



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:05 PM UTC

PDB ID : 2ONO / pdb_00002ono
Title : Arg475Gln Mutant of Mitochondrial Aldehyde Dehydrogenase, apo form,
pseudo-merohedrally twinned
Authors : Larson, H.N.; Hurley, T.D.
Deposited on : 2007-01-24
Resolution : 2.15 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
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

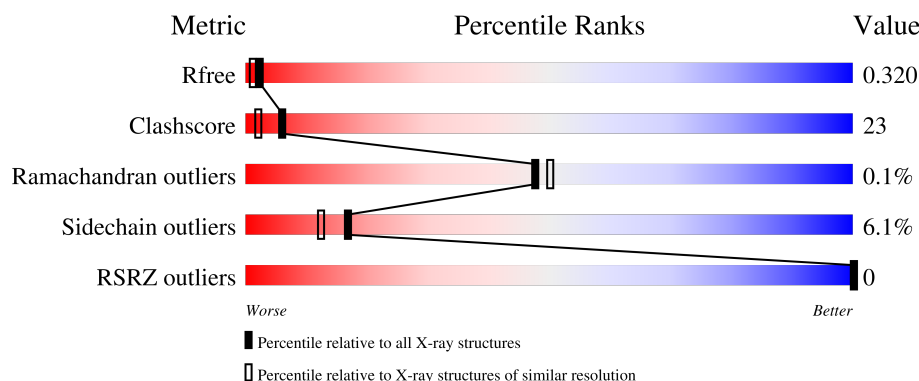
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	500	
1	B	500	
1	C	500	
1	D	500	
1	E	500	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	500	 60% 36% ..
1	G	500	 58% 38% . .
1	H	500	 58% 39% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31388 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	B	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	C	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	D	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	E	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	F	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	G	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	H	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	ARG	engineered mutation	UNP P05091
B	475	GLN	ARG	engineered mutation	UNP P05091
C	475	GLN	ARG	engineered mutation	UNP P05091
D	475	GLN	ARG	engineered mutation	UNP P05091
E	475	GLN	ARG	engineered mutation	UNP P05091
F	475	GLN	ARG	engineered mutation	UNP P05091
G	475	GLN	ARG	engineered mutation	UNP P05091
H	475	GLN	ARG	engineered mutation	UNP P05091

- Molecule 2 is water.

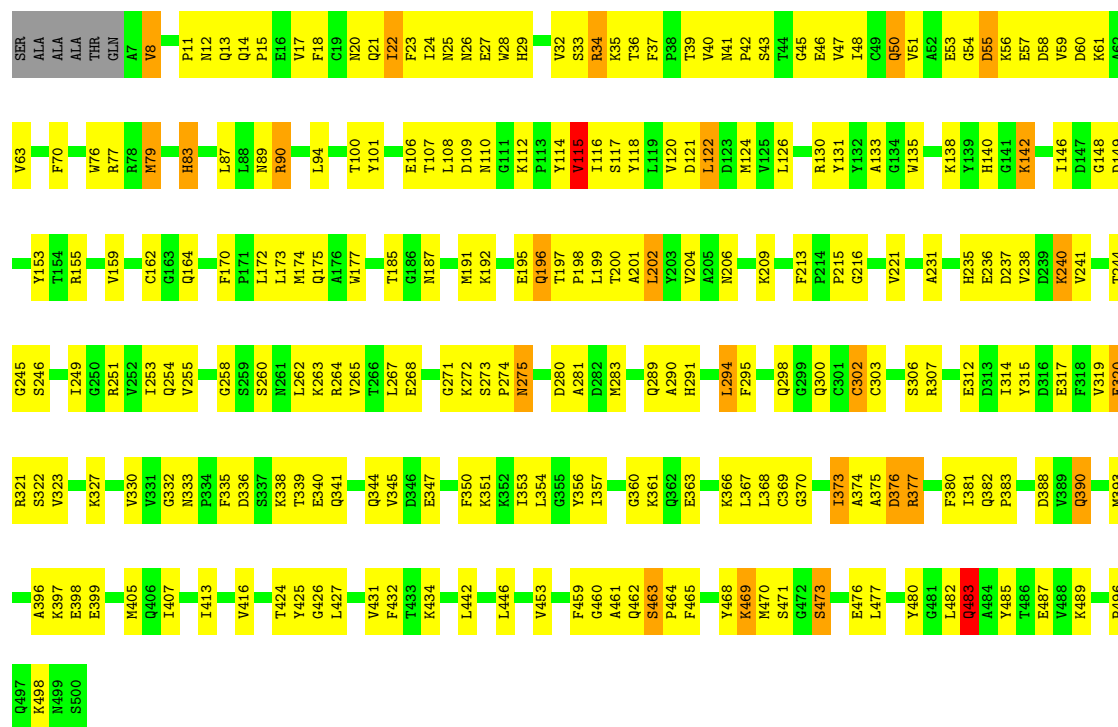
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	134	Total 134	O 134	0	0
2	B	131	Total 131	O 131	0	0
2	C	145	Total 145	O 145	0	0
2	D	133	Total 133	O 133	0	0
2	E	140	Total 140	O 140	0	0
2	F	114	Total 114	O 114	0	0
2	G	118	Total 118	O 118	0	0
2	H	105	Total 105	O 105	0	0

3 Residue-property plots

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.

