



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:03 AM UTC

PDB ID : 3HYM / pdb_00003hym
Title : Insights into Anaphase Promoting Complex TPR subdomain assembly from a CDC26-APC6 structure
Authors : Wang, J.; Dye, B.T.; Rajashankar, K.R.; Kurinov, I.; Schulman, B.A.
Deposited on : 2009-06-22
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

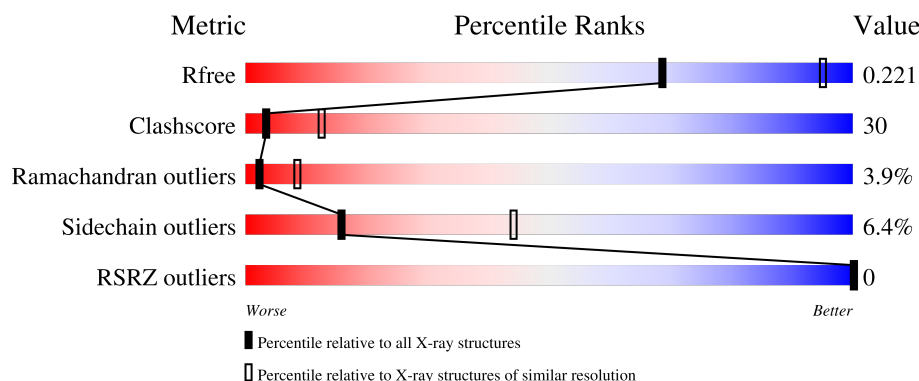
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	29	
1	C	29	
1	E	29	
1	G	29	
1	I	29	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	29	31%38%10%21%
2	B	330	49%38%.9%
2	D	330	41%46%..9%
2	F	330	52%35%.9%
2	H	330	52%34%5%.8%
2	J	330	41%45%5%9%
2	L	330	43%43%.9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15517 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 Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	26	Total	C	N	O	Se	0	0	0
			214	134	41	38	1			
1	C	23	Total	C	N	O	Se	0	0	0
			199	125	38	35	1			
1	E	26	Total	C	N	O	Se	0	0	0
			208	131	38	38	1			
1	G	25	Total	C	N	O	Se	0	0	0
			213	133	40	39	1			
1	I	26	Total	C	N	O	Se	0	0	0
			208	131	38	38	1			
1	K	23	Total	C	N	O	Se	0	0	0
			197	124	35	37	1			

- Molecule 2 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	301	Total	C	N	O	S	Se	0	0
			2344	1514	383	430	7	10		
2	D	301	Total	C	N	O	S	Se	0	0
			2348	1517	384	430	7	10		
2	F	301	Total	C	N	O	S	Se	0	0
			2356	1520	389	430	7	10		
2	H	302	Total	C	N	O	S	Se	0	0
			2345	1513	382	433	7	10		
2	J	301	Total	C	N	O	S	Se	0	0
			2346	1514	385	430	7	10		
2	L	299	Total	C	N	O	S	Se	0	0
			2328	1504	383	424	7	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	210	GLY	-	expression tag	UNP Q13042

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	211	SER	-	expression tag	UNP Q13042
D	210	GLY	-	expression tag	UNP Q13042
D	211	SER	-	expression tag	UNP Q13042
F	210	GLY	-	expression tag	UNP Q13042
F	211	SER	-	expression tag	UNP Q13042
H	210	GLY	-	expression tag	UNP Q13042
H	211	SER	-	expression tag	UNP Q13042
J	210	GLY	-	expression tag	UNP Q13042
J	211	SER	-	expression tag	UNP Q13042
L	210	GLY	-	expression tag	UNP Q13042
L	211	SER	-	expression tag	UNP Q13042

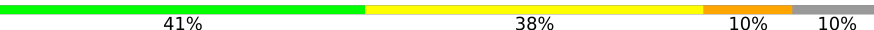
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	32	Total O 32 32	0	0
3	C	4	Total O 4 4	0	0
3	D	31	Total O 31 31	0	0
3	E	5	Total O 5 5	0	0
3	F	19	Total O 19 19	0	0
3	G	4	Total O 4 4	0	0
3	H	48	Total O 48 48	0	0
3	I	1	Total O 1 1	0	0
3	J	29	Total O 29 29	0	0
3	K	3	Total O 3 3	0	0
3	L	33	Total O 33 33	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Anaphase-promoting complex subunit CDC26

Chain A: 

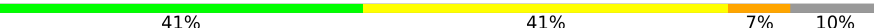


- Molecule 1: Anaphase-promoting complex subunit CDC26

Chain C: 

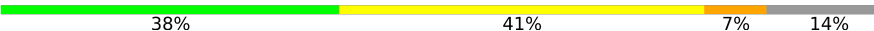


- Molecule 1: Anaphase-promoting complex subunit CDC26

Chain E: 

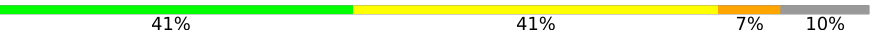


- Molecule 1: Anaphase-promoting complex subunit CDC26

Chain G: 

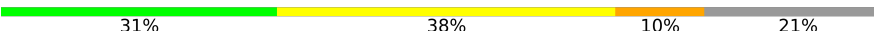


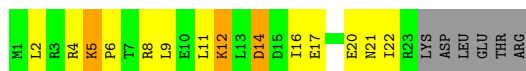
- Molecule 1: Anaphase-promoting complex subunit CDC26

Chain I: 



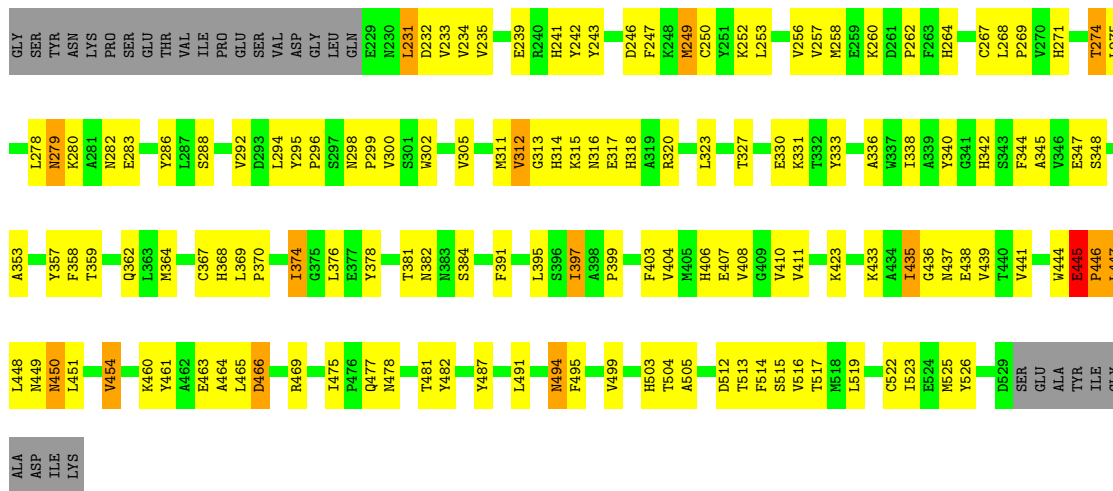
- Molecule 1: Anaphase-promoting complex subunit CDC26

Chain K: 



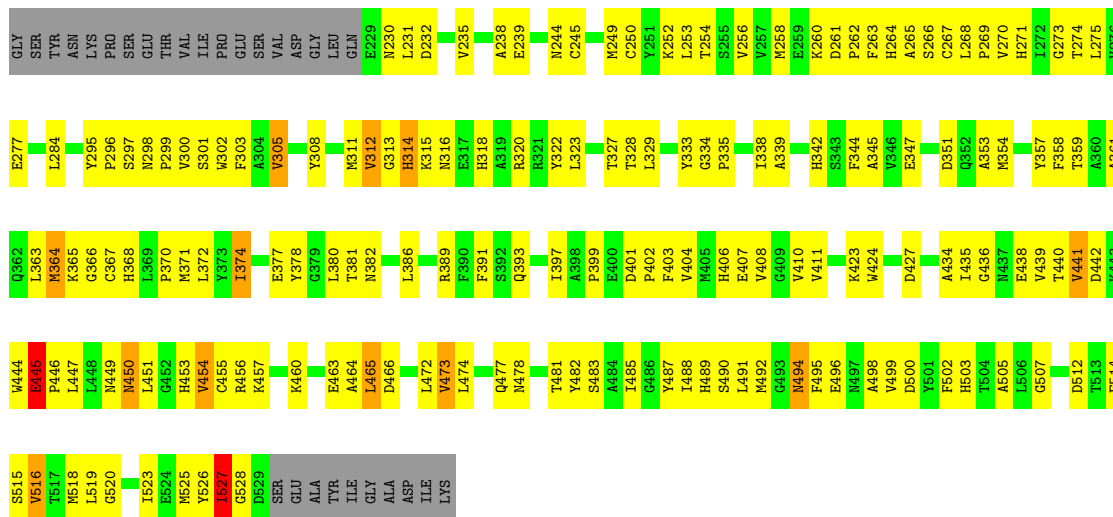
• Molecule 2: Cell division cycle protein 16 homolog

Chain B: 49% 38% 9%



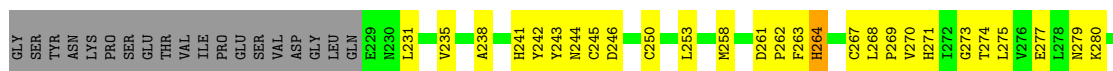
• Molecule 2: Cell division cycle protein 16 homolog

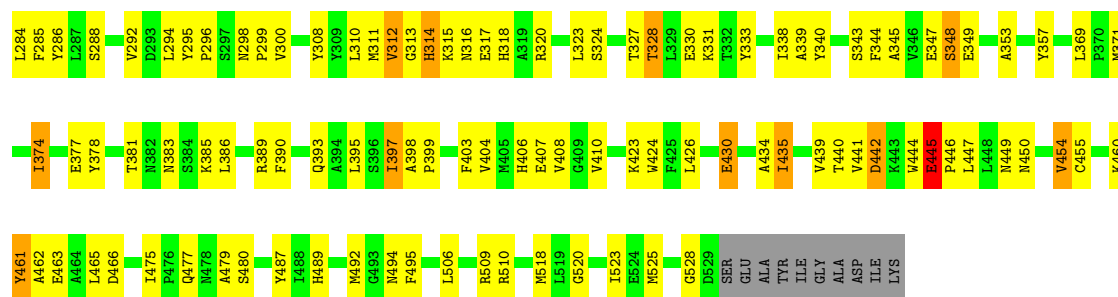
Chain D: 41% 46% 9%



• Molecule 2: Cell division cycle protein 16 homolog

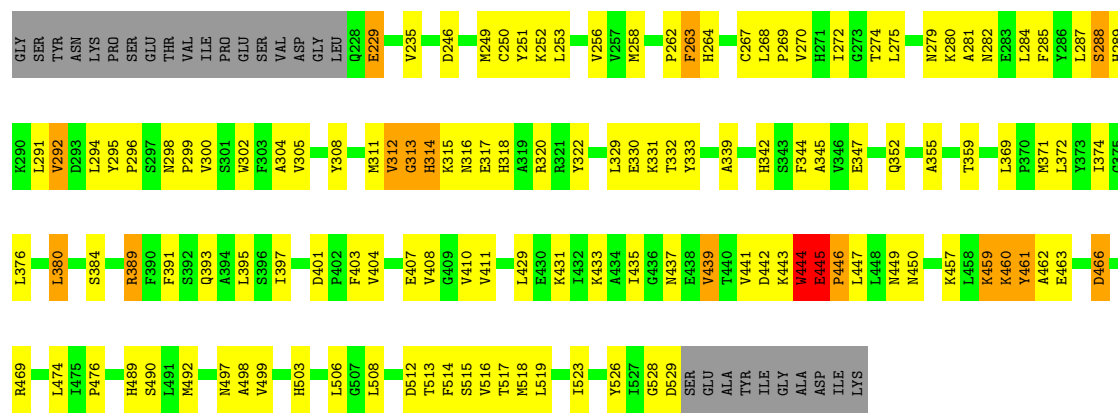
Chain F: 52% 35% 9%





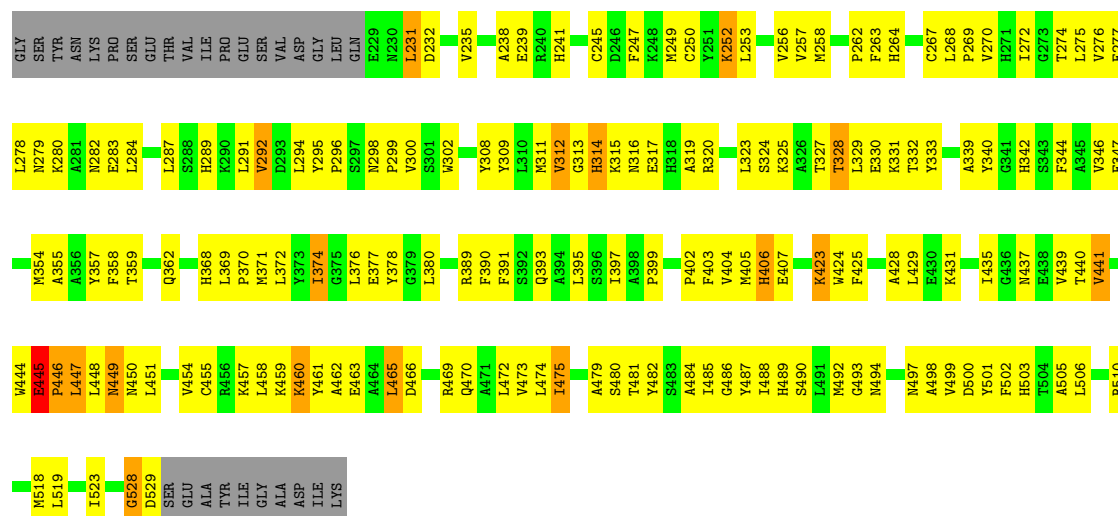
- Molecule 2: Cell division cycle protein 16 homolog

