:HA	5:J:116:LYS:HE3	2.02	0.42
5:J:304:GLN:N	5:J:304:GLN:OE1	2.50	0.42
5:J:323:ARG:O	5:J:324:SER:OG	2.28	0.42
5:J:386:ASN:N	5:J:386:ASN:ND2	2.60	0.42
1:B:257:GLN:HG3	1:B:257:GLN:H	1.58	0.42
2:C:53:GLN:OE1	2:C:53:GLN:N	2.53	0.42
3:E:272:LYS:O	3:E:273:CYS:HB2	2.20	0.42
3:E:352:GLU:HG3	3:E:369:LYS:C	2.40	0.42
3:E:384:VAL:HB	3:E:401:VAL:HG22	2.01	0.42
5:J:134:VAL:HG23	5:J:270:TYR:O	2.19	0.42
1:A:22:VAL:HA	1:A:25:LYS:HG3	2.02	0.42
2:D:212:LYS:N	6:D:401:PO4:O4	2.53	0.42
3:E:274:GLN:CD	3:E:274:GLN:N	2.72	0.42
3:E:36:PRO:HD2	4:H:143:PRO:HG2	2.02	0.42
3:E:442:ALA:O	3:E:444:GLY:N	2.53	0.42
3:F:147:SER:HB2	3:F:241:HIS:CE1	2.55	0.42
3:F:385:ILE:CG1	3:F:402:VAL:HG21	2.46	0.42
5:J:33:PRO:HG2	5:J:419:ARG:CG	2.49	0.42
5:J:418:LYS:NZ	5:J:419:ARG:C	2.72	0.42
5:J:431:LEU:HD23	5:J:432:ASN:N	2.35	0.42
2:C:93:LEU:HD12	2:C:96:THR:OG1	2.19	0.42
3:E:267:ILE:HB	3:E:268:PRO:HD3	2.02	0.42
3:F:124:ASP:C	3:F:126:LYS:H	2.21	0.42
4:H:122:ILE:HD11	4:H:123:PHE:CZ	2.55	0.42
4:H:208:SER:HB2	4:H:344:HIS:NE2	2.35	0.42
5:I:211:GLU:O	5:I:212:LEU:HG	2.19	0.42
5:I:63:VAL:O	5:I:93:PHE:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:MET:HB3	1:A:35:MET:HE2	1.95	0.42
3:E:207:TYR:CE1	3:E:209:LYS:HB2	2.55	0.42
3:E:169:SER:OG	3:E:313:ILE:HG13	2.20	0.41
3:E:274:GLN:C	3:E:276:GLN:NE2	2.73	0.41
4:G:403:ASN:C	4:G:403:ASN:ND2	2.73	0.41
5:I:19:GLN:OE1	5:I:120:THR:N	2.45	0.41
1:A:175:GLY:O	1:A:179:THR:OG1	2.30	0.41
1:A:47:LEU:C	1:A:50:SER:OG	2.58	0.41
3:E:81:GLU:OE1	3:E:110:GLY:O	2.38	0.41
3:E:355:LEU:HD21	3:E:370:ASP:HA	1.83	0.41
3:F:274:GLN:HG3	3:F:274:GLN:H	1.57	0.41
3:F:367:THR:O	3:F:384:VAL:CB	2.68	0.41
3:F:385:ILE:CG2	3:F:386:GLY:N	2.82	0.41
2:C:287:LEU:HB2	2:C:358:ILE:HB	2.02	0.41
2:D:140:MET:HB3	2:D:140:MET:HE2	1.99	0.41
3:F:172:ALA:O	3:F:317:GLY:HA2	2.20	0.41
3:F:423:SER:HA	3:F:438:ALA:O	2.21	0.41
4:H:347:LEU:HD23	4:H:386:GLN:H	1.85	0.41
5:I:409:GLY:CA	5:I:433:ASP:HB2	2.50	0.41
1:B:276:THR:HG23	1:B:278:HIS:HB3	1.28	0.41
1:B:322:ASP:OD1	1:B:322:ASP:N	2.41	0.41
3:E:266:LEU:HB3	3:E:267:ILE:HD13	2.03	0.41
3:F:199:GLU:C	3:F:200:GLU:O	2.57	0.41