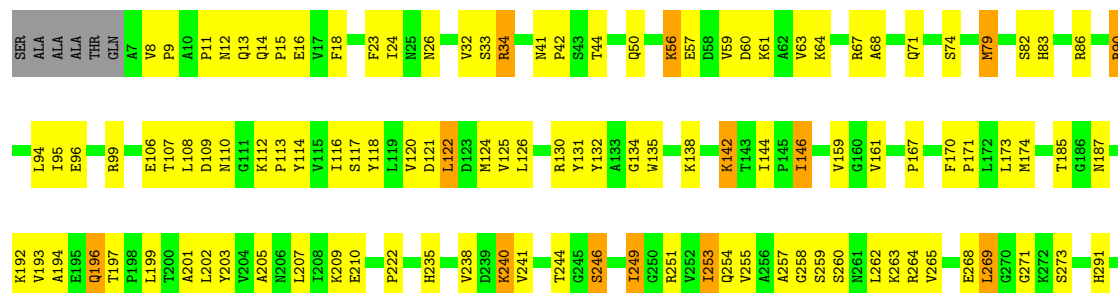
- Molecule 1: Aldehyde dehydrogenase

Chain A: 



- Molecule 1: Aldehyde dehydrogenase

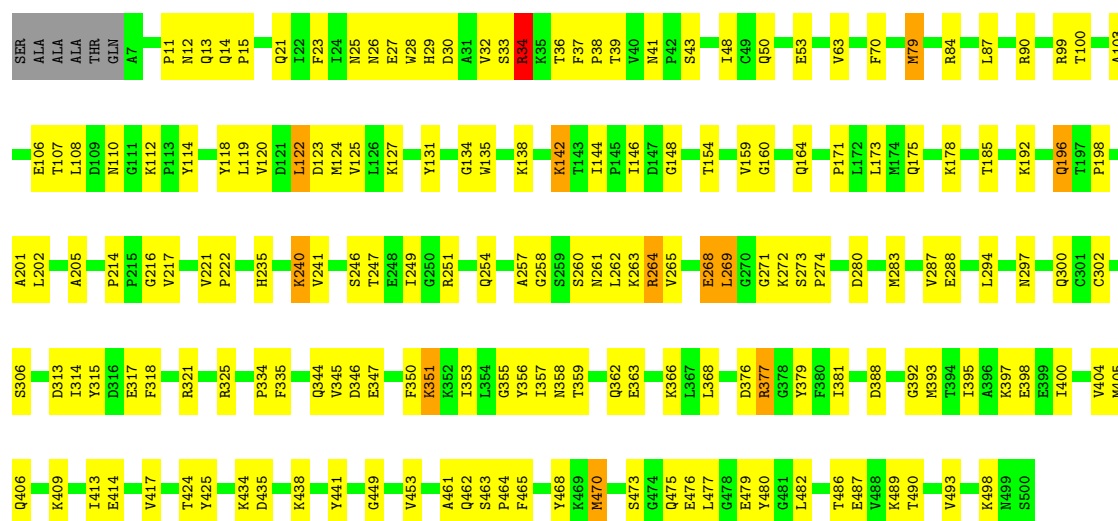
Chain B: 