Chain H: 52% 34% 5% 8%



- Molecule 2: Cell division cycle protein 16 homolog

Chain J: 41% 45% 5% 9%



- Molecule 2: Cell division cycle protein 16 homolog

Chain L: 43% 43% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	301.90Å 301.90Å 80.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.40 – 2.80 49.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.40-2.80) 98.7 (49.40-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.188 , 0.220 0.194 , 0.221	Depositor DCC
R_{free} test set	4998 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.459 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15517	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% 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

5.1 Standard geometry

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	0.42	0/215	0.82	0/286
1	C	0.31	0/200	0.84	0/265
1	E	0.37	0/209	0.76	0/279
1	G	0.39	0/214	0.93	0/284
1	I	0.39	0/209	0.82	0/279
1	K	0.35	0/198	0.79	0/263
2	B	0.40	0/2401	0.77	0/3254
2	D	0.40	0/2405	0.77	2/3258 (0.1%)
2	F	0.39	0/2413	0.77	2/3268 (0.1%)
2	H	0.38	0/2402	0.77	1/3258 (0.0%)
2	J	0.39	0/2403	0.83	4/3257 (0.1%)
2	L	0.38	0/2384	0.81	2/3230 (0.1%)
All	All	0.39	0/15653	0.79	11/21181 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	401	ASP	CA-C-N	7.90	127.18	118.97
2	L	401	ASP	C-N-CA	7.90	127.18	118.97
2	F	475	ILE	CA-C-N	7.19	127.35	119.87
2	F	475	ILE	C-N-CA	7.19	127.35	119.87
2	J	445	GLU	CA-C-N	6.42	127.87	119.84
2	J	445	GLU	C-N-CA	6.42	127.87	119.84
2	J	475	ILE	CA-C-N	6.15	126.05	119.28
2	J	475	ILE	C-N-CA	6.15	126.05	119.28
2	H	433	LYS	N-CA-C	-5.75	106.43	113.50
2	D	366	GLY	N-CA-C	-5.40	108.28	115.40
2	D	507	GLY	N-CA-C	-5.35	108.47	114.40

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	214	0	218	23	0
1	C	199	0	212	32	0
1	E	208	0	207	18	0
1	G	213	0	220	17	0
1	I	208	0	207	19	0
1	K	197	0	205	26	0
2	B	2344	0	2194	133	0
2	D	2348	0	2205	177	0
2	F	2356	0	2216	112	0
2	H	2345	0	2178	132	0
2	J	2346	0	2194	162	0
2	L	2328	0	2181	161	0
3	A	2	0	0	0	0
3	B	32	0	0	6	0
3	C	4	0	0	0	0
3	D	31	0	0	7	0
3	E	5	0	0	0	0
3	F	19	0	0	1	0
3	G	4	0	0	0	0
3	H	48	0	0	7	0
3	I	1	0	0	0	0
3	J	29	0	0	6	0
3	K	3	0	0	2	0
3	L	33	0	0	6	0
All	All	15517	0	14437	899	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 30.