3:F:351:SER:HG	3:F:355:LEU:CD1	2.29	0.41
3:F:388:GLY:C	3:F:405:GLY:HA2	2.40	0.41
4:G:175:ILE:O	4:G:178:TYR:HB3	2.20	0.41
4:H:117:GLU:C	4:H:119:GLN:NE2	2.73	0.41
1:A:264:ARG:CZ	1:A:303:ARG:HD2	2.50	0.41
1:A:330:SER:O	1:A:334:GLU:HG3	2.20	0.41
2:C:193:VAL:HA	2:C:220:PHE:CE1	2.55	0.41
2:C:378:LEU:HD23	2:C:381:ILE:HD12	2.02	0.41
3:E:181:GLU:OE1	3:E:182:HIS:N	2.53	0.41
3:F:335:CYS:O	3:F:338:LYS:HB3	2.21	0.41
5:I:16:HIS:ND1	5:I:16:HIS:C	2.74	0.41
5:J:140:LEU:O	5:J:144:ARG:HG3	2.21	0.41
5:J:383:ILE:O	5:J:384:LEU:HD23	2.20	0.41
1:A:66:SER:HA	1:A:69:LEU:HB3	2.02	0.41
1:B:81:ALA:HB2	1:B:250:VAL:HB	2.03	0.41
3:E:276:GLN:CD	3:E:276:GLN:N	2.73	0.41
3:E:434:HIS:ND1	3:E:448:VAL:HA	2.35	0.41
3:F:129:ALA:HB2	3:F:262:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:278:SER:OG	3:F:278:SER:O	2.26	0.41
4:H:359:SER:OG	4:H:433:ASP:OD2	2.34	0.41
5:I:230:VAL:HB	5:I:231:PRO:HD3	2.02	0.41
5:J:436:LEU:HA	5:J:437:VAL:HA	1.97	0.41
3:E:332:LEU:O	3:E:336:ILE:HG13	2.19	0.41
4:H:411:GLU:CD	4:H:411:GLU:N	2.73	0.41
5:I:160:ARG:HB3	5:I:219:ILE:HB	2.03	0.41
5:I:293:TYR:CG	5:I:294:PRO:HA	2.56	0.41
1:A:148:VAL:HG13	1:A:208:LEU:HD23	2.03	0.41
3:F:214:VAL:CG2	3:F:218:PHE:HD1	2.33	0.41
4:G:139:LYS:H	4:G:139:LYS:CD	2.32	0.41
4:G:241:LYS:O	4:G:245:TYR:CB	2.67	0.41
4:G:403:ASN:ND2	4:G:407:ASP:O	2.54	0.41
2:C:377:TYR:HH	4:H:460:ASN:ND2	2.17	0.41
5:I:293:TYR:CD1	5:I:294:PRO:HA	2.56	0.41
5:I:436:LEU:CD1	5:I:436:LEU:C	2.85	0.41
5:J:293:TYR:CD1	5:J:294:PRO:HA	2.56	0.41
1:A:217:ASN:HB3	1:A:253:PHE:CZ	2.56	0.41
2:C:289:THR:OG1	2:C:290:TYR:N	2.54	0.41
2:D:187:ILE:HG13	2:D:188:ASN:N	2.36	0.41
2:D:294:GLN:HG2	2:D:298:GLN:HG2	2.02	0.41
3:F:205:LEU:C	3:F:206:LEU:HD12	2.41	0.41
3:F:429:GLU:HG3	3:F:445:GLU:HB2	2.03	0.41
4:G:238:LEU:HD23	4:G:238:LEU:HA	1.76	0.41
4:G:240:GLU:CD	4:G:241:LYS:HG2	2.41	0.41
4:G:274:TYR:CZ	4:G:275:LEU:HD11	2.55	0.41
4:H:332:ILE:HD12	4:H:332:ILE:HA	1.96	0.41
1:A:19:ILE:CG2	1:A:20:VAL:N	2.84	0.41
1:A:21:GLN:O	1:A:25:LYS:HG3	2.21	0.41
1:B:126:ALA:HA	1:B:151:VAL:HG22	2.03	0.41
2:C:313:ILE:HG13	2:C:369:ASN:OD1	2.21	0.41