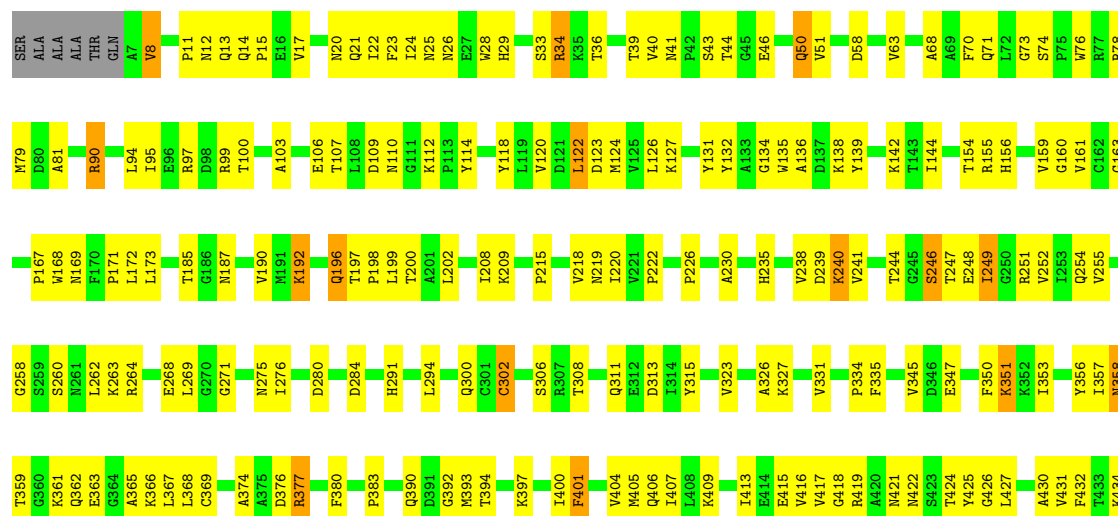
• Molecule 1: Aldehyde dehydrogenase

Chain C: 63% 33% ..



• Molecule 1: Aldehyde dehydrogenase

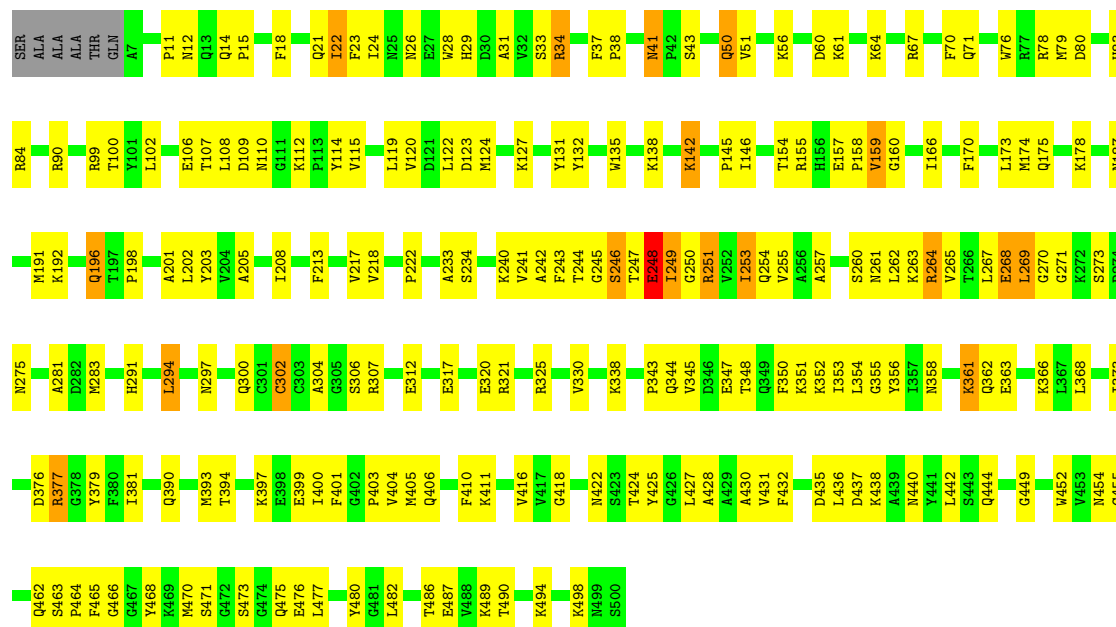
Chain D: 55% 41% ..