All (899) 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)
2:J:489:HIS:HB2	2:J:498:ALA:HB2	1.42	1.00
1:C:17:GLU:HA	1:C:20:GLU:HG3	1.46	0.98
2:D:445:GLU:H	2:D:446:PRO:CD	1.79	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:GLU:H	2:B:446:PRO:CD	1.78	0.95
2:D:445:GLU:H	2:D:446:PRO:HD3	1.34	0.90
2:H:445:GLU:H	2:H:446:PRO:CD	1.86	0.88
2:D:312:VAL:HG13	2:D:313:GLY:H	1.38	0.87
2:J:445:GLU:N	2:J:446:PRO:HD2	1.90	0.86
2:B:499:VAL:HG13	2:B:519:LEU:HD11	1.56	0.85
2:B:279:ASN:HA	2:B:311:MSE:HE1	1.57	0.85
2:L:249:MSE:HE3	2:L:253:LEU:HD21	1.58	0.85
2:L:404:VAL:O	2:L:408:VAL:HG23	1.76	0.85
2:L:445:GLU:H	2:L:446:PRO:CD	1.89	0.84
1:A:8:ARG:HH12	2:B:445:GLU:CD	1.85	0.84
2:J:320:ARG:HH22	2:J:347:GLU:HG3	1.43	0.84
2:F:250:CYS:SG	2:F:274:THR:HG21	2.17	0.84
2:F:445:GLU:H	2:F:446:PRO:HD2	1.43	0.83
2:H:523:ILE:HG13	2:H:526:TYR:HB3	1.60	0.83
2:D:489:HIS:HB2	2:D:498:ALA:HB2	1.61	0.83
2:J:264:HIS:HB3	2:J:267:CYS:HB3	1.63	0.81
2:J:376:LEU:HD13	2:J:407:GLU:HB3	1.63	0.81
2:J:312:VAL:HG22	2:J:313:GLY:H	1.43	0.80
1:K:8:ARG:HG3	2:L:446:PRO:HB3	1.63	0.78
2:L:271:HIS:O	2:L:275:LEU:HG	1.85	0.77
2:F:312:VAL:HG13	2:F:313:GLY:H	1.48	0.76
1:C:16:ILE:HA	2:D:487:TYR:OH	1.85	0.76
2:B:445:GLU:H	2:B:446:PRO:HD3	1.49	0.76
2:H:284:LEU:O	2:H:288:SER:HB3	1.84	0.76
1:C:19:PHE:HB2	2:D:491:LEU:HD23	1.67	0.76
1:I:9:LEU:HG	2:J:450:ASN:OD1	1.87	0.75
1:A:15:ASP:O	1:A:18:GLU:HG3	1.86	0.75
2:L:475:ILE:HG23	2:L:477:GLN:NE2	2.01	0.75
2:H:445:GLU:H	2:H:446:PRO:HD3	1.51	0.74
2:L:456:ARG:HD3	2:L:488:ILE:HG13	1.68	0.74
2:D:441:VAL:HA	2:D:444:TRP:HB3	1.69	0.74
2:J:309:TYR:HB2	2:J:319:ALA:HB2	1.69	0.74
2:B:445:GLU:OE1	2:B:475:ILE:HD12	1.87	0.73
1:C:5:LYS:HD3	1:C:5:LYS:H	1.53	0.73
2:D:444:TRP:HZ2	2:D:447:LEU:HB3	1.53	0.73
2:D:265:ALA:HA	3:D:46:HOH:O	1.88	0.73
2:D:463:GLU:HA	2:D:466:ASP:OD2	1.88	0.72
2:J:445:GLU:H	2:J:446:PRO:HD2	1.50	0.72
2:H:298:ASN:OD1	2:H:299:PRO:HD2	1.90	0.72
2:F:445:GLU:H	2:F:446:PRO:CD	2.02	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:HIS:HB3	2:D:322:TYR:HE2	1.55	0.71
2:D:477:GLN:HB3	2:L:477:GLN:HG3	1.71	0.71
2:L:295:TYR:N	2:L:296:PRO:HD3	2.06	0.71
2:J:458:LEU:HD13	2:J:460:LYS:HD2	1.72	0.70
1:A:4:ARG:NH2	2:B:376:LEU:HD23	2.06	0.70
2:J:461:TYR:O	2:J:465:LEU:HD12	1.92	0.70
2:D:483:SER:HB2	2:D:515:SER:OG	1.92	0.69
2:B:300:VAL:HG22	2:B:333:TYR:OH	1.92	0.69
2:L:418:TRP:HA	2:L:421:ALA:HB3	1.74	0.69
1:E:8:ARG:HH12	2:F:445:GLU:CD	2.00	0.69
2:J:482:TYR:HB3	2:J:505:ALA:HB2	1.73	0.69
2:L:478:ASN:HB3	2:L:481:THR:OG1	1.92	0.69
2:B:378:TYR:OH	2:D:359:THR:HG22	1.91	0.69
2:D:295:TYR:N	2:D:296:PRO:HD3	2.07	0.69
2:D:312:VAL:HG13	2:D:313:GLY:N	2.07	0.69
2:B:463:GLU:HA	2:B:466:ASP:OD2	1.93	0.69
2:D:249:MSE:HE3	2:D:253:LEU:HG	1.75	0.69
2:D:477:GLN:O	2:D:477:GLN:HG2	1.91	0.69
2:J:359:THR:HG22	2:L:378:TYR:OH	1.93	0.69
2:J:445:GLU:N	2:J:446:PRO:CD	2.56	0.69
1:K:17:GLU:HA	1:K:20:GLU:CG	2.23	0.69
2:B:407:GLU:O	2:B:411:VAL:HG23	1.93	0.69
2:D:445:GLU:N	2:D:446:PRO:HD3	2.08	0.69
2:J:405:MSE:SE	3:J:13:HOH:O	2.61	0.68
2:L:445:GLU:H	2:L:446:PRO:HD3	1.59	0.68
2:B:359:THR:HG22	2:D:378:TYR:OH	1.93	0.68
1:K:8:ARG:HH22	2:L:481:THR:HG23	1.57	0.68
2:L:502:PHE:O	2:L:505:ALA:HB3	1.93	0.68
2:F:295:TYR:N	2:F:296:PRO:HD3	2.09	0.68
2:H:312:VAL:HG22	2:H:313:GLY:N	2.08	0.68
2:J:451:LEU:HD12	2:J:451:LEU:H	1.59	0.68
2:F:292:VAL:O	2:F:296:PRO:HG3	1.93	0.67
2:F:385:LYS:HD3	2:H:332:THR:HG21	1.76	0.67
2:L:279:ASN:HA	2:L:311:MSE:HE1	1.77	0.67
2:L:300:VAL:HG22	2:L:333:TYR:OH	1.94	0.67
2:J:325:LYS:O	2:J:329:LEU:HB2	1.94	0.67
2:H:302:TRP:HA	2:H:305:VAL:HG12	1.76	0.67
2:B:295:TYR:N	2:B:296:PRO:HD3	2.10	0.67
2:B:450:ASN:HD22	2:B:450:ASN:H	1.42	0.67
2:D:496:GLU:HA	2:L:286:TYR:OH	1.94	0.67
2:H:371:MSE:HE1	2:H:397:ILE:HD12	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:284:LEU:HD23	2:F:311:MSE:SE	2.45	0.66
2:B:445:GLU:N	2:B:446:PRO:HD3	2.10	0.66
1:C:22:ILE:HG22	1:C:22:ILE:O	1.96	0.66
2:H:312:VAL:HG13	2:H:313:GLY:H	1.61	0.66
2:H:444:TRP:CD1	2:H:446:PRO:HD2	2.31	0.66
2:B:232:ASP:HB2	3:B:38:HOH:O	1.96	0.66
2:D:492:MSE:SE	3:D:30:HOH:O	2.63	0.66
2:F:450:ASN:O	2:F:454:VAL:HG23	1.96	0.66
2:D:250:CYS:SG	2:D:274:THR:HG21	2.36	0.65
2:H:355:ALA:O	2:H:359:THR:HG23	1.96	0.65
1:E:5:LYS:H	1:E:5:LYS:HD3	1.61	0.65
2:B:513:THR:O	2:B:517:THR:HG23	1.96	0.64
2:D:444:TRP:CZ2	2:D:447:LEU:HB3	2.32	0.64
2:H:462:ALA:HB3	3:H:172:HOH:O	1.97	0.64
2:J:368:HIS:HB3	2:J:397:ILE:HG21	1.78	0.64
2:L:292:VAL:O	2:L:296:PRO:HG3	1.98	0.64
2:H:300:VAL:HG22	2:H:333:TYR:OH	1.96	0.64
2:D:512:ASP:O	2:D:516:VAL:HG23	1.98	0.64
2:F:288:SER:O	2:F:292:VAL:HG23	1.96	0.64
2:H:499:VAL:HG12	2:H:503:HIS:CD2	2.33	0.64
1:C:19:PHE:HB2	2:D:491:LEU:CD2	2.28	0.64
2:B:250:CYS:HA	2:B:253:LEU:HD12	1.79	0.64
2:J:376:LEU:O	2:J:380:LEU:HG	1.97	0.64
2:F:404:VAL:O	2:F:408:VAL:HG23	1.97	0.64
2:B:376:LEU:HD22	3:B:2:HOH:O	1.96	0.63
2:H:403:PHE:O	2:H:407:GLU:HG2	1.99	0.63
2:D:445:GLU:N	2:D:446:PRO:CD	2.57	0.63
2:J:403:PHE:O	2:J:407:GLU:HG2	1.98	0.63
2:B:481:THR:HG22	3:B:57:HOH:O	1.98	0.63
2:J:249:MSE:HE3	2:J:253:LEU:HD21	1.81	0.63
2:F:312:VAL:HG13	2:F:313:GLY:N	2.13	0.63
2:H:444:TRP:CE3	2:H:444:TRP:C	2.76	0.63
1:C:17:GLU:HA	1:C:20:GLU:CG	2.26	0.63
2:J:295:TYR:N	2:J:296:PRO:HD3	2.14	0.63
2:B:495:PHE:HD2	2:B:522:CYS:HG	1.47	0.63
1:E:17:GLU:HA	1:E:20:GLU:CG	2.29	0.63
2:B:407:GLU:HA	2:B:410:VAL:HB	1.81	0.62
2:B:242:TYR:HD2	2:B:274:THR:HG23	1.63	0.62
2:B:523:ILE:HB	2:F:285:PHE:CZ	2.34	0.62
2:F:506:LEU:HA	2:F:509:ARG:O	1.99	0.62
1:A:5:LYS:HD3	1:A:5:LYS:H	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:512:ASP:O	2:L:516:VAL:HG23	2.00	0.62
2:J:423:LYS:HG3	2:J:424:TRP:N	2.12	0.62
1:K:2:LEU:CD2	2:L:339:ALA:HB2	2.30	0.62
2:L:448:LEU:HA	2:L:451:LEU:HD12	1.81	0.62
2:L:499:VAL:HG12	2:L:503:HIS:CD2	2.35	0.62
2:D:308:TYR:OH	2:L:503:HIS:HE1	1.83	0.62
1:E:16:ILE:HA	2:F:487:TYR:OH	1.99	0.62
2:L:481:THR:HB	3:L:28:HOH:O	2.00	0.61
2:L:449:ASN:ND2	2:L:481:THR:HG22	2.15	0.61
2:D:323:LEU:O	2:D:327:THR:HG23	1.99	0.61
1:G:5:LYS:H	1:G:5:LYS:HD3	1.65	0.61
2:L:475:ILE:HG22	2:L:478:ASN:HB2	1.83	0.61
2:H:295:TYR:N	2:H:296:PRO:HD3	2.14	0.61
2:F:269:PRO:HG3	2:F:333:TYR:OH	2.01	0.61
2:B:264:HIS:HD2	2:B:267:CYS:H	1.48	0.61
2:J:313:GLY:C	2:J:315:LYS:H	2.08	0.61
2:L:318:HIS:HA	3:L:59:HOH:O	2.00	0.61
2:D:342:HIS:HD2	2:D:357:TYR:OH	1.84	0.60
2:B:445:GLU:H	2:B:446:PRO:HD2	1.64	0.60
1:K:12:LYS:HA	1:K:12:LYS:HE3	1.84	0.60
1:K:17:GLU:HA	1:K:20:GLU:HG2	1.82	0.60
2:D:264:HIS:HB3	2:D:267:CYS:HB3	1.84	0.60
2:D:442:ASP:C	2:D:444:TRP:H	2.09	0.60
2:H:447:LEU:HA	2:H:450:ASN:HD22	1.67	0.60
2:L:264:HIS:HD2	2:L:267:CYS:H	1.50	0.60
2:D:377:GLU:O	2:D:381:THR:HG23	2.01	0.60
2:D:460:LYS:HE2	2:D:463:GLU:OE1	2.01	0.60
1:E:17:GLU:HA	1:E:20:GLU:HG3	1.83	0.60
2:B:314:HIS:CG	2:B:314:HIS:O	2.55	0.60
2:H:313:GLY:C	2:H:315:LYS:H	2.10	0.60
2:J:446:PRO:O	2:J:447:LEU:C	2.45	0.59
2:L:425:PHE:HB3	2:L:451:LEU:HD23	1.84	0.59
1:K:14:ASP:N	1:K:14:ASP:OD1	2.35	0.59
2:L:449:ASN:O	2:L:453:HIS:HD2	1.85	0.59
2:B:435:ILE:C	2:B:437:ASN:H	2.10	0.59
2:D:273:GLY:O	2:D:277:GLU:HG2	2.01	0.59
2:L:355:ALA:O	2:L:359:THR:HG23	2.02	0.59
1:A:11:LEU:HD13	2:B:514:PHE:CE2	2.38	0.59
2:L:450:ASN:N	2:L:450:ASN:HD22	2.01	0.59
1:A:23:ARG:HH12	2:B:525:MSE:SE	2.35	0.59
2:H:264:HIS:HB3	2:H:267:CYS:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:312:VAL:HG22	2:H:313:GLY:H	1.67	0.59
2:H:320:ARG:HH22	2:H:347:GLU:HG3	1.68	0.59
2:F:347:GLU:O	2:F:348:SER:HB2	2.03	0.59
1:E:1:MSE:HG3	2:F:243:TYR:OH	2.02	0.58
2:H:299:PRO:HA	2:H:329:LEU:HD23	1.84	0.58
1:K:8:ARG:HH22	2:L:481:THR:CG2	2.16	0.58
2:H:250:CYS:HA	2:H:253:LEU:HD12	1.85	0.58
2:H:445:GLU:O	2:H:445:GLU:HG2	2.02	0.58
2:J:331:LYS:HE3	2:L:382:ASN:HB2	1.84	0.58
2:L:506:LEU:HA	2:L:509:ARG:O	2.03	0.58
2:D:296:PRO:O	2:D:302:TRP:HH2	1.86	0.58
2:D:320:ARG:HD3	2:D:344:PHE:CE1	2.38	0.58
2:D:231:LEU:HD23	2:D:260:LYS:HD3	1.86	0.58
2:F:299:PRO:HG2	2:F:330:GLU:HB3	1.84	0.58
2:F:489:HIS:HB3	2:F:494:ASN:HB2	1.85	0.58
2:D:250:CYS:O	2:D:253:LEU:HB2	2.03	0.58
2:D:478:ASN:HB3	2:D:481:THR:OG1	2.02	0.58
2:D:249:MSE:HE3	2:D:253:LEU:CG	2.34	0.58
2:D:403:PHE:O	2:D:407:GLU:HG2	2.03	0.58
1:G:17:GLU:HA	1:G:20:GLU:CG	2.34	0.58
2:L:446:PRO:HB2	3:L:152:HOH:O	2.02	0.58
2:B:403:PHE:O	2:B:407:GLU:HG2	2.04	0.58
2:B:446:PRO:O	2:B:449:ASN:N	2.37	0.58
2:D:302:TRP:HB3	2:D:322:TYR:O	2.04	0.58
2:D:444:TRP:CE3	2:D:445:GLU:HA	2.38	0.58
2:F:250:CYS:HA	2:F:253:LEU:HD12	1.85	0.58
2:H:503:HIS:HE1	2:J:308:TYR:OH	1.86	0.58
2:D:487:TYR:O	2:D:490:SER:HB3	2.03	0.58
2:J:313:GLY:O	2:J:315:LYS:N	2.36	0.58
2:B:258:MSE:HE2	2:B:271:HIS:CD2	2.39	0.58
2:J:444:TRP:CG	2:J:445:GLU:N	2.72	0.57
2:L:298:ASN:OD1	2:L:299:PRO:HD2	2.03	0.57
2:J:300:VAL:HG22	2:J:333:TYR:OH	2.04	0.57
2:D:397:ILE:O	2:D:399:PRO:HD3	2.04	0.57
2:H:447:LEU:N	3:H:10:HOH:O	2.36	0.57
2:J:314:HIS:C	2:J:316:ASN:H	2.13	0.57
2:L:241:HIS:HB2	2:L:250:CYS:HB2	1.85	0.57
2:F:344:PHE:HB2	2:F:353:ALA:HB2	1.86	0.57
2:D:320:ARG:NH2	2:D:347:GLU:HG3	2.19	0.57
2:J:298:ASN:OD1	2:J:300:VAL:HG23	2.04	0.57
2:J:359:THR:HG22	2:L:378:TYR:CE1	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:435:ILE:C	2:J:437:ASN:H	2.11	0.57
2:F:423:LYS:HG3	2:F:424:TRP:N	2.20	0.57
2:J:484:ALA:O	2:J:488:ILE:HG13	2.04	0.57
2:L:313:GLY:C	2:L:315:LYS:H	2.13	0.57
1:I:14:ASP:N	1:I:14:ASP:OD1	2.38	0.57
2:D:252:LYS:O	2:D:256:VAL:HG23	2.05	0.56
2:F:480:SER:HA	2:F:509:ARG:NH1	2.20	0.56
2:H:372:LEU:HD11	2:H:407:GLU:HG3	1.87	0.56
2:B:439:VAL:C	2:B:441:VAL:H	2.12	0.56
2:B:477:GLN:HB2	2:F:477:GLN:HG3	1.86	0.56
2:F:403:PHE:O	2:F:407:GLU:HG2	2.05	0.56
2:J:247:PHE:CE2	2:J:277:GLU:HB3	2.41	0.56
2:J:402:PRO:HA	3:J:13:HOH:O	2.04	0.56
2:J:470:GLN:O	2:J:473:VAL:HB	2.05	0.56
2:H:263:PHE:HA	2:H:268:LEU:HD11	1.85	0.56
2:F:377:GLU:O	2:F:381:THR:HG23	2.06	0.56
2:H:512:ASP:O	2:H:516:VAL:HG23	2.04	0.56
2:D:454:VAL:O	2:D:457:LYS:HB2	2.05	0.56