3:F:353:ARG:O	3:F:354:ALA:CB	2.69	0.41
3:F:368:ILE:CG2	3:F:385:ILE:HB	2.47	0.41
3:F:434:HIS:CD2	3:F:448:VAL:HG21	2.52	0.41
5:I:322:ALA:O	5:I:325:CYS:HB3	2.20	0.41
1:A:62:LEU:HG	1:A:62:LEU:H	1.61	0.41
2:C:235:PHE:CD1	2:C:236:PRO:HA	2.56	0.41
3:E:267:ILE:H	3:E:267:ILE:HD13	1.78	0.41
3:E:364:GLU:C	3:E:366:THR:H	2.23	0.41
3:F:355:LEU:CD2	3:F:368:ILE:O	2.69	0.41
3:F:49:ASN:N	3:F:49:ASN:OD1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HB3	1:A:174:SER:HB3	2.03	0.40
3:E:94:GLU:OE2	3:E:120:THR:HA	2.22	0.40
3:E:414:ALA:HB3	3:E:431:GLY:O	2.20	0.40
3:F:259:ILE:H	3:F:259:ILE:HG13	1.60	0.40
3:F:275:TYR:O	3:F:277:LYS:N	2.51	0.40
3:F:340:THR:HG23	3:F:342:GLU:HG3	2.03	0.40
4:H:300:ASP:OD1	4:H:301:SER:N	2.50	0.40
5:J:431:LEU:O	5:J:432:ASN:CB	2.62	0.40
5:J:63:VAL:O	5:J:93:PHE:HB3	2.21	0.40
1:A:132:LEU:HD12	1:A:320:ILE:HD11	2.02	0.40
1:B:142:HIS:CE1	1:B:225:GLY:HA3	2.56	0.40
1:B:341:LEU:HA	1:B:341:LEU:HD12	1.91	0.40
2:D:235:PHE:CD1	2:D:236:PRO:HA	2.56	0.40
3:E:266:LEU:HD23	3:E:266:LEU:C	2.41	0.40
3:E:333:ASN:HB2	3:E:412:ILE:HD11	2.04	0.40
3:E:67:ILE:HG22	3:E:68:GLY:N	2.36	0.40
1:A:18:ASP:CG	1:A:21:GLN:HG3	2.41	0.40
1:A:31:PRO:HB3	1:B:285:PRO:HD3	2.03	0.40
3:E:272:LYS:O	3:E:273:CYS:CB	2.68	0.40
3:E:354:ALA:HB3	3:E:370:ASP:CB	2.50	0.40
3:E:65:LEU:HB2	3:E:72:MET:HE3	2.03	0.40
3:F:385:ILE:HG22	3:F:386:GLY:N	2.36	0.40
4:G:288:LYS:HE3	4:G:288:LYS:HB2	1.90	0.40
4:H:418:ASN:O	4:H:422:VAL:HG23	2.21	0.40
5:I:337:THR:HG23	5:I:354:CYS:HB2	2.04	0.40
5:I:381:LYS:HA	5:I:381:LYS:HD3	1.93	0.40
5:I:419:ARG:C	5:I:420:LEU:HD23	2.41	0.40
2:C:331:SER:OG	2:C:332:SER:N	2.52	0.40
2:D:40:ARG:HG3	2:D:174:ILE:HD12	2.04	0.40
2:D:32:ALA:HB2	2:D:74:SER:OG	2.22	0.40
4:G:134:THR:O	4:G:137:ILE:HB	2.22	0.40
4:G:264:LYS:HA	4:G:264:LYS:HD3	1.85	0.40
5:I:57:PHE:CD1	5:I:132:SER:HB3	2.57	0.40
5:I:257:LEU:O	5:I:259:LYS:HD3	2.22	0.40
5:J:140:LEU:HD23	5:J:225:ILE:HD13	2.02	0.40
1:B:230:ALA:HB1	1:B:315:PHE:HB3	2.03	0.40
3:F:367:THR:N	3:F:383:CYS:O	2.55	0.40
4:G:273:THR:O	4:G:273:THR:HG23	2.21	0.40
4:H:202:VAL:HG22	4:H:207:LEU:HG	2.03	0.40