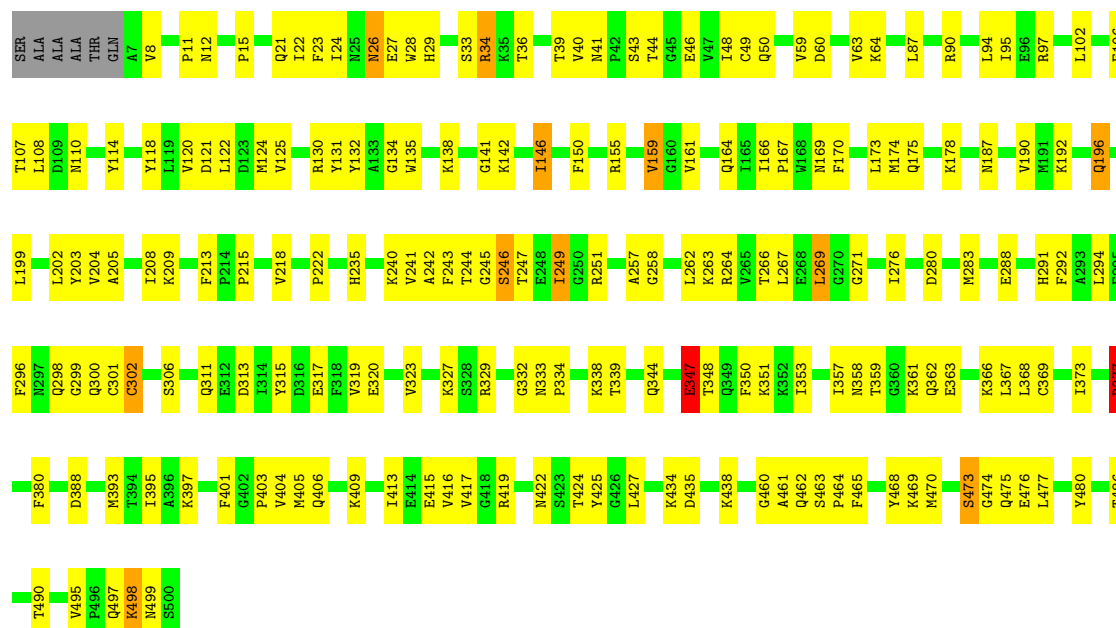
• Molecule 1: Aldehyde dehydrogenase

Chain E: 57% 38% ..



• Molecule 1: Aldehyde dehydrogenase

Chain F: 60% 36% ..



• Molecule 1: Aldehyde dehydrogenase

[illegible]

Chain H: 58% 39% ..