2:L:255:SER:HA	2:L:258:MSE:HB2	1.88	0.56
2:L:475:ILE:HG23	2:L:477:GLN:HE21	1.67	0.56
2:D:244:ASN:O	2:D:245:CYS:HB2	2.03	0.56
2:H:506:LEU:C	2:H:508:LEU:H	2.14	0.56
1:I:8:ARG:NH1	2:J:445:GLU:OE2	2.37	0.56
1:K:12:LYS:N	1:K:12:LYS:HD2	2.21	0.56
2:J:239:GLU:HG2	2:J:270:VAL:HG21	1.87	0.56
1:E:5:LYS:H	1:E:5:LYS:CD	2.16	0.55
2:B:312:VAL:HG22	2:B:313:GLY:N	2.21	0.55
2:L:299:PRO:HG3	2:L:329:LEU:HD23	1.88	0.55
2:L:344:PHE:HB2	2:L:353:ALA:HB2	1.87	0.55
2:D:477:GLN:CB	2:L:477:GLN:HG3	2.35	0.55
2:L:405:MSE:HG2	2:L:424:TRP:HZ3	1.72	0.55
2:B:241:HIS:CD2	2:B:249:MSE:HG2	2.41	0.55
2:J:466:ASP:O	2:J:469:ARG:HB3	2.06	0.55
2:L:368:HIS:HB3	2:L:397:ILE:HD12	1.89	0.55
2:H:288:SER:O	2:H:292:VAL:HG23	2.07	0.55
2:J:358:PHE:O	2:J:362:GLN:HG2	2.06	0.55
2:L:296:PRO:O	2:L:302:TRP:HH2	1.90	0.55
2:L:450:ASN:O	2:L:453:HIS:HB2	2.07	0.55
2:H:407:GLU:O	2:H:411:VAL:HG23	2.07	0.55
2:D:364:MSE:HE2	2:D:367:CYS:SG	2.47	0.54
2:D:499:VAL:HG12	2:D:503:HIS:CD2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:489:HIS:CB	2:J:498:ALA:HB2	2.28	0.54
1:K:8:ARG:NH2	2:L:481:THR:HG23	2.21	0.54
1:K:14:ASP:O	1:K:17:GLU:HB3	2.07	0.54
1:A:5:LYS:HD3	1:A:5:LYS:N	2.22	0.54
2:F:308:TYR:O	2:F:312:VAL:HG12	2.07	0.54
1:I:3:ARG:HH11	2:J:403:PHE:HD2	1.55	0.54
2:L:405:MSE:HG2	2:L:424:TRP:CZ3	2.42	0.54
1:A:16:ILE:O	1:A:20:GLU:HG2	2.07	0.54
2:H:445:GLU:H	2:H:446:PRO:HD2	1.72	0.54
2:J:447:LEU:HD21	3:J:55:HOH:O	2.06	0.54
2:L:506:LEU:C	2:L:508:LEU:H	2.15	0.54
2:J:252:LYS:O	2:J:256:VAL:HG23	2.06	0.54
2:F:520:GLY:O	2:F:523:ILE:HG22	2.07	0.54
1:C:23:ARG:HH12	2:D:525:MSE:SE	2.41	0.54
2:H:289:HIS:HB2	2:J:523:ILE:HD11	1.89	0.54
2:H:308:TYR:O	2:H:312:VAL:HG12	2.07	0.54
2:B:260:LYS:O	2:B:262:PRO:HD3	2.08	0.54
2:D:391:PHE:HE2	2:D:411:VAL:HG21	1.72	0.54
2:D:261:ASP:O	2:D:264:HIS:HB2	2.08	0.54
2:F:298:ASN:OD1	2:F:300:VAL:HG23	2.08	0.54
2:F:261:ASP:O	2:F:264:HIS:HB2	2.08	0.53
2:H:296:PRO:HA	2:H:302:TRP:CH2	2.44	0.53
2:J:332:THR:HG21	2:L:385:LYS:HD3	1.89	0.53
2:F:509:ARG:O	2:F:509:ARG:HG2	2.06	0.53
2:H:489:HIS:HA	2:H:492:MSE:HE2	1.89	0.53
2:J:312:VAL:HG22	2:J:313:GLY:N	2.19	0.53
2:J:313:GLY:C	2:J:315:LYS:N	2.63	0.53
2:B:331:LYS:HE3	2:D:382:ASN:HB2	1.91	0.53
2:D:473:VAL:HG12	2:D:474:LEU:HD23	1.88	0.53
1:K:5:LYS:CD	1:K:5:LYS:H	2.22	0.53
2:D:488:ILE:O	2:D:492:MSE:HG3	2.08	0.53
1:K:8:ARG:HB2	2:L:446:PRO:HG3	1.89	0.53
2:D:499:VAL:HG11	2:L:285:PHE:HD2	1.74	0.53
1:K:17:GLU:HA	1:K:20:GLU:HG3	1.91	0.53
2:L:472:LEU:HD23	2:L:475:ILE:O	2.08	0.53
2:B:311:MSE:HG3	2:B:312:VAL:HG12	1.90	0.53
2:H:246:ASP:OD2	2:H:249:MSE:HB3	2.09	0.53
2:H:312:VAL:HG13	2:H:313:GLY:N	2.24	0.53
1:I:16:ILE:O	1:I:20:GLU:HG2	2.09	0.53
2:J:354:MSE:HE1	2:J:377:GLU:HB3	1.89	0.53
2:D:451:LEU:HA	2:D:454:VAL:HG23	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:244:ASN:HA	3:F:3:HOH:O	2.09	0.53
2:J:458:LEU:CD1	2:J:460:LYS:HD2	2.39	0.53
1:K:8:ARG:HG3	2:L:446:PRO:CB	2.36	0.53
2:L:445:GLU:H	2:L:446:PRO:HD2	1.69	0.53
2:D:271:HIS:O	2:D:275:LEU:HG	2.09	0.52
2:B:370:PRO:O	2:B:374:ILE:HG12	2.10	0.52
2:D:406:HIS:HD2	2:D:447:LEU:HD13	1.74	0.52
2:D:455:CYS:HB3	2:D:460:LYS:HB2	1.91	0.52
2:F:357:TYR:HB2	2:F:374:ILE:HG23	1.90	0.52
2:H:313:GLY:O	2:H:315:LYS:N	2.41	0.52
2:L:241:HIS:CB	2:L:250:CYS:HB2	2.39	0.52
2:L:320:ARG:NH2	2:L:347:GLU:HG3	2.24	0.52
2:L:451:LEU:HA	2:L:454:VAL:HG23	1.92	0.52
1:A:5:LYS:H	1:A:5:LYS:CD	2.19	0.52
2:B:279:ASN:HA	2:B:311:MSE:CE	2.36	0.52
2:D:318:HIS:HB3	2:D:322:TYR:CE2	2.40	0.52
2:F:389:ARG:O	2:F:393:GLN:HG3	2.09	0.52
2:H:384:SER:HB3	3:H:7:HOH:O	2.10	0.52
1:I:3:ARG:NH1	2:J:403:PHE:HD2	2.07	0.52
2:B:241:HIS:HB2	2:B:250:CYS:HB2	1.90	0.52
2:B:503:HIS:C	2:B:505:ALA:H	2.18	0.52
1:C:22:ILE:O	1:C:22:ILE:CG2	2.58	0.52
1:E:3:ARG:HD3	2:F:403:PHE:CD2	2.45	0.52
2:B:242:TYR:CD2	2:B:274:THR:HG23	2.44	0.52
1:E:12:LYS:HD2	1:E:12:LYS:N	2.25	0.52
2:F:479:ALA:HB1	2:F:509:ARG:HD2	1.92	0.52
2:F:487:TYR:CE1	2:F:518:MSE:HE2	2.44	0.52
2:H:503:HIS:CE1	2:J:308:TYR:OH	2.62	0.52
2:L:368:HIS:CB	2:L:397:ILE:HD12	2.39	0.52
2:B:446:PRO:O	2:B:447:LEU:C	2.52	0.52
1:I:19:PHE:CD1	2:J:518:MSE:HE1	2.45	0.52
2:L:450:ASN:HD22	2:L:450:ASN:H	1.55	0.52
2:B:381:THR:O	2:B:382:ASN:HB2	2.09	0.52
2:D:527:ILE:O	2:D:527:ILE:HG22	2.09	0.52
2:H:518:MSE:O	2:H:518:MSE:HE3	2.10	0.52
2:J:489:HIS:O	2:J:493:GLY:N	2.33	0.52
2:J:444:TRP:CD2	2:J:445:GLU:N	2.78	0.52
2:L:368:HIS:HA	2:L:371:MSE:HE2	1.91	0.52
2:D:503:HIS:HE1	2:L:308:TYR:OH	1.93	0.52
2:H:287:LEU:O	2:H:291:LEU:HG	2.09	0.52
2:H:391:PHE:CG	2:H:408:VAL:HG22	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:245:CYS:SG	2:J:402:PRO:HD2	2.50	0.52
2:J:355:ALA:O	2:J:359:THR:HG23	2.09	0.52
2:F:378:TYR:OH	2:H:359:THR:HG22	2.10	0.51
2:L:295:TYR:C	2:L:297:SER:H	2.17	0.51
2:L:449:ASN:HD22	2:L:481:THR:HG22	1.75	0.51
1:C:5:LYS:H	1:C:5:LYS:CD	2.15	0.51
2:F:328:THR:HG23	2:F:331:LYS:HE2	1.92	0.51
1:G:17:GLU:HA	1:G:20:GLU:HG3	1.92	0.51
2:H:281:ALA:O	2:H:285:PHE:HB2	2.11	0.51
2:B:444:TRP:CD1	2:B:446:PRO:HD2	2.45	0.51
2:F:445:GLU:N	2:F:446:PRO:CD	2.66	0.51
2:J:299:PRO:HG2	2:J:330:GLU:HB2	1.91	0.51
2:J:357:TYR:HB2	2:J:374:ILE:HG23	1.92	0.51
2:B:445:GLU:O	2:B:445:GLU:HG2	2.10	0.51
1:C:13:LEU:C	1:C:15:ASP:H	2.19	0.51
2:D:358:PHE:O	2:D:361:ALA:HB3	2.09	0.51
2:D:450:ASN:N	2:D:450:ASN:HD22	2.07	0.51
2:F:298:ASN:OD1	2:F:299:PRO:HD2	2.10	0.51
2:F:300:VAL:HG22	2:F:333:TYR:OH	2.11	0.51
2:H:401:ASP:CG	2:H:404:VAL:HG23	2.36	0.51
2:B:450:ASN:HD22	2:B:450:ASN:N	2.09	0.51
2:J:354:MSE:SE	2:J:374:ILE:HG22	2.60	0.51
2:J:423:LYS:CG	2:J:424:TRP:N	2.73	0.51
2:B:342:HIS:HD2	2:B:357:TYR:OH	1.94	0.51
2:L:489:HIS:HB2	2:L:498:ALA:HB2	1.91	0.51
2:F:312:VAL:HG22	2:F:313:GLY:N	2.26	0.51
3:H:141:HOH:O	2:J:503:HIS:CE1	2.63	0.51
2:L:490:SER:OG	2:L:518:MSE:HE1	2.09	0.51
2:D:250:CYS:HA	2:D:253:LEU:HD12	1.93	0.51
2:D:258:MSE:HE1	2:D:268:LEU:HD21	1.92	0.51
1:G:4:ARG:NH2	2:H:376:LEU:HD23	2.26	0.51
2:J:444:TRP:CG	2:J:445:GLU:H	2.29	0.51
2:B:302:TRP:HA	2:B:305:VAL:HG12	1.92	0.51
2:B:344:PHE:HB2	2:B:353:ALA:HB2	1.93	0.51
2:B:444:TRP:CD2	2:B:445:GLU:N	2.79	0.51
2:D:231:LEU:HD12	2:D:232:ASP:N	2.26	0.51
2:L:357:TYR:HB2	2:L:374:ILE:HG23	1.91	0.51
2:B:441:VAL:HA	2:B:444:TRP:CE3	2.46	0.51
1:E:4:ARG:NH1	2:F:345:ALA:HB1	2.26	0.51
2:F:460:LYS:O	2:F:461:TYR:C	2.54	0.51
2:D:300:VAL:HG22	2:D:333:TYR:OH	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:ARG:O	2:D:393:GLN:HG3	2.10	0.50
2:H:499:VAL:HG13	2:H:519:LEU:HD21	1.93	0.50
2:D:308:TYR:O	2:D:312:VAL:HG12	2.12	0.50
2:D:313:GLY:C	2:D:315:LYS:H	2.19	0.50
2:F:487:TYR:CD1	2:F:518:MSE:HE2	2.46	0.50
2:J:241:HIS:HB2	2:J:250:CYS:HB2	1.93	0.50
2:L:497:ASN:O	2:L:501:TYR:HD2	1.94	0.50
2:H:344:PHE:CE1	2:H:352:GLN:NE2	2.80	0.50
2:B:446:PRO:O	2:B:448:LEU:N	2.44	0.50
2:F:495:PHE:CZ	2:F:525:MSE:HE1	2.45	0.50
2:H:459:LYS:C	2:H:461:TYR:H	2.19	0.50
1:C:8:ARG:NH1	2:D:445:GLU:CD	2.69	0.50
1:C:13:LEU:CD2	2:D:514:PHE:HD1	2.24	0.50
2:J:458:LEU:O	2:J:459:LYS:HB2	2.11	0.50
2:B:323:LEU:O	2:B:327:THR:HG23	2.12	0.50
2:D:499:VAL:HG11	2:L:285:PHE:CD2	2.46	0.50
2:L:450:ASN:N	2:L:450:ASN:ND2	2.59	0.50
2:D:262:PRO:C	2:D:264:HIS:H	2.20	0.50
2:D:487:TYR:HA	2:D:502:PHE:HZ	1.76	0.50
2:F:441:VAL:HA	2:F:444:TRP:HE3	1.75	0.50
2:H:279:ASN:HA	2:H:311:MSE:HE1	1.94	0.50
2:H:444:TRP:CG	2:H:445:GLU:N	2.79	0.50
2:J:461:TYR:C	2:J:465:LEU:HD12	2.36	0.50
2:B:239:GLU:O	2:B:243:TYR:HD2	1.94	0.50
2:J:309:TYR:CB	2:J:319:ALA:HB2	2.39	0.50
2:L:448:LEU:HA	2:L:451:LEU:CD1	2.41	0.50
2:F:320:ARG:HD3	2:F:344:PHE:CE1	2.47	0.49
2:D:301:SER:O	2:D:305:VAL:HG12	2.12	0.49
2:F:479:ALA:CB	2:F:509:ARG:HD2	2.42	0.49
2:J:287:LEU:O	2:J:291:LEU:HG	2.13	0.49
2:F:463:GLU:O	2:F:466:ASP:HB2	2.12	0.49
1:E:2:LEU:HA	2:F:242:TYR:OH	2.13	0.49
2:L:309:TYR:HB2	2:L:319:ALA:HB2	1.94	0.49
2:B:512:ASP:HB3	2:B:515:SER:HB2	1.95	0.49
1:A:16:ILE:HA	2:B:487:TYR:OH	2.13	0.49
2:B:233:VAL:HG23	3:B:112:HOH:O	2.13	0.49
2:B:247:PHE:HB3	2:B:278:LEU:HD21	1.94	0.49
2:D:489:HIS:HB3	2:D:494:ASN:HB2	1.95	0.49
2:F:371:MSE:HE1	2:F:397:ILE:CD1	2.43	0.49
2:H:251:TYR:CE1	2:H:280:LYS:HE3	2.47	0.49
2:B:314:HIS:HB2	2:F:510:ARG:CZ	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:LEU:HB2	2:F:269:PRO:HD3	1.95	0.49
2:F:323:LEU:O	2:F:327:THR:HG23	2.13	0.49
2:J:473:VAL:HG12	2:J:474:LEU:HD23	1.95	0.49
2:J:479:ALA:O	2:J:482:TYR:HB2	2.12	0.49
2:B:526:TYR:CZ	2:F:286:TYR:HB3	2.48	0.49
2:D:314:HIS:C	2:D:316:ASN:H	2.21	0.49
2:D:472:LEU:O	2:D:473:VAL:C	2.56	0.49
2:D:367:CYS:SG	2:D:370:PRO:HD3	2.52	0.49
2:H:282:ASN:O	2:H:285:PHE:HB3	2.13	0.49
2:D:391:PHE:CE2	2:D:411:VAL:HG21	2.48	0.49
2:H:513:THR:HG23	2:H:514:PHE:N	2.28	0.49
2:J:370:PRO:O	2:J:374:ILE:HG12	2.13	0.49
2:J:296:PRO:O	2:J:302:TRP:HH2	1.96	0.48
2:L:483:SER:HB2	2:L:515:SER:OG	2.13	0.48
2:F:455:CYS:O	2:F:460:LYS:N	2.44	0.48
1:G:12:LYS:HD2	1:G:12:LYS:N	2.28	0.48
2:B:234:VAL:HG11	2:B:257:VAL:HG23	1.95	0.48
1:E:3:ARG:HG2	2:F:369:LEU:HD21	1.94	0.48
1:I:12:LYS:HD2	1:I:12:LYS:N	2.29	0.48
2:J:253:LEU:O	2:J:257:VAL:HG23	2.13	0.48
2:J:461:TYR:O	2:J:462:ALA:C	2.56	0.48
2:H:252:LYS:O	2:H:256:VAL:HG23	2.12	0.48
1:I:8:ARG:CZ	2:J:449:ASN:ND2	2.77	0.48
2:J:377:GLU:OE1	2:J:377:GLU:HA	2.13	0.48
2:B:232:ASP:N	3:B:112:HOH:O	2.47	0.48
2:B:444:TRP:CG	2:B:445:GLU:N	2.82	0.48
1:C:9:LEU:HD12	2:D:450:ASN:HA	1.96	0.48
1:C:16:ILE:O	1:C:20:GLU:HG2	2.13	0.48
2:D:444:TRP:CZ3	2:D:445:GLU:HA	2.49	0.48
2:H:371:MSE:HE1	2:H:397:ILE:CD1	2.42	0.48
1:I:19:PHE:CE1	2:J:518:MSE:HE1	2.48	0.48
2:J:450:ASN:O	2:J:454:VAL:HG23	2.13	0.48
1:K:16:ILE:O	1:K:20:GLU:HG2	2.13	0.48
2:L:327:THR:C	2:L:329:LEU:H	2.22	0.48
2:B:264:HIS:HD2	2:B:267:CYS:N	2.12	0.48
2:D:381:THR:O	2:D:382:ASN:HB2	2.12	0.48
2:D:338:ILE:CG2	2:D:339:ALA:N	2.76	0.48
2:D:344:PHE:HB2	2:D:353:ALA:HB2	1.96	0.48
2:D:490:SER:OG	2:D:518:MSE:HE2	2.14	0.48
1:E:16:ILE:O	1:E:20:GLU:HG2	2.14	0.48
1:I:17:GLU:HA	1:I:20:GLU:HG3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:444:TRP:HZ3	2:L:474:LEU:CD1	2.27	0.48