5:I:439:ILE:HD11	5:I:441:GLY:HA2	2.00	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:113:ARG:NH2	5:J:443:GLY:C[2_555]	0.64	1.56
3:F:113:ARG:CZ	5:J:443:GLY:O[2_555]	0.66	1.54
3:F:113:ARG:NH2	5:J:443:GLY:O[2_555]	0.96	1.24
3:F:113:ARG:NH1	5:J:443:GLY:O[2_555]	1.51	0.69
3:F:113:ARG:CZ	5:J:443:GLY:C[2_555]	1.76	0.44
3:F:113:ARG:NE	5:J:443:GLY:O[2_555]	1.83	0.37
2:D:56:ASP:OD2	5:I:432:ASN:OD1[3_645]	1.95	0.25
3:F:113:ARG:NH2	5:J:443:GLY:CA[2_555]	2.04	0.16

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	313/341 (92%)	293 (94%)	17 (5%)	3 (1%)	17	56
1	B	315/341 (92%)	302 (96%)	12 (4%)	1 (0%)	43	80
2	C	343/399 (86%)	330 (96%)	13 (4%)	0	100	100
2	D	340/399 (85%)	327 (96%)	13 (4%)	0	100	100
3	E	378/458 (82%)	334 (88%)	36 (10%)	8 (2%)	8	36
3	F	377/458 (82%)	334 (89%)	40 (11%)	3 (1%)	21	61
4	G	347/467 (74%)	331 (95%)	15 (4%)	1 (0%)	43	80
4	H	347/467 (74%)	339 (98%)	8 (2%)	0	100	100
5	I	426/678 (63%)	400 (94%)	24 (6%)	2 (0%)	31	71
5	J	426/678 (63%)	385 (90%)	37 (9%)	4 (1%)	19	59
All	All	3612/4686 (77%)	3375 (93%)	215 (6%)	22 (1%)	27	67

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	262	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	442	ALA
3	E	270	LEU
3	E	277	LYS
5	J	432	ASN
5	I	432	ASN
1	A	61	ILE
3	E	273	CYS
3	E	340	THR
1	B	274	PRO
3	E	327	PRO
3	F	331	GLU
3	F	341	PRO
3	E	150	SER
5	J	32	ARG
5	J	434	PRO
1	A	97	VAL
1	A	274	PRO
3	F	402	VAL
5	J	437	VAL
5	I	33	PRO
4	G	303	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	276/298 (93%)	264 (96%)	12 (4%)	32	70
1	B	278/298 (93%)	274 (99%)	4 (1%)	69	90
2	C	301/350 (86%)	290 (96%)	11 (4%)	37	74
2	D	298/350 (85%)	295 (99%)	3 (1%)	78	93
3	E	330/395 (84%)	299 (91%)	31 (9%)	9	35
3	F	329/395 (83%)	306 (93%)	23 (7%)	16	50
4	G	314/408 (77%)	307 (98%)	7 (2%)	55	84
4	H	314/408 (77%)	307 (98%)	7 (2%)	55	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	379/596 (64%)	363 (96%)	16 (4%)	32	71
5	J	378/596 (63%)	365 (97%)	13 (3%)	40	76
All	All	3197/4094 (78%)	3070 (96%)	127 (4%)	34	72

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	21	GLN
1	A	28	GLN
1	A	49	ARG