Q462	T359	L267	K178	R78	SER
S463		E268	L179	M79	ALA
P464	Q362	O269	G180	M79	ALA
F465	E363	G270	P181	R86	ALA
		G271		L87	THR
Y468	I373		T185	R90	GLN
K469	A374	P274	G186	R90	A7
M470	A375	M275	N187	L94	
S471	D376	L276		L95	P11
G472	R377		K192		M12
S473	G378	L294		R99	P15
	Y379		Q196	T100	
E476	F380	Q298		Y101	F18
L477		G299	L199	L102	
	Q390	Q300	T200		
L482		G301	A201		Q21
T486	M393	C302	L202	E106	I22
	T394	C303	Y203	T107	F23
K489	K397	S306		L108	I24
V493	E398	R307	L207	D109	N25
	I400			N110	N26
	L408	V310	F213	G111	E27
Q497	K409	Q311	G216	K112	V28
K498	F410	E312		P113	H29
N499	K411		N219	Y114	
S500	T412	S316	V221	I116	
	I413	E317	P222		
		F318		V120	S32
	V417	S320	H235	D121	R34
	C418	R321	V238	L122	K35
	Y425		D239	M124	T36
	G426	R329	K240	V125	V40
			V241	L126	N41
	A429	N333	E242	Y131	P42
	C430	P334	F243	Y132	S43
	V431	C335	T244	T44	T44
		D336	G245	W135	G45
		S337	G246	V47	E46
	D435	K338	T247	K138	V47
	L436	T339	E248		I48
	G437	E340	I249	I146	C49
	K438	Q341	G250		Q50
			R251	D149	
	L442	P343	V252		E53
	S443	Q344	I253	R155	
	Q444	V345	Q254		E57
	A445	D346	V255	V159	
	L446	E347	A256		K61
			A257	W168	R67
	G449	F350			A68
	T450	K351	S260	P171	
	V451	R352	N261	L172	Q71
		I353	L262	L173	
	V458		K263	M174	S74
	F459	Y356	R264	O175	P75
		T357	V265	A176	P76
	G460	R352	T266	L177	R77
	A461				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.47Å 175.85Å 101.46Å 90.00° 94.79° 90.00°	Depositor
Resolution (Å)	10.00 – 2.15 10.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.5 (10.00-2.15) 96.6 (10.00-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.15Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.251 , 0.314 0.264 , 0.320	Depositor DCC
R_{free} test set	9469 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.467 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31388	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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	0.39	2/3880 (0.1%)	1.08	11/5265 (0.2%)
1	B	0.33	0/3880	0.95	6/5265 (0.1%)
1	C	0.37	2/3880 (0.1%)	1.02	8/5265 (0.2%)
1	D	0.36	1/3880 (0.0%)	0.96	6/5265 (0.1%)
1	E	0.37	1/3880 (0.0%)	1.11	6/5265 (0.1%)
1	F	0.33	0/3880	0.96	6/5265 (0.1%)
1	G	0.36	1/3880 (0.0%)	1.02	7/5265 (0.1%)
1	H	0.35	1/3880 (0.0%)	0.97	5/5265 (0.1%)
All	All	0.36	8/31040 (0.0%)	1.01	55/42120 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	ILE	CG1-CD1	8.13	1.83	1.51
1	G	361	LYS	CD-CE	7.27	1.74	1.52
1	E	248	GLU	CD-OE1	6.30	1.37	1.25
1	H	409	LYS	CD-CE	6.18	1.71	1.52
1	A	115	VAL	CB-CG1	5.93	1.72	1.52
1	C	268	GLU	CG-CD	5.28	1.65	1.52
1	A	83	HIS	CE1-NE2	5.26	1.37	1.32
1	C	268	GLU	CD-OE2	5.00	1.34	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	90	ARG	CD-NE-CZ	37.22	176.51	124.40
1	A	90	ARG	CD-NE-CZ	26.23	161.12	124.40
1	C	377	ARG	CD-NE-CZ	18.59	150.43	124.40
1	G	377	ARG	CD-NE-CZ	17.40	148.75	124.40
1	C	34	ARG	CD-NE-CZ	15.60	146.24	124.40
1	G	377	ARG	NE-CZ-NH2	14.66	132.40	119.20
1	E	99	ARG	NE-CZ-NH2	-13.03	107.48	119.20
1	C	377	ARG	NE-CZ-NH2	12.97	130.87	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	ARG	NE-CZ-NH1	12.63	134.13	121.50
1	C	34	ARG	NE-CZ-NH1	12.53	134.03	121.50
1	C	34	ARG	NE-CZ-NH2	-11.58	108.78	119.20
1	E	99	ARG	CD-NE-CZ	11.16	140.03	124.40
1	C	377	ARG	NE-CZ-NH1	-10.88	110.62	121.50
1	G	377	ARG	NE-CZ-NH1	-10.53	110.97	121.50
1	A	483	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	B	377	ARG	CD-NE-CZ	9.41	137.57	124.40
1	G	34	ARG	CD-NE-CZ	9.34	137.48	124.40
1	A	90	ARG	NE-CZ-NH2	-8.96	111.14	119.20
1	A	90	ARG	NE-CZ-NH1	8.95	130.45	121.50
1	H	377	ARG	CD-NE-CZ	8.56	136.38	124.40
1	E	377	ARG	CD-NE-CZ	8.37	136.11	124.40
1	A	320	GLU	CA-CB-CG	8.09	130.29	114.10
1	A	275	ASN	CB-CG-ND2	-7.97	104.44	116.40
1	A	275	ASN	CB-CG-OD1	7.73	136.26	120.80
1	D	377	ARG	CD-NE-CZ	7.53	134.95	124.40
1	A	483	GLN	CG-CD-NE2	6.69	126.43	116.40
1	C	90	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	D	249	ILE	CB-CG1-CD1	-6.14	100.90	113.80
1	D	469	LYS	CB-CA-C	-6.11	109.52	116.54
1	H	90	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	F	90	ARG	CD-NE-CZ	6.07	132.89	124.40
1	D	90	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	C	90	ARG	CD-NE-CZ	5.95	132.73	124.40
1	B	90	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	A	469	LYS	CB-CA-C	-5.93	109.72	116.54
1	F	90	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	B	90	ARG	CD-NE-CZ	5.91	132.67	124.40
1	B	469	LYS	CB-CA-C	-5.84	109.83	116.54
1	H	90	ARG	CD-NE-CZ	5.75	132.45	124.40
1	D	34	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	B	34	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	H	409	LYS	CG-CD-CE	-5.59	98.44	111.30
1	A	377	ARG	CD-NE-CZ	5.54	132.16	124.40
1	G	248	GLU	CA-CB-CG	5.50	125.11	114.10
1	F	469	LYS	CB-CA-C	-5.47	110.24	116.54
1	F	347	GLU	CA-CB-CG	5.45	125.01	114.10
1	G	90	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	F	377	ARG	CD-NE-CZ	5.36	131.91	124.40
1	F	377	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	A	34	ARG	NE-CZ-NH2	5.32	123.99	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	34	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	D	90	ARG	CD-NE-CZ	5.18	131.65	124.40
1	E	34	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	144	ILE	N-CA-CB	-5.06	107.01	112.37
1	G	90	ARG	CD-NE-CZ	5.04	131.45	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3796	0	3740	220	0
1	B	3796	0	3740	179	0
1	C	3796	0	3740	144	0
1	D	3796	0	3740	185	0
1	E	3796	0	3740	200	0
1	F	3796	0	3740	175	0
1	G	3796	0	3740	185	0
1	H	3796	0	3740	184	0
2	A	134	0	0	27	0
2	B	131	0	0	9	0
2	C	145	0	0	10	0
2	D	133	0	0	12	0
2	E	140	0	0	14	0
2	F	114	0	0	11	0
2	G	118	0	0	18	0
2	H	105	0	0	19	0
All	All	31388	0	29920	1369	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 23.