2:F:300:VAL:HG22	2:F:333:TYR:CZ	2.49	0.48
1:G:4:ARG:NH1	2:H:345:ALA:HB1	2.29	0.48
2:H:474:LEU:C	2:H:476:PRO:HD3	2.39	0.48
2:L:230:ASN:OD1	2:L:230:ASN:C	2.56	0.48
2:L:305:VAL:O	2:L:308:TYR:N	2.47	0.48
2:B:444:TRP:HZ2	2:B:447:LEU:HB3	1.79	0.48
1:C:9:LEU:HD12	2:D:450:ASN:CB	2.44	0.48
2:H:317:GLU:H	2:H:317:GLU:CD	2.21	0.48
2:H:444:TRP:C	2:H:444:TRP:CD2	2.92	0.48
2:L:481:THR:O	2:L:485:ILE:HG13	2.13	0.48
1:E:8:ARG:NH1	2:F:445:GLU:OE1	2.46	0.48
2:H:330:GLU:HA	3:H:164:HOH:O	2.13	0.48
2:J:299:PRO:HG2	2:J:330:GLU:CB	2.43	0.48
2:J:472:LEU:HD21	2:J:481:THR:OG1	2.14	0.48
2:D:446:PRO:O	2:D:449:ASN:N	2.47	0.47
2:D:526:TYR:CZ	2:L:286:TYR:HB3	2.48	0.47
2:H:314:HIS:C	2:H:316:ASN:H	2.22	0.47
2:J:320:ARG:NH2	2:J:347:GLU:HG3	2.22	0.47
2:J:487:TYR:O	2:J:490:SER:HB2	2.14	0.47
2:L:495:PHE:O	2:L:499:VAL:HG23	2.14	0.47
2:D:284:LEU:HD23	2:D:311:MSE:SE	2.64	0.47
2:D:298:ASN:OD1	2:D:299:PRO:HD2	2.14	0.47
2:D:445:GLU:O	2:D:445:GLU:HG2	2.13	0.47
2:J:481:THR:O	2:J:485:ILE:HG13	2.14	0.47
2:L:377:GLU:OE1	2:L:377:GLU:HA	2.14	0.47
1:A:23:ARG:NH1	2:B:525:MSE:SE	2.97	0.47
2:B:358:PHE:O	2:B:362:GLN:HG2	2.14	0.47
2:B:512:ASP:O	2:B:516:VAL:HG23	2.14	0.47
2:D:351:ASP:HB2	3:D:67:HOH:O	2.14	0.47
2:J:378:TYR:OH	2:L:359:THR:HG22	2.14	0.47
2:B:460:LYS:O	2:B:461:TYR:C	2.58	0.47
2:D:436:GLY:HA3	3:D:154:HOH:O	2.13	0.47
2:L:387:ALA:O	2:L:391:PHE:CD2	2.67	0.47
2:H:302:TRP:HB3	2:H:322:TYR:O	2.14	0.47
2:J:320:ARG:HD3	2:J:344:PHE:CE1	2.50	0.47
2:F:455:CYS:HB3	2:F:460:LYS:HB2	1.96	0.47
2:J:359:THR:HG22	2:L:378:TYR:CZ	2.50	0.47
2:J:374:ILE:HD12	2:J:390:PHE:HE1	1.79	0.47
1:K:20:GLU:OE1	1:K:20:GLU:HA	2.15	0.47
2:B:252:LYS:O	2:B:256:VAL:HG23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:CYS:O	2:D:254:THR:HG23	2.14	0.47
2:J:372:LEU:HD11	2:J:407:GLU:HG3	1.97	0.47
2:J:499:VAL:O	2:J:503:HIS:CD2	2.67	0.47
2:D:338:ILE:HG23	2:D:339:ALA:N	2.30	0.47
2:B:288:SER:O	2:B:292:VAL:HG23	2.15	0.47
2:F:268:LEU:HD13	2:F:300:VAL:HG11	1.97	0.47
2:F:313:GLY:C	2:F:315:LYS:H	2.23	0.47
2:F:426:LEU:O	2:F:430:GLU:HG3	2.15	0.47
2:H:372:LEU:HD12	2:H:391:PHE:HE1	1.79	0.47
2:H:506:LEU:HD21	2:H:512:ASP:HB3	1.97	0.47
2:J:272:ILE:O	2:J:276:VAL:HG23	2.15	0.47
2:J:324:SER:O	2:J:328:THR:OG1	2.33	0.47
2:J:389:ARG:O	2:J:393:GLN:HG3	2.15	0.47
2:L:357:TYR:CB	2:L:374:ILE:HG23	2.44	0.47
2:L:527:ILE:HG22	2:L:527:ILE:O	2.14	0.47
2:F:279:ASN:HA	2:F:311:MSE:CE	2.45	0.47
2:F:338:ILE:HG23	2:F:339:ALA:N	2.29	0.47
2:H:229:GLU:OE2	2:H:229:GLU:HA	2.15	0.47
2:L:472:LEU:HD22	2:L:476:PRO:HA	1.96	0.47
2:B:314:HIS:C	2:B:316:ASN:H	2.24	0.46
2:H:315:LYS:O	2:H:318:HIS:HB2	2.15	0.46
2:H:376:LEU:HD11	2:H:380:LEU:HD21	1.97	0.46
1:K:16:ILE:HG12	2:L:514:PHE:CE1	2.50	0.46
2:B:357:TYR:CB	2:B:374:ILE:HG23	2.44	0.46
2:B:475:ILE:HG22	2:B:475:ILE:O	2.14	0.46
2:D:520:GLY:HA3	3:D:74:HOH:O	2.14	0.46
2:L:295:TYR:N	2:L:296:PRO:CD	2.77	0.46
1:C:6:PRO:O	1:C:7:THR:C	2.59	0.46
2:H:258:MSE:HE1	2:H:268:LEU:HD21	1.98	0.46
2:L:445:GLU:N	2:L:446:PRO:HD3	2.26	0.46
2:D:235:VAL:O	2:D:239:GLU:HG3	2.16	0.46
2:H:443:LYS:O	2:H:444:TRP:O	2.33	0.46
2:J:323:LEU:HD13	2:J:340:TYR:HA	1.97	0.46
2:J:499:VAL:HG13	2:J:519:LEU:HD21	1.97	0.46
2:J:510:ARG:NH1	3:J:58:HOH:O	2.48	0.46
2:L:410:VAL:O	2:L:413:PHE:HB3	2.16	0.46
2:L:528:GLY:O	2:L:529:ASP:C	2.57	0.46
2:D:464:ALA:O	2:D:465:LEU:C	2.59	0.46
2:F:250:CYS:O	2:F:253:LEU:HB2	2.16	0.46
2:H:376:LEU:O	2:H:380:LEU:HG	2.15	0.46
1:K:14:ASP:HB3	3:K:176:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:475:ILE:HG12	3:L:62:HOH:O	2.16	0.46
2:B:478:ASN:O	2:B:482:TYR:HD2	1.99	0.46
1:C:1:MSE:H1	2:D:364:MSE:HE3	1.80	0.46
2:H:445:GLU:N	2:H:446:PRO:HD3	2.24	0.46
2:J:235:VAL:O	2:J:239:GLU:HG3	2.15	0.46
2:J:395:LEU:HG	2:J:404:VAL:HG11	1.96	0.46
2:B:296:PRO:HA	2:B:302:TRP:CH2	2.50	0.46
2:D:238:ALA:HA	2:D:253:LEU:HD13	1.97	0.46
2:F:262:PRO:C	2:F:264:HIS:H	2.23	0.46
2:H:294:LEU:O	2:H:295:TYR:CD1	2.69	0.46
2:L:444:TRP:HZ3	2:L:474:LEU:HD12	1.81	0.46
2:L:447:LEU:HD12	2:L:447:LEU:C	2.38	0.46
2:L:493:GLY:O	2:L:495:PHE:HD1	1.99	0.46
2:H:459:LYS:O	2:H:461:TYR:N	2.45	0.46
1:I:2:LEU:O	2:J:342:HIS:HE1	1.98	0.46
2:L:325:LYS:O	2:L:329:LEU:HB2	2.15	0.46
2:L:455:CYS:HB3	2:L:460:LYS:HB2	1.97	0.46
2:L:477:GLN:H	2:L:477:GLN:CD	2.24	0.46
1:A:13:LEU:HD23	2:B:514:PHE:HD1	1.81	0.46
2:B:271:HIS:O	2:B:275:LEU:HG	2.15	0.46
1:C:8:ARG:NH1	2:D:445:GLU:OE1	2.49	0.46
2:J:238:ALA:HA	2:J:253:LEU:CD1	2.46	0.46
2:L:413:PHE:C	2:L:413:PHE:CD2	2.94	0.46
1:I:9:LEU:HD12	2:J:450:ASN:HA	1.96	0.46
2:J:528:GLY:O	2:J:529:ASP:C	2.58	0.46
2:F:258:MSE:HE1	2:F:268:LEU:HD21	1.98	0.45
2:H:528:GLY:O	2:H:529:ASP:C	2.60	0.45
2:J:368:HIS:HB3	2:J:397:ILE:CG2	2.46	0.45
2:J:499:VAL:HG12	2:J:503:HIS:NE2	2.30	0.45
2:L:335:PRO:O	2:L:338:ILE:HG22	2.16	0.45
2:B:495:PHE:HD2	2:B:522:CYS:SG	2.39	0.45
1:C:21:ASN:C	1:C:23:ARG:H	2.24	0.45
2:D:444:TRP:CD2	2:D:445:GLU:N	2.85	0.45
2:F:324:SER:O	2:F:328:THR:OG1	2.33	0.45
1:K:8:ARG:NE	3:K:52:HOH:O	2.49	0.45
2:L:372:LEU:HD22	2:L:404:VAL:HG22	1.97	0.45
2:F:386:LEU:O	2:F:390:PHE:HD2	2.00	0.45
2:F:444:TRP:CG	2:F:445:GLU:N	2.84	0.45
2:J:327:THR:C	2:J:329:LEU:H	2.23	0.45
2:J:403:PHE:O	2:J:406:HIS:HB3	2.16	0.45
2:L:288:SER:O	2:L:292:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:MSE:HE2	2:B:271:HIS:HD2	1.82	0.45
2:H:513:THR:HG23	2:H:514:PHE:H	1.81	0.45
2:B:395:LEU:HG	2:B:404:VAL:HG11	1.98	0.45
2:B:451:LEU:HA	2:B:454:VAL:HG23	1.98	0.45
1:G:17:GLU:HA	1:G:20:GLU:HG2	1.99	0.45
2:H:282:ASN:HA	2:J:503:HIS:NE2	2.32	0.45
2:H:298:ASN:OD1	2:H:300:VAL:HG23	2.16	0.45
2:B:311:MSE:CG	2:B:312:VAL:HG12	2.46	0.45
2:D:312:VAL:O	2:D:313:GLY:C	2.60	0.45
2:H:497:ASN:O	2:H:498:ALA:C	2.59	0.45
2:J:445:GLU:OE1	2:J:475:ILE:HD12	2.17	0.45
2:J:499:VAL:HG13	2:J:519:LEU:CD2	2.46	0.45
2:J:510:ARG:HD3	3:J:58:HOH:O	2.16	0.45
2:D:295:TYR:N	2:D:296:PRO:CD	2.79	0.45
2:D:455:CYS:C	2:D:457:LYS:N	2.70	0.45
2:F:268:LEU:CB	2:F:269:PRO:HD3	2.46	0.45
2:H:466:ASP:O	2:H:469:ARG:HB3	2.17	0.45
2:J:276:VAL:HG13	2:J:311:MSE:HB3	1.99	0.45
2:L:358:PHE:O	2:L:362:GLN:HG2	2.17	0.45
1:A:12:LYS:NZ	1:A:12:LYS:HA	2.32	0.45
1:A:23:ARG:H	1:A:23:ARG:HG2	1.43	0.45
1:C:14:ASP:OD1	1:C:14:ASP:N	2.50	0.45
2:D:523:ILE:HD12	2:D:526:TYR:HB3	1.99	0.45
2:H:499:VAL:HG13	2:H:519:LEU:CD2	2.47	0.45
2:J:289:HIS:HA	2:J:292:VAL:HG23	1.98	0.45
1:G:8:ARG:HG3	2:H:446:PRO:HB3	1.99	0.45
2:H:445:GLU:C	3:H:10:HOH:O	2.60	0.45
2:J:299:PRO:HG3	2:J:329:LEU:HD23	1.99	0.45
2:L:381:THR:O	2:L:382:ASN:HB2	2.17	0.45
2:D:249:MSE:O	2:D:250:CYS:C	2.60	0.44
2:D:456:ARG:HD3	2:D:488:ILE:HG13	1.99	0.44
2:D:494:ASN:OD1	2:D:494:ASN:N	2.50	0.44
2:D:512:ASP:CG	2:D:515:SER:HB2	2.41	0.44
2:F:241:HIS:HB3	2:F:246:ASP:O	2.17	0.44
2:F:264:HIS:HD2	2:F:267:CYS:H	1.65	0.44
2:F:264:HIS:CD2	2:F:267:CYS:HB2	2.52	0.44
2:F:340:TYR:O	2:F:343:SER:OG	2.34	0.44
2:F:480:SER:HA	2:F:509:ARG:HH12	1.81	0.44
2:H:339:ALA:O	2:H:342:HIS:HB2	2.17	0.44
2:J:448:LEU:HD13	2:J:470:GLN:HB3	1.98	0.44
1:K:4:ARG:CZ	2:L:345:ALA:HB1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:320:ARG:HD3	2:L:344:PHE:CE1	2.52	0.44
2:L:484:ALA:O	2:L:488:ILE:HD12	2.16	0.44
1:A:4:ARG:NH1	2:B:345:ALA:HB1	2.33	0.44
2:B:336:ALA:O	2:B:340:TYR:HB2	2.17	0.44
2:B:435:ILE:O	2:B:437:ASN:N	2.46	0.44
1:C:4:ARG:NH1	2:D:345:ALA:HB1	2.32	0.44
1:C:12:LYS:HD2	1:C:12:LYS:N	2.33	0.44
1:G:4:ARG:HD3	2:H:342:HIS:HD2	1.82	0.44
2:H:404:VAL:O	2:H:408:VAL:HG23	2.17	0.44
2:H:512:ASP:HB3	2:H:515:SER:HB2	1.97	0.44
2:J:231:LEU:HD22	2:J:257:VAL:HG13	1.99	0.44
2:J:486:GLY:HA2	2:J:489:HIS:HD2	1.82	0.44
2:B:478:ASN:O	2:B:482:TYR:CD2	2.70	0.44
2:D:334:GLY:HA2	2:D:363:LEU:CD1	2.47	0.44
2:F:294:LEU:CD1	2:F:295:TYR:HD1	2.30	0.44
2:H:252:LYS:HB3	2:H:252:LYS:HE2	1.74	0.44
2:H:268:LEU:O	2:H:272:ILE:HG13	2.17	0.44
2:L:447:LEU:N	3:L:152:HOH:O	2.51	0.44
2:L:490:SER:OG	2:L:518:MSE:CE	2.66	0.44
2:B:404:VAL:O	2:B:408:VAL:HG23	2.18	0.44
2:D:299:PRO:HA	2:D:329:LEU:HD23	2.00	0.44
2:H:389:ARG:O	2:H:393:GLN:HG3	2.18	0.44
2:J:282:ASN:O	2:J:283:GLU:C	2.61	0.44
1:A:2:LEU:O	2:B:342:HIS:HE1	2.00	0.44
2:D:423:LYS:HG3	2:D:424:TRP:N	2.31	0.44
2:D:503:HIS:CE1	2:L:308:TYR:OH	2.71	0.44
1:G:14:ASP:O	1:G:17:GLU:HB3	2.17	0.44
2:H:443:LYS:C	2:H:444:TRP:O	2.60	0.44
1:I:2:LEU:HD23	2:J:339:ALA:HB2	2.00	0.44
2:L:266:SER:O	2:L:269:PRO:HD2	2.18	0.44
2:D:499:VAL:HG22	2:D:519:LEU:CD2	2.48	0.44
2:J:397:ILE:O	2:J:399:PRO:HD3	2.17	0.44
2:J:497:ASN:O	2:J:500:ASP:HB3	2.18	0.44
1:G:4:ARG:HH21	2:H:376:LEU:HD23	1.82	0.44
2:H:282:ASN:HD21	2:J:500:ASP:HA	1.83	0.44
2:J:250:CYS:SG	2:J:274:THR:HG21	2.58	0.44
2:L:249:MSE:CE	2:L:253:LEU:HD21	2.40	0.44
1:A:13:LEU:C	1:A:15:ASP:N	2.76	0.44
2:B:264:HIS:CD2	2:B:267:CYS:HB3	2.52	0.44
2:B:298:ASN:OD1	2:B:299:PRO:HD2	2.18	0.44
2:B:316:ASN:ND2	2:B:347:GLU:HG2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:483:SER:HB2	2:D:515:SER:HG	1.82	0.44
1:G:3:ARG:NH1	2:H:403:PHE:HD2	2.16	0.44
2:F:383:ASN:OD1	2:H:331:LYS:HD2	2.18	0.44
2:H:391:PHE:HE2	2:H:411:VAL:HG21	1.83	0.44
2:H:445:GLU:N	2:H:446:PRO:CD	2.61	0.44
2:J:300:VAL:HG22	2:J:333:TYR:CZ	2.53	0.44
2:J:502:PHE:O	2:J:506:LEU:HD12	2.18	0.44
1:K:11:LEU:HD13	2:L:514:PHE:CE2	2.53	0.44
1:C:16:ILE:HD13	2:D:518:MSE:SE	2.68	0.43
2:D:499:VAL:O	2:D:503:HIS:CD2	2.71	0.43
2:F:460:LYS:O	2:F:463:GLU:N	2.51	0.43
2:H:429:LEU:C	2:H:431:LYS:H	2.26	0.43
2:H:460:LYS:O	2:H:462:ALA:N	2.51	0.43
2:L:264:HIS:CD2	2:L:267:CYS:HB3	2.52	0.43
2:L:425:PHE:HB3	2:L:451:LEU:CD2	2.47	0.43
2:B:397:ILE:O	2:B:399:PRO:HD3	2.18	0.43
2:D:249:MSE:HE3	2:D:253:LEU:CD2	2.48	0.43
2:D:485:ILE:HA	2:D:488:ILE:HD12	2.00	0.43
2:D:489:HIS:CB	2:D:498:ALA:HB2	2.41	0.43
2:J:342:HIS:O	2:J:346:VAL:HG13	2.17	0.43
2:L:313:GLY:O	2:L:315:LYS:N	2.49	0.43
2:L:324:SER:HB3	2:L:340:TYR:CE1	2.53	0.43
2:D:303:PHE:HE1	2:D:335:PRO:O	2.01	0.43
2:D:314:HIS:HB2	2:L:510:ARG:CZ	2.49	0.43
2:D:442:ASP:C	2:D:444:TRP:N	2.72	0.43
2:D:500:ASP:HB2	2:L:282:ASN:HD21	1.83	0.43