1	A	50	SER
1	A	51	GLN
1	A	57	GLU
1	A	61	ILE
1	A	62	LEU
1	A	93	SER
1	A	100	PHE
1	A	113	LEU
1	B	87	GLN
1	B	106	HIS
1	B	187	ILE
1	B	276	THR
2	C	1	MET
2	C	2	SER
2	C	44	SER
2	C	49	SER
2	C	87	ARG
2	C	90	TYR
2	C	92	GLU
2	C	93	LEU
2	C	139	SER
2	C	162	ARG
2	C	164	THR
2	D	47	ARG
2	D	49	SER
2	D	167	MET
3	E	31	GLN
3	E	33	GLN
3	E	34	SER
3	E	94	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	133	ARG
3	E	135	VAL
3	E	181	GLU
3	E	218	PHE
3	E	221	ARG
3	E	254	ARG
3	E	256	LYS
3	E	267	ILE
3	E	269	TYR
3	E	273	CYS
3	E	274	GLN
3	E	276	GLN
3	E	277	LYS
3	E	324	ASN
3	E	326	LEU
3	E	327	PRO
3	E	328	ASN
3	E	331	GLU
3	E	332	LEU
3	E	334	LYS
3	E	353	ARG
3	E	355	LEU
3	E	367	THR
3	E	370	ASP
3	E	397	MET
3	E	424	LYS
3	E	448	VAL
3	F	113	ARG
3	F	120	THR
3	F	183	ILE
3	F	200	GLU
3	F	217	ASP
3	F	268	PRO
3	F	272	LYS
3	F	277	LYS
3	F	279	PHE
3	F	281	VAL
3	F	315	LYS
3	F	319	ILE
3	F	339	LEU
3	F	342	GLU
3	F	344	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	345	LEU
3	F	360	CYS
3	F	428	CYS
3	F	429	GLU
3	F	435	ARG
3	F	440	ARG
3	F	443	ARG
3	F	450	MET
4	G	228	ASP
4	G	232	ASP
4	G	237	LEU
4	G	240	GLU
4	G	278	SER
4	G	403	ASN
4	G	412	LYS
4	H	156	LYS
4	H	355	ARG
4	H	404	MET
4	H	407	ASP
4	H	408	ASP
4	H	410	GLU
4	H	411	GLU
5	I	16	HIS
5	I	18	LEU
5	I	26	SER
5	I	29	TYR
5	I	30	ARG
5	I	149	ASP
5	I	205	ILE
5	I	210	GLU
5	I	268	GLU
5	I	418	LYS
5	I	419	ARG
5	I	430	THR
5	I	431	LEU
5	I	432	ASN
5	I	436	LEU
5	I	439	ILE
5	J	381	LYS
5	J	386	ASN
5	J	394	CYS
5	J	398	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	417	ASN
5	J	418	LYS
5	J	419	ARG
5	J	426	HIS
5	J	427	SER
5	J	428	GLN
5	J	435	SER
5	J	437	VAL
5	J	442	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	95	HIS
1	B	305	ASN
2	C	142	ASN
2	D	239	GLN
3	E	182	HIS
3	E	276	GLN
3	F	325	ASN
3	F	343	GLN
4	G	403	ASN
4	G	460	ASN
4	H	119	GLN
4	H	460	ASN
5	I	188	HIS
5	I	347	ASN
5	I	417	ASN
5	J	386	ASN
5	J	393	ASN
5	J	417	ASN
5	J	428	GLN

5.3.3 RNA ⓘ

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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	A	401	-	4,4,4	0.77	0	6,6,6	0.38	0