All (1369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ILE:CD1	1:D:249:ILE:CG1	1.83	1.52
1:E:424:THR:HG22	1:E:470:MET:HB2	1.20	1.11
1:A:262:LEU:HD21	1:B:251:ARG:HG2	1.41	1.02
1:A:424:THR:CG2	1:A:470:MET:HE3	1.91	1.01
1:E:424:THR:HG21	1:E:470:MET:SD	2.02	0.99
1:H:247:THR:HA	1:H:269:LEU:HD22	1.45	0.99
1:D:247:THR:HG23	1:D:269:LEU:HD13	1.46	0.97
1:E:424:THR:HG22	1:E:470:MET:CB	1.95	0.97
1:A:196:GLN:H	1:A:196:GLN:HE21	1.09	0.97
1:C:461:ALA:HA	1:C:477:LEU:HD22	1.45	0.95
1:A:272:LYS:HE3	1:A:306:SER:HB2	1.46	0.95
1:F:26:ASN:HB3	1:F:209:LYS:HD2	1.49	0.95
1:H:247:THR:HG23	1:H:269:LEU:HD13	1.47	0.95
1:A:405:MET:HE3	1:A:407:ILE:HD11	1.47	0.93
1:G:196:GLN:H	1:G:196:GLN:HE21	1.16	0.92
1:C:424:THR:HG22	1:C:470:MET:HB2	1.51	0.92
1:D:196:GLN:H	1:D:196:GLN:HE21	1.16	0.92
1:E:424:THR:HG23	1:E:470:MET:HE3	1.53	0.91
1:A:461:ALA:HA	1:A:477:LEU:HD22	1.53	0.90
1:D:120:VAL:HG12	1:D:124:MET:HE2	1.54	0.90
1:A:424:THR:HG21	1:A:470:MET:HE3	1.49	0.90
1:F:461:ALA:HA	1:F:477:LEU:HD22	1.53	0.89
1:C:120:VAL:HG12	1:C:124:MET:HE2	1.53	0.88
1:E:424:THR:CG2	1:E:470:MET:SD	2.61	0.88
1:G:248:GLU:HG2	1:G:249:ILE:HD13	1.56	0.88
1:G:41:ASN:HD22	1:G:43:SER:H	1.16	0.87
1:G:475:GLN:OE1	1:G:480:TYR:HB3	1.75	0.86
1:E:120:VAL:HG12	1:E:124:MET:HE2	1.56	0.85
1:F:120:VAL:HG12	1:F:124:MET:HE2	1.58	0.84
1:H:298:GLN:HG3	1:H:341:GLN:HG3	1.60	0.84
1:G:258:GLY:HA3	1:H:254:GLN:HG2	1.60	0.83
1:E:247:THR:HG23	1:E:269:LEU:HD13	1.58	0.83
1:F:247:THR:HA	1:F:269:LEU:HD22	1.61	0.82
1:A:360:GLY:HA2	2:A:9084:HOH:O	1.78	0.82
1:C:453:VAL:HB	1:D:493:VAL:HG13	1.61	0.82
1:G:255:VAL:HG22	1:H:255:VAL:HG13	1.60	0.82
1:E:247:THR:HA	1:E:269:LEU:HD22	1.60	0.81
1:G:120:VAL:HG12	1:G:124:MET:HE2	1.63	0.80
1:F:196:GLN:H	1:F:196:GLN:HE21	1.30	0.80
1:A:322:SER:HB3	1:A:405:MET:HE1	1.64	0.79
1:C:393:MET:O	1:C:397:LYS:HG3	1.82	0.79
1:H:276:ILE:HD12	1:H:446:LEU:HD11	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HH21	1:A:94:LEU:HD21	1.47	0.79
1:G:294:LEU:HD12	1:G:306:SER:HA	1.64	0.79
1:H:294:LEU:HD12	1:H:306:SER:HA	1.63	0.79
1:A:336:ASP:HB3	1:A:339:THR:OG1	1.83	0.78
1:E:41:ASN:HD22	1:E:43:SER:H	1.31	0.78
1:D:249:ILE:CD1	1:D:249:ILE:CB	2.61	0.78
1:H:32:VAL:HG11	1:H:57:GLU:OE2	1.84	0.78
1:D:21:GLN:HB3	1:D:29:HIS:O	1.84	0.77
1:E:247:THR:HA	1:E:269:LEU:HB3	1.66	0.77
1:D:294:LEU:HD12	1:D:306:SER:HA	1.65	0.77
1:C:359:THR:O	1:C:363:GLU:HG3	1.85	0.77
1:A:41:ASN:HD22	1:A:43:SER:H	1.33	0.77