1:E:3:ARG:HD3	2:F:403:PHE:HD2	1.82	0.43
2:F:440:THR:C	2:F:442:ASP:H	2.25	0.43
2:F:445:GLU:O	2:F:445:GLU:HG2	2.15	0.43
2:F:463:GLU:HA	2:F:466:ASP:OD2	2.18	0.43
2:H:229:GLU:C	2:H:229:GLU:CD	2.86	0.43
2:J:448:LEU:HD12	2:J:474:LEU:HD11	2.00	0.43
1:K:9:LEU:HD12	2:L:450:ASN:HB3	1.99	0.43
2:L:340:TYR:CD2	2:L:344:PHE:HE2	2.37	0.43
1:A:4:ARG:O	1:A:5:LYS:C	2.62	0.43
1:C:8:ARG:NH2	2:D:481:THR:HG23	2.33	0.43
2:D:303:PHE:CE1	2:D:335:PRO:O	2.72	0.43
2:H:314:HIS:HB2	2:J:510:ARG:NE	2.33	0.43
2:J:317:GLU:CD	2:J:317:GLU:H	2.27	0.43
2:J:428:ALA:HB3	3:J:55:HOH:O	2.17	0.43
2:J:455:CYS:HB3	2:J:460:LYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:395:LEU:C	2:L:397:ILE:H	2.25	0.43
1:C:13:LEU:C	1:C:15:ASP:N	2.74	0.43
2:D:320:ARG:HH22	2:D:347:GLU:HG3	1.83	0.43
2:H:352:GLN:H	2:H:352:GLN:HG3	1.61	0.43
2:L:268:LEU:O	2:L:272:ILE:HG13	2.18	0.43
1:E:7:THR:O	2:F:406:HIS:CE1	2.71	0.43
2:J:439:VAL:O	2:J:441:VAL:N	2.52	0.43
2:J:492:MSE:HE3	2:J:494:ASN:OD1	2.18	0.43
1:A:18:GLU:HB2	2:B:491:LEU:HD21	2.01	0.43
2:D:451:LEU:HA	2:D:454:VAL:CG2	2.48	0.43
2:D:520:GLY:O	2:D:523:ILE:HG22	2.18	0.43
2:J:314:HIS:C	2:J:316:ASN:N	2.72	0.43
2:B:243:TYR:HD1	2:B:368:HIS:CE1	2.37	0.43
2:B:313:GLY:HA3	2:B:314:HIS:HA	1.74	0.43
2:D:239:GLU:HG2	2:D:270:VAL:HG21	2.01	0.43
2:H:289:HIS:CB	2:J:523:ILE:HD11	2.48	0.43
2:H:514:PHE:O	2:H:515:SER:C	2.61	0.43
1:I:8:ARG:NH2	2:J:480:SER:OG	2.52	0.43
2:J:506:LEU:O	2:J:510:ARG:HG2	2.19	0.43
1:K:17:GLU:CA	1:K:20:GLU:HG2	2.47	0.43
2:L:231:LEU:HD22	2:L:257:VAL:HG13	2.00	0.43
2:L:446:PRO:HB2	2:L:447:LEU:H	1.60	0.43
2:B:439:VAL:C	2:B:441:VAL:N	2.77	0.43
2:B:466:ASP:HB3	2:B:469:ARG:NH2	2.34	0.43
2:B:499:VAL:HG12	2:B:503:HIS:NE2	2.33	0.43
1:C:13:LEU:HD22	2:D:514:PHE:HD1	1.83	0.43
2:D:503:HIS:C	2:D:505:ALA:N	2.76	0.43
1:I:12:LYS:HB2	1:I:15:ASP:OD2	2.18	0.43
2:J:327:THR:C	2:J:329:LEU:N	2.76	0.43
2:J:446:PRO:O	2:J:450:ASN:ND2	2.52	0.43
2:B:280:LYS:HB3	2:B:283:GLU:HB2	2.00	0.43
2:B:315:LYS:O	2:B:318:HIS:HB2	2.19	0.43
2:B:317:GLU:CD	2:B:317:GLU:H	2.26	0.43
2:F:320:ARG:HH22	2:F:347:GLU:HG3	1.83	0.43
2:F:460:LYS:O	2:F:462:ALA:N	2.51	0.43
2:H:270:VAL:O	2:H:274:THR:HG23	2.18	0.43
1:I:6:PRO:HG3	2:J:403:PHE:CE1	2.54	0.43
2:J:270:VAL:O	2:J:274:THR:HG23	2.19	0.43
2:J:276:VAL:HG22	2:J:284:LEU:HD22	1.99	0.43
2:L:249:MSE:O	2:L:250:CYS:C	2.61	0.43
2:L:446:PRO:CB	3:L:152:HOH:O	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:THR:O	2:B:278:LEU:HG	2.19	0.42
2:B:475:ILE:HG22	2:B:478:ASN:HB2	2.01	0.42
2:D:230:ASN:OD1	2:D:230:ASN:C	2.62	0.42
2:F:314:HIS:C	2:F:316:ASN:H	2.27	0.42
1:C:16:ILE:HA	2:D:487:TYR:HH	1.81	0.42
2:H:268:LEU:N	2:H:269:PRO:CD	2.82	0.42
2:L:357:TYR:HB2	2:L:374:ILE:CG2	2.49	0.42
2:B:268:LEU:N	2:B:269:PRO:CD	2.82	0.42
2:D:354:MSE:HE2	2:D:354:MSE:HB2	1.98	0.42
2:D:495:PHE:O	2:D:496:GLU:C	2.62	0.42
2:F:338:ILE:CG2	2:F:339:ALA:N	2.82	0.42
1:G:23:ARG:H	1:G:23:ARG:HG2	1.57	0.42
2:H:457:LYS:HD2	2:H:457:LYS:HA	1.75	0.42
2:J:231:LEU:HD12	2:J:232:ASP:N	2.33	0.42
2:J:372:LEU:HD12	2:J:391:PHE:HE1	1.83	0.42
2:B:464:ALA:O	2:B:465:LEU:C	2.63	0.42
2:H:262:PRO:C	2:H:264:HIS:H	2.27	0.42
2:J:262:PRO:C	2:J:264:HIS:H	2.27	0.42
1:A:18:GLU:O	1:A:22:ILE:HG13	2.20	0.42
2:B:231:LEU:HD23	2:B:260:LYS:HD2	2.00	0.42
2:D:318:HIS:O	2:D:322:TYR:CD2	2.73	0.42
2:D:404:VAL:O	2:D:408:VAL:HG23	2.19	0.42
2:H:499:VAL:HG12	2:H:503:HIS:NE2	2.33	0.42
2:B:397:ILE:C	2:B:399:PRO:HD3	2.44	0.42
2:D:260:LYS:O	2:D:262:PRO:HD3	2.20	0.42
2:D:478:ASN:O	2:D:482:TYR:HD2	2.02	0.42
1:E:6:PRO:HA	2:F:407:GLU:OE2	2.19	0.42
2:J:268:LEU:HB2	2:J:269:PRO:HD3	2.01	0.42
2:L:409:GLY:O	2:L:410:VAL:C	2.62	0.42
2:L:499:VAL:HG12	2:L:503:HIS:HD2	1.82	0.42
1:A:8:ARG:NH1	2:B:445:GLU:OE1	2.53	0.42
2:B:316:ASN:HD21	2:B:347:GLU:HG2	1.84	0.42
2:D:268:LEU:HD23	2:D:268:LEU:HA	1.93	0.42
2:F:444:TRP:CD2	2:F:445:GLU:N	2.87	0.42
1:I:5:LYS:HA	1:I:6:PRO:HD3	1.93	0.42
2:L:395:LEU:C	2:L:397:ILE:N	2.78	0.42
2:L:445:GLU:N	2:L:446:PRO:CD	2.61	0.42
2:L:507:GLY:O	2:L:508:LEU:HG	2.19	0.42
2:B:252:LYS:HB3	2:B:252:LYS:HE2	1.59	0.42
2:D:258:MSE:O	2:D:262:PRO:HG3	2.20	0.42
2:D:374:ILE:H	2:D:374:ILE:HG12	1.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:LEU:O	2:H:369:LEU:HD13	2.20	0.42
2:J:371:MSE:HA	2:J:374:ILE:HG13	2.01	0.42
2:J:519:LEU:O	2:J:523:ILE:HG22	2.20	0.42
2:L:402:PRO:O	2:L:406:HIS:N	2.45	0.42
2:B:435:ILE:C	2:B:437:ASN:N	2.75	0.42
2:D:335:PRO:O	2:D:338:ILE:HG22	2.20	0.42
2:D:386:LEU:HD23	2:D:386:LEU:HA	1.83	0.42
2:F:465:LEU:HD11	2:F:492:MSE:SE	2.69	0.42
2:H:250:CYS:SG	2:H:274:THR:HG21	2.60	0.42
2:L:320:ARG:HD3	2:L:344:PHE:CZ	2.55	0.42
2:L:430:GLU:O	2:L:431:LYS:CB	2.68	0.42
1:A:7:THR:O	2:B:406:HIS:HE1	2.02	0.42
2:B:247:PHE:CB	2:B:278:LEU:HD21	2.48	0.42
2:D:268:LEU:N	2:D:269:PRO:CD	2.83	0.42
2:D:328:THR:HG23	3:D:14:HOH:O	2.19	0.42
2:D:372:LEU:HD12	2:D:391:PHE:HE1	1.85	0.42
2:F:328:THR:HA	2:F:331:LYS:HE2	2.01	0.42
2:J:294:LEU:CD1	2:J:295:TYR:HD1	2.32	0.42
2:J:455:CYS:HA	2:J:458:LEU:HD12	2.02	0.42
2:L:252:LYS:O	2:L:256:VAL:HG23	2.20	0.42
2:L:395:LEU:HG	2:L:404:VAL:HG11	2.02	0.42
2:H:391:PHE:CE2	2:H:411:VAL:HG21	2.56	0.41
2:H:466:ASP:OD1	2:H:466:ASP:N	2.53	0.41
1:A:8:ARG:NH1	2:B:445:GLU:CD	2.66	0.41
2:B:241:HIS:CG	2:B:249:MSE:HG2	2.54	0.41
2:B:364:MSE:O	2:B:367:CYS:HB3	2.20	0.41
1:C:8:ARG:NH1	2:D:445:GLU:OE2	2.53	0.41
2:D:264:HIS:HD2	2:D:266:SER:H	1.67	0.41
2:F:238:ALA:HA	2:F:253:LEU:HD13	2.02	0.41
2:H:429:LEU:HD13	2:H:447:LEU:HD23	2.02	0.41
2:J:369:LEU:HB2	2:J:370:PRO:HD3	2.03	0.41
2:L:401:ASP:HA	2:L:402:PRO:HD3	1.78	0.41
2:B:369:LEU:HB2	2:B:370:PRO:HD3	2.01	0.41
2:D:401:ASP:CG	2:D:404:VAL:HG23	2.45	0.41
2:H:371:MSE:CE	2:H:397:ILE:HD12	2.47	0.41
2:H:506:LEU:C	2:H:508:LEU:N	2.78	0.41
2:J:258:MSE:SE	2:J:268:LEU:CD2	3.18	0.41
2:L:473:VAL:HG12	2:L:474:LEU:HD23	2.02	0.41
2:F:395:LEU:O	2:F:399:PRO:HG3	2.19	0.41
2:B:526:TYR:CE2	2:F:286:TYR:HB3	2.54	0.41
2:F:398:ALA:N	2:F:399:PRO:HD3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:457:LYS:HA	3:H:137:HOH:O	2.19	0.41
2:L:303:PHE:O	2:L:307:CYS:SG	2.78	0.41
1:C:20:GLU:HG2	1:C:20:GLU:H	1.61	0.41
2:D:365:LYS:HG2	3:D:92:HOH:O	2.21	0.41
2:F:273:GLY:O	2:F:277:GLU:HG2	2.20	0.41
1:G:18:GLU:OE2	2:H:457:LYS:HD3	2.19	0.41
2:H:460:LYS:O	2:H:463:GLU:N	2.53	0.41
1:I:19:PHE:O	1:I:20:GLU:C	2.63	0.41
2:J:369:LEU:N	2:J:370:PRO:CD	2.84	0.41
2:J:485:ILE:HG21	2:J:501:TYR:CE1	2.56	0.41
2:L:371:MSE:HA	2:L:374:ILE:HD11	2.03	0.41
2:L:371:MSE:HE1	2:L:397:ILE:HD11	2.02	0.41
2:B:320:ARG:HD3	2:B:344:PHE:CE1	2.56	0.41
2:B:391:PHE:CG	2:B:408:VAL:HG22	2.55	0.41
2:D:264:HIS:CD2	2:D:266:SER:OG	2.73	0.41
2:D:372:LEU:HD11	2:D:407:GLU:HG3	2.02	0.41
1:G:3:ARG:HH11	2:H:403:PHE:HD2	1.68	0.41
2:J:278:LEU:O	2:J:279:ASN:HB2	2.21	0.41
2:L:320:ARG:HH22	2:L:347:GLU:HG3	1.86	0.41
2:B:494:ASN:OD1	2:B:494:ASN:N	2.54	0.41
2:D:368:HIS:HB3	2:D:397:ILE:HG21	2.02	0.41
2:D:401:ASP:HA	2:D:402:PRO:HD3	1.88	0.41
2:F:310:LEU:HD23	2:F:310:LEU:HA	1.92	0.41
2:F:315:LYS:O	2:F:318:HIS:HB2	2.21	0.41
2:H:251:TYR:CD2	2:H:251:TYR:C	2.99	0.41
2:H:312:VAL:O	2:H:313:GLY:C	2.64	0.41
2:H:437:ASN:C	2:H:439:VAL:N	2.79	0.41
2:J:354:MSE:HG2	2:L:355:ALA:HB1	2.03	0.41
1:K:5:LYS:HA	1:K:6:PRO:HD3	1.88	0.41
2:L:286:TYR:O	2:L:287:LEU:C	2.63	0.41
2:L:487:TYR:CD1	2:L:514:PHE:HZ	2.39	0.41
2:B:450:ASN:N	2:B:450:ASN:ND2	2.69	0.41
2:F:271:HIS:O	2:F:275:LEU:HG	2.20	0.41
2:F:295:TYR:N	2:F:296:PRO:CD	2.80	0.41
2:F:377:GLU:OE1	2:F:377:GLU:HA	2.21	0.41
2:L:279:ASN:C	2:L:281:ALA:H	2.28	0.41
2:B:241:HIS:HB3	2:B:246:ASP:O	2.21	0.40
2:D:438:GLU:O	2:D:439:VAL:C	2.64	0.40
2:D:478:ASN:O	2:D:482:TYR:CD2	2.74	0.40
2:D:503:HIS:C	2:D:505:ALA:H	2.29	0.40
2:H:272:ILE:HD13	2:H:304:ALA:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:457:LYS:C	2:J:459:LYS:H	2.29	0.40
2:L:272:ILE:HD13	2:L:304:ALA:HA	2.03	0.40
2:L:311:MSE:HG3	2:L:312:VAL:HG22	2.03	0.40
2:L:347:GLU:O	2:L:348:SER:CB	2.69	0.40
2:L:370:PRO:O	2:L:374:ILE:HG12	2.21	0.40
2:B:314:HIS:CG	2:F:510:ARG:NH2	2.89	0.40
1:C:5:LYS:HD3	1:C:5:LYS:N	2.28	0.40
1:C:8:ARG:HH22	2:D:481:THR:HG23	1.85	0.40
2:D:449:ASN:O	2:D:453:HIS:HD2	2.04	0.40
2:F:434:ALA:O	2:F:435:ILE:C	2.63	0.40
1:K:20:GLU:C	1:K:22:ILE:H	2.30	0.40
2:L:441:VAL:HA	2:L:444:TRP:HE3	1.87	0.40
2:D:295:TYR:C	2:D:297:SER:H	2.30	0.40
2:D:406:HIS:CD2	2:D:447:LEU:HD13	2.54	0.40
2:D:444:TRP:CE3	2:D:444:TRP:C	3.00	0.40
2:F:312:VAL:HG22	2:F:313:GLY:H	1.87	0.40
2:F:444:TRP:HZ2	2:F:447:LEU:HB3	1.86	0.40
1:G:7:THR:HG23	2:H:407:GLU:OE1	2.22	0.40
2:B:357:TYR:HB3	2:B:374:ILE:HG23	2.03	0.40
2:B:407:GLU:HB3	3:B:2:HOH:O	2.21	0.40
2:B:444:TRP:HZ2	2:B:447:LEU:CB	2.35	0.40
2:D:231:LEU:HD12	2:D:231:LEU:C	2.47	0.40
2:J:258:MSE:SE	2:J:268:LEU:HD23	2.71	0.40
2:J:314:HIS:O	2:J:314:HIS:ND1	2.53	0.40
2:L:472:LEU:HD23	2:L:472:LEU:HA	1.68	0.40
2:B:282:ASN:O	2:B:286:TYR:CD2	2.74	0.40
2:D:407:GLU:O	2:D:411:VAL:HG23	2.21	0.40
2:D:438:GLU:C	2:D:440:THR:N	2.76	0.40
1:E:3:ARG:NH2	2:F:245:CYS:SG	2.94	0.40
2:H:395:LEU:C	2:H:397:ILE:H	2.29	0.40
2:H:437:ASN:C	2:H:439:VAL:H	2.28	0.40
2:J:275:LEU:O	2:J:280:LYS:HB2	2.22	0.40
2:J:316:ASN:HD21	2:J:347:GLU:HG2	1.87	0.40
2:J:359:THR:HG22	2:L:378:TYR:HE1	1.82	0.40
2:L:391:PHE:O	2:L:395:LEU:HD12	2.22	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	24/29 (83%)	21 (88%)	3 (12%)	0	100	100
1	C	21/29 (72%)	17 (81%)	4 (19%)	0	100	100
1	E	24/29 (83%)	21 (88%)	2 (8%)	1 (4%)	2	7
1	G	23/29 (79%)	21 (91%)	2 (9%)	0	100	100
1	I	24/29 (83%)	21 (88%)	3 (12%)	0	100	100
1	K	21/29 (72%)	17 (81%)	3 (14%)	1 (5%)	2	6
2	B	299/330 (91%)	255 (85%)	34 (11%)	10 (3%)	3	11
2	D	299/330 (91%)	260 (87%)	28 (9%)	11 (4%)	2	9
2	F	299/330 (91%)	255 (85%)	29 (10%)	15 (5%)	1	5
2	H	300/330 (91%)	259 (86%)	28 (9%)	13 (4%)	2	7
2	J	299/330 (91%)	253 (85%)	34 (11%)	12 (4%)	2	8
2	L	295/330 (89%)	237 (80%)	45 (15%)	13 (4%)	2	7
All	All	1928/2154 (90%)	1637 (85%)	215 (11%)	76 (4%)	2	8