6	PO4	B	401	-	4,4,4	0.78	0	6,6,6	0.40	0
6	PO4	C	401	-	4,4,4	0.75	0	6,6,6	0.38	0
6	PO4	D	401	-	4,4,4	0.77	0	6,6,6	0.39	0
6	PO4	G	501	-	4,4,4	0.76	0	6,6,6	0.39	0
6	PO4	G	502	-	4,4,4	0.75	0	6,6,6	0.38	0
6	PO4	H	501	-	4,4,4	0.75	0	6,6,6	0.40	0
6	PO4	H	502	-	4,4,4	0.77	0	6,6,6	0.41	0
6	PO4	I	701	-	4,4,4	0.74	0	6,6,6	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PO4	A	401	-	-	0/0/0/0	0/0/0/0
6	PO4	B	401	-	-	0/0/0/0	0/0/0/0
6	PO4	C	401	-	-	0/0/0/0	0/0/0/0
6	PO4	D	401	-	-	0/0/0/0	0/0/0/0
6	PO4	G	501	-	-	0/0/0/0	0/0/0/0
6	PO4	G	502	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PO4	H	501	-	-	0/0/0/0	0/0/0/0
6	PO4	H	502	-	-	0/0/0/0	0/0/0/0
6	PO4	I	701	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	401	PO4	1	0
6	G	501	PO4	1	0
6	I	701	PO4	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	317/341 (92%)	0.60	30 (9%) 8 3	55, 86, 150, 173	0
1	B	319/341 (93%)	0.49	18 (5%) 24 8	49, 80, 123, 180	0
2	C	349/399 (87%)	0.46	23 (6%) 18 6	42, 68, 138, 165	0
2	D	346/399 (86%)	0.19	10 (2%) 51 23	41, 66, 111, 161	0
3	E	384/458 (83%)	0.67	42 (10%) 5 2	61, 99, 142, 163	0
3	F	383/458 (83%)	0.79	56 (14%) 2 1	66, 108, 153, 168	0
4	G	349/467 (74%)	0.45	20 (5%) 24 8	44, 75, 136, 167	0
4	H	349/467 (74%)	0.19	12 (3%) 45 19	44, 65, 116, 153	0
5	I	428/678 (63%)	0.23	10 (2%) 60 31	42, 73, 115, 148	0
5	J	428/678 (63%)	0.39	25 (5%) 23 8	50, 87, 122, 153	0
All	All	3652/4686 (77%)	0.44	246 (6%) 18 5	41, 80, 137, 180	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	423	SER	7.7
2	C	8	HIS	7.5
3	E	450	MET	6.5
4	G	226	ASP	6.0
2	C	4	ILE	5.7
2	C	-3	ILE	5.6
5	I	442	ARG	5.6
5	J	433	ASP	5.5
2	C	2	SER	5.5
1	A	52	ALA	5.4
3	E	31	GLN	5.2
4	G	182	TYR	5.2
1	A	58	PHE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	G	183	GLY	5.1
4	G	184	THR	5.0
1	A	94	LEU	4.9
5	J	436	LEU	4.9
3	F	450	MET	4.8
2	C	169	MET	4.8
5	I	432	ASN	4.7
1	A	97	VAL	4.6
3	F	401	VAL	4.5
2	C	173	ILE	4.4
3	F	122	LEU	4.4
1	A	51	GLN	4.3
2	D	137	TYR	4.3
3	F	211	SER	4.3
2	D	165	GLY	4.2
4	G	229	LEU	4.1
1	B	277	VAL	4.1
2	D	90	TYR	4.1
5	J	16	HIS	4.1
3	F	434	HIS	4.0
2	C	48	TRP	4.0