1:F:266:THR:O	1:F:267:LEU:HD23	1.85	0.77
1:B:329:ARG:HE	1:B:341:GLN:HB2	1.49	0.77
1:H:300:GLN:HE22	1:H:345:VAL:H	1.32	0.77
1:G:77:ARG:HD2	2:G:8877:HOH:O	1.85	0.76
1:H:238:VAL:O	1:H:263:LYS:HE3	1.85	0.76
1:C:351:LYS:HB3	1:E:38:PRO:HG2	1.67	0.76
1:D:172:LEU:HD21	1:D:200:THR:HB	1.65	0.76
1:A:350:PHE:O	1:A:354:LEU:HG	1.86	0.76
1:A:40:VAL:HG13	1:A:46:GLU:O	1.86	0.76
1:G:157:GLU:OE2	1:G:489:LYS:HD2	1.85	0.76
1:G:424:THR:HG22	1:G:470:MET:HB2	1.68	0.76
1:H:196:GLN:HE21	1:H:196:GLN:H	1.33	0.76
1:E:22:ILE:HD13	1:E:222:PRO:HD2	1.66	0.76
1:G:393:MET:O	1:G:397:LYS:HG3	1.85	0.76
1:D:12:ASN:O	1:D:15:PRO:HD3	1.86	0.76
1:F:240:LYS:NZ	1:F:242:ALA:HB2	2.01	0.76
1:E:436:LEU:HB3	2:H:8628:HOH:O	1.86	0.75
1:F:393:MET:O	1:F:397:LYS:HG3	1.85	0.75
1:G:257:ALA:HB1	1:G:263:LYS:HG3	1.69	0.75
1:H:22:ILE:HG12	1:H:222:PRO:HD2	1.69	0.75
1:C:317:GLU:O	1:C:321:ARG:HG3	1.87	0.74
1:H:244:THR:HG23	1:H:268:GLU:HB2	1.66	0.74
1:A:172:LEU:HD21	1:A:200:THR:HB	1.67	0.74
1:A:235:HIS:HB3	1:A:238:VAL:HG23	1.68	0.74
1:E:449:GLY:HA3	1:E:466:GLY:O	1.87	0.74
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.70	0.74
1:E:475:GLN:OE1	1:E:480:TYR:HB3	1.88	0.74
1:F:298:GLN:HB2	1:F:300:GLN:HE21	1.53	0.74
1:B:424:THR:CG2	1:B:470:MET:HE3	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:THR:O	1:G:363:GLU:HG3	1.87	0.73
1:B:60:ASP:O	1:B:64:LYS:HG3	1.89	0.73
1:A:244:THR:HG23	1:A:268:GLU:O	1.88	0.73
1:A:424:THR:HG23	1:A:470:MET:HE3	1.68	0.73
1:E:244:THR:HG23	1:E:268:GLU:HB3	1.69	0.73
1:E:317:GLU:O	1:E:321:ARG:HG3	1.89	0.73
1:F:247:THR:HA	1:F:269:LEU:HB3	1.71	0.73
1:F:257:ALA:HB1	1:F:263:LYS:HG3	1.71	0.73
1:A:196:GLN:HE21	1:A:196:GLN:N	1.87	0.73
1:F:240:LYS:HZ3	1:F:242:ALA:HB2	1.54	0.73
1:A:32:VAL:HG11	1:A:57:GLU:OE2	1.89	0.72
1:B:240:LYS:HE3	1:B:484:ALA:O	1.89	0.72
1:C:413:ILE:O	1:C:417:VAL:HG23	1.89	0.72
1:E:300:GLN:HE22	1:E:345:VAL:H	1.36	0.72
1:E:424:THR:CG2	1:E:470:MET:HE3	2.17	0.72
1:B:194:ALA:HB3	1:B:197:THR:OG1	1.90	0.72
1:H:100:THR:HG22	2:H:9608:HOH:O	1.88	0.72
1:D:40:VAL:HG13	1:D:46:GLU:O	1.90	0.72
1:E:12:ASN:O	1:E:15:PRO:HD3	1.88	0.72
1:G:262:LEU:HD22	1:H:254:GLN:OE1	1.89	0.72
1:G:489:LYS:HB2	1:H:468:TYR:OH	1.89	0.72
1:E:41:ASN:HD21	1:E:43:SER:HB2	1.54	0.72
1:H:185:THR:HG23	1:H:482:LEU:HD22	1.72	0.72
1:G:41:ASN:ND2	1:G:43:SER:H	1.88	0.71
1:G:366:LYS:HE2	1:G:368:LEU:HD21	1.71	0.71
1:C:353:ILE:O	1:C:357:ILE:HG13	1.91	0.71
1:D:156:HIS:HB3	1:D:486:THR:HG21	1.73	0.71
1:D:300:GLN:HE22	1:D:345:VAL:H	1.37	0.71