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	433	LYS
2	B	435	ILE
2	B	438	GLU
2	B	445	GLU
2	B	447	LEU
2	D	441	VAL
2	D	445	GLU
2	F	445	GLU
2	H	444	TRP
2	H	445	GLU
2	J	314	HIS
2	J	431	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	445	GLU
2	L	431	LYS
2	L	432	ILE
2	L	446	PRO
2	L	447	LEU
2	D	312	VAL
2	F	264	HIS
2	F	312	VAL
2	F	439	VAL
2	F	442	ASP
2	H	314	HIS
2	H	442	ASP
2	J	312	VAL
2	J	440	THR
2	J	441	VAL
2	J	460	LYS
2	L	312	VAL
2	L	435	ILE
2	L	445	GLU
2	L	528	GLY
2	B	446	PRO
2	D	314	HIS
2	D	473	VAL
1	E	25	ASP
2	F	348	SER
2	H	312	VAL
2	H	460	LYS
2	H	461	TYR
2	J	447	LEU
2	L	280	LYS
2	B	504	THR
2	D	263	PHE
2	D	434	ALA
2	D	527	ILE
2	F	349	GLU
2	F	461	TYR
2	H	435	ILE
2	H	439	VAL
1	K	21	ASN
2	L	314	HIS
2	F	314	HIS
2	F	430	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	263	PHE
2	J	263	PHE
2	J	406	HIS
2	L	423	LYS
2	B	330	GLU
2	D	465	LEU
2	D	528	GLY
2	F	263	PHE
2	F	280	LYS
2	J	446	PRO
2	F	528	GLY
2	B	397	ILE
2	H	313	GLY
2	F	397	ILE
2	F	435	ILE
2	H	441	VAL
2	J	528	GLY
2	B	436	GLY
2	D	435	ILE
2	H	446	PRO
2	L	262	PRO
2	L	296	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	22/28 (79%)	19 (86%)	3 (14%)	3	13
1	C	22/28 (79%)	17 (77%)	5 (23%)	1	3
1	E	21/28 (75%)	18 (86%)	3 (14%)	3	11
1	G	23/28 (82%)	19 (83%)	4 (17%)	2	7
1	I	21/28 (75%)	18 (86%)	3 (14%)	3	11
1	K	22/28 (79%)	19 (86%)	3 (14%)	3	13
2	B	238/270 (88%)	221 (93%)	17 (7%)	13	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	239/270 (88%)	226 (95%)	13 (5%)	20	51
2	F	240/270 (89%)	230 (96%)	10 (4%)	26	61
2	H	237/270 (88%)	221 (93%)	16 (7%)	14	42
2	J	238/270 (88%)	226 (95%)	12 (5%)	22	54
2	L	236/270 (87%)	225 (95%)	11 (5%)	23	57
All	All	1559/1788 (87%)	1459 (94%)	100 (6%)	16	44