1	B	17	PHE	4.0
3	F	34	SER	3.9
1	A	23	TYR	3.9
1	B	285	PRO	3.9
3	E	252	LEU	3.8
3	F	259	ILE	3.8
2	C	10	TYR	3.8
3	E	356	VAL	3.8
1	A	101	GLU	3.7
3	F	132	LEU	3.7
1	A	17	PHE	3.6
4	H	184	THR	3.6
2	C	9	THR	3.6
2	D	166	GLY	3.6
3	F	418	GLN	3.6
4	G	227	ILE	3.6
3	E	253	ILE	3.5
1	A	86	PHE	3.5
3	E	440	ARG	3.4
5	J	393	ASN	3.4
4	G	175	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	G	405	GLY	3.3
4	H	119	GLN	3.3
5	J	414	ILE	3.3
3	E	402	VAL	3.3
4	G	224	VAL	3.2
3	E	273	CYS	3.2
3	E	418	GLN	3.2
3	E	220	PHE	3.2
1	A	289	ASP	3.2
3	E	32	LEU	3.2
3	F	367	THR	3.2
2	C	3	THR	3.1
3	E	278	SER	3.1
3	F	44	PHE	3.1
4	G	114	ILE	3.1
2	D	97	ALA	3.1
3	F	385	ILE	3.1
1	B	58	PHE	3.1
1	B	54	THR	3.1
3	F	384	VAL	3.1
3	F	408	LEU	3.0
3	E	47	PHE	3.0
3	F	402	VAL	3.0
3	E	355	LEU	3.0
3	F	218	PHE	3.0
3	F	351	SER	3.0
5	J	435	SER	3.0
1	B	47	LEU	3.0
3	E	385	ILE	3.0
4	H	408	ASP	3.0
3	F	355	LEU	2.9
3	F	425	LEU	2.9
3	E	351	SER	2.9
1	A	295	LEU	2.9
3	F	252	LEU	2.9
3	F	123	ASP	2.9
3	F	419	ILE	2.9
3	E	279	PHE	2.9
1	B	94	LEU	2.9
3	E	256	LYS	2.8
2	C	-4	PRO	2.8
3	F	125	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	G	230	THR	2.8
3	F	56	GLY	2.8
1	B	55	ILE	2.8
4	G	198	ILE	2.8
2	C	46	THR	2.8
3	F	431	GLY	2.8
4	G	235	LYS	2.8
2	D	93	LEU	2.8
2	D	164	THR	2.8
3	F	436	VAL	2.8
3	F	253	ILE	2.8
1	A	291	ILE	2.7
1	B	53	LYS	2.7
3	E	268	PRO	2.7
5	J	434	PRO	2.7
5	I	374	GLY	2.7
1	A	53	LYS	2.7
1	A	56	SER	2.7
3	F	145	CYS	2.7
4	H	120	VAL	2.7
3	E	218	PHE	2.6
3	F	220	PHE	2.6
3	F	406	VAL	2.6
5	J	379	ILE	2.6
1	A	107	LEU	2.6
5	J	420	LEU	2.6
5	J	37	ASP	2.6
2	C	90	TYR	2.6
1	A	50	SER	2.6
1	A	290	ALA	2.6
1	A	59	MET	2.6
3	F	32	LEU	2.6
3	F	276	GLN	2.6
5	J	431	LEU	2.6
1	B	72	GLY	2.6
4	H	405	GLY	2.6
1	A	65	GLY	2.6
3	E	206	LEU	2.5
5	J	256	LEU	2.5
3	E	281	VAL	2.5
3	F	347	ASP	2.5
3	F	91	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	18	ASP	2.5
3	E	192	ALA	2.5
1	B	20	VAL	2.5
3	E	369	LYS	2.5
1	B	51	GLN	2.5
5	J	356	ILE	2.5
1	A	293	ASN	2.5
5	J	402	VAL	2.5
3	F	47	PHE	2.5
3	F	182	HIS	2.5
3	E	272	LYS	2.4
4	G	189	HIS	2.4
3	F	254	ARG	2.4
3	F	400	ILE	2.4
3	E	404	ASP	2.4
3	F	449	ASP	2.4
1	B	61	ILE	2.4
3	E	254	ARG	2.4
3	E	374	ILE	2.4
1	B	19	ILE	2.4
4	G	225	LEU	2.4
3	F	124	ASP	2.4
2	C	5	ASN	2.4
1	B	52	ALA	2.4
1	A	286	THR	2.4
4	H	116	GLU	2.4
3	F	412	ILE	2.4
3	E	45	ALA	2.4
4	H	158	PHE	2.3
5	J	259	LYS	2.3
3	F	379	ILE	2.3
4	H	226	ASP	2.3
4	G	115	PHE	2.3
1	A	96	ASP	2.3
2	C	177	ILE	2.3
3	F	313	ILE	2.3
5	J	154	ILE	2.3
3	F	210	SER	2.3
3	E	330	PHE	2.3
4	G	186	LEU	2.3
5	I	198	TYR	2.3
1	A	54	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	99	ASP	2.3
3	E	216	SER	2.3
1	A	43	LEU	2.3
3	E	60	LEU	2.3
3	E	33	GLN	2.3
2	C	58	VAL	2.3
5	I	357	GLY	2.2
4	H	227	ILE	2.2
5	J	326	ILE	2.2
1	B	86	PHE	2.2
5	J	396	ILE	2.2
3	E	315	LYS	2.2
3	F	206	LEU	2.2
2	C	174	ILE	2.2
3	F	273	CYS	2.2
1	A	100	PHE	2.2
3	E	441	ILE	2.2
3	F	55	THR	2.2
5	I	15	LYS	2.2
3	E	346	VAL	2.2
3	E	92	CYS	2.2
4	H	407	ASP	2.2
3	E	443	ARG	2.2
2	D	54	LEU	2.2
4	G	180	THR	2.2
5	I	379	ILE	2.2
3	E	258	SER	2.2
3	F	368	ILE	2.1
5	I	396	ILE	2.1
5	J	411	ASN	2.1
3	E	134	ALA	2.1
3	F	121	ILE	2.1
1	A	103	CYS	2.1
3	F	369	LYS	2.1
5	J	374	GLY	2.1
2	C	170	ARG	2.1
5	I	238	PHE	2.1
3	F	94	GLU	2.1
5	J	320	VAL	2.1
3	F	407	ARG	2.1
5	I	408	ILE	2.1
5	J	118	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	57	GLU	2.1
2	C	94	LEU	2.1
4	G	123	PHE	2.1
5	J	257	LEU	2.1
1	B	100	PHE	2.1
2	D	254	ILE	2.1
3	E	265	ASP	2.1
3	E	419	ILE	2.1
4	G	157	ILE	2.1
3	F	424	LYS	2.1
5	J	407	VAL	2.1
2	C	0	PHE	2.1
4	H	115	PHE	2.1
5	J	367	LEU	2.0
2	C	86	ILE	2.0
2	C	361	ASP	2.0
3	F	327	PRO	2.0
1	B	65	GLY	2.0
1	A	102	GLN	2.0
3	F	92	CYS	2.0
2	C	51	VAL	2.0
2	D	94	LEU	2.0
4	H	416	LEU	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. 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PO4	G	501	5/5	0.88	0.17	91,94,118,136	0
6	PO4	G	502	5/5	0.89	0.18	62,67,102,104	0
6	PO4	H	501	5/5	0.89	0.17	81,85,101,134	0
6	PO4	I	701	5/5	0.90	0.15	101,102,127,141	0
6	PO4	H	502	5/5	0.95	0.20	71,82,90,98	0
6	PO4	D	401	5/5	0.97	0.22	50,53,72,73	0
6	PO4	A	401	5/5	0.98	0.16	70,71,84,89	0
6	PO4	B	401	5/5	0.98	0.19	63,67,86,93	0
6	PO4	C	401	5/5	0.99	0.18	51,53,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.