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	12	LYS
1	A	23	ARG
2	B	231	LEU
2	B	235	VAL
2	B	249	MSE
2	B	274	THR
2	B	279	ASN
2	B	294	LEU
2	B	312	VAL
2	B	338	ILE
2	B	348	SER
2	B	374	ILE
2	B	384	SER
2	B	423	LYS
2	B	445	GLU
2	B	450	ASN
2	B	454	VAL
2	B	466	ASP
2	B	494	ASN
1	C	5	LYS
1	C	7	THR
1	C	14	ASP
1	C	20	GLU
1	C	23	ARG
2	D	305	VAL
2	D	364	MSE
2	D	371	MSE
2	D	374	ILE
2	D	380	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	410	VAL
2	D	427	ASP
2	D	445	GLU
2	D	450	ASN
2	D	454	VAL
2	D	494	ASN
2	D	516	VAL
2	D	527	ILE
1	E	5	LYS
1	E	7	THR
1	E	22	ILE
2	F	231	LEU
2	F	235	VAL
2	F	270	VAL
2	F	317	GLU
2	F	328	THR
2	F	374	ILE
2	F	410	VAL
2	F	445	GLU
2	F	449	ASN
2	F	454	VAL
1	G	5	LYS
1	G	16	ILE
1	G	22	ILE
1	G	23	ARG
2	H	229	GLU
2	H	235	VAL
2	H	275	LEU
2	H	288	SER
2	H	292	VAL
2	H	374	ILE
2	H	380	LEU
2	H	389	ARG
2	H	410	VAL
2	H	444	TRP
2	H	445	GLU
2	H	449	ASN
2	H	459	LYS
2	H	466	ASP
2	H	490	SER
2	H	517	THR
1	I	8	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	14	ASP
1	I	22	ILE
2	J	231	LEU
2	J	252	LYS
2	J	292	VAL
2	J	328	THR
2	J	374	ILE
2	J	423	LYS
2	J	425	PHE
2	J	429	LEU
2	J	445	GLU
2	J	449	ASN
2	J	463	GLU
2	J	465	LEU
1	K	5	LYS
1	K	12	LYS
1	K	14	ASP
2	L	231	LEU
2	L	235	VAL
2	L	274	THR
2	L	292	VAL
2	L	294	LEU
2	L	312	VAL
2	L	374	ILE
2	L	395	LEU
2	L	450	ASN
2	L	451	LEU
2	L	494	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	264	HIS
2	B	271	HIS
2	B	342	HIS
2	B	352	GLN
2	B	406	HIS
2	B	450	ASN
2	D	282	ASN
2	D	314	HIS
2	D	342	HIS
2	D	362	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	406	HIS
2	D	450	ASN
2	D	503	HIS
2	F	264	HIS
2	F	342	HIS
2	F	350	HIS
2	F	468	HIS
2	F	503	HIS
2	H	264	HIS
2	H	271	HIS
2	H	282	ASN
2	H	352	GLN
2	H	362	GLN
2	H	450	ASN
2	H	503	HIS
2	J	282	ASN
2	J	342	HIS
2	J	450	ASN
2	J	477	GLN
2	J	489	HIS
2	J	521	HIS
2	L	264	HIS
2	L	271	HIS
2	L	279	ASN
2	L	350	HIS
2	L	352	GLN
2	L	449	ASN
2	L	453	HIS
2	L	470	GLN
2	L	477	GLN
2	L	489	HIS
2	L	503	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	25/29 (86%)	-1.86	0 100 100	33, 54, 78, 119	0
1	C	22/29 (75%)	-1.84	0 100 100	41, 53, 75, 80	0
1	E	25/29 (86%)	-1.89	0 100 100	38, 54, 89, 119	0
1	G	24/29 (82%)	-1.91	0 100 100	38, 56, 81, 119	0
1	I	25/29 (86%)	-1.85	0 100 100	36, 54, 81, 121	0
1	K	22/29 (75%)	-1.86	0 100 100	36, 51, 71, 82	0
2	B	291/330 (88%)	-1.82	0 100 100	27, 54, 96, 196	0
2	D	291/330 (88%)	-1.76	0 100 100	32, 56, 99, 141	0
2	F	291/330 (88%)	-1.79	0 100 100	24, 54, 98, 170	0
2	H	292/330 (88%)	-1.77	0 100 100	36, 56, 99, 140	0
2	J	291/330 (88%)	-1.73	0 100 100	35, 58, 115, 201	0
2	L	289/330 (87%)	-1.72	0 100 100	35, 58, 106, 152	0
All	All	1888/2154 (87%)	-1.77	0 100 100	24, 56, 103, 201	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.