1:B:313:ASP:HB3	2:B:9435:HOH:O	1.91	0.71
1:B:257:ALA:HB1	1:B:263:LYS:HG3	1.71	0.71
1:F:247:THR:HG23	1:F:269:LEU:HD13	1.72	0.71
1:F:366:LYS:HD3	1:F:388:ASP:OD2	1.90	0.71
1:F:22:ILE:HG12	1:F:222:PRO:HD2	1.73	0.70
1:A:238:VAL:HB	1:A:263:LYS:HE2	1.72	0.70
1:B:159:VAL:HG23	2:B:9130:HOH:O	1.90	0.70
1:H:359:THR:O	1:H:363:GLU:HG3	1.92	0.70
1:A:142:LYS:HD2	1:B:480:TYR:OH	1.91	0.70
1:B:294:LEU:HD12	1:B:306:SER:HA	1.74	0.70
1:B:44:THR:HB	1:B:377:ARG:NH2	2.07	0.70
1:D:359:THR:O	1:D:363:GLU:HG3	1.92	0.70
1:G:41:ASN:HD21	1:G:43:SER:HB2	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:ND2	1:A:43:SER:H	1.88	0.70
1:B:393:MET:O	1:B:397:LYS:HG3	1.92	0.70
1:D:124:MET:HE3	1:D:173:LEU:HD22	1.73	0.69
1:F:134:GLY:O	1:F:138:LYS:HD2	1.92	0.69
1:F:12:ASN:O	1:F:15:PRO:HD3	1.91	0.69
1:D:246:SER:OG	1:D:249:ILE:HD12	1.92	0.69
1:B:358:ASN:O	1:B:362:GLN:HG2	1.92	0.69
1:B:86:ARG:HD3	2:D:9167:HOH:O	1.92	0.69
1:F:190:VAL:HG23	2:F:8853:HOH:O	1.92	0.69
1:H:257:ALA:HB1	1:H:263:LYS:HG3	1.75	0.69
1:A:294:LEU:HD22	1:A:405:MET:HB2	1.74	0.69
1:G:117:SER:O	1:G:121:ASP:HB2	1.92	0.69
1:B:121:ASP:O	1:B:125:VAL:HG23	1.93	0.69
1:G:196:GLN:HE21	1:G:196:GLN:N	1.89	0.69
1:F:283:MET:HE3	1:F:317:GLU:OE2	1.93	0.69
1:A:425:TYR:O	1:A:469:LYS:HD2	1.93	0.68
1:F:124:MET:HE3	1:F:173:LEU:HD22	1.75	0.68
1:B:378:GLY:HA2	2:B:8708:HOH:O	1.93	0.68
1:E:424:THR:CG2	1:E:470:MET:CG	2.71	0.68
1:A:317:GLU:O	1:A:321:ARG:HG3	1.92	0.68
1:A:330:VAL:HG23	1:A:340:GLU:OE2	1.93	0.68
1:H:120:VAL:HG12	1:H:124:MET:HE2	1.75	0.68
1:A:109:ASP:OD2	1:A:197:THR:HA	1.92	0.68
1:B:244:THR:HG23	1:B:268:GLU:HB2	1.75	0.68
1:D:413:ILE:O	1:D:417:VAL:HG23	1.94	0.68
1:E:196:GLN:H	1:E:196:GLN:HE21	1.41	0.68
1:D:235:HIS:HB3	1:D:238:VAL:HG23	1.75	0.68
1:F:298:GLN:HE21	1:F:300:GLN:HE21	1.40	0.68
1:B:315:TYR:O	1:B:319:VAL:HG23	1.94	0.68
1:D:358:ASN:O	1:D:362:GLN:HG2	1.93	0.68
1:G:258:GLY:CA	1:H:254:GLN:HG2	2.23	0.68
1:H:468:TYR:O	1:H:471:SER:HB2	1.94	0.68
1:G:26:ASN:HB3	1:G:209:LYS:HD2	1.76	0.68
1:C:241:VAL:HG12	1:C:265:VAL:HG22	1.77	0.67
1:C:294:LEU:HD12	1:C:306:SER:HA	1.74	0.67
1:B:196:GLN:H	1:B:196:GLN:NE2	1.92	0.67
1:H:46:GLU:HB2	2:H:8788:HOH:O	1.93	0.67
1:A:185:THR:HG23	1:A:482:LEU:HD22	1.75	0.67
1:G:177:TRP:NE1	1:G:477:LEU:HD21	2.09	0.67
1:H:426:GLY:O	1:H:468:TYR:HB2	1.94	0.67
1:E:283:MET:HE3	1:E:317:GLU:OE2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLN:H	1:B:196:GLN:HE21	1.41	0.67
1:F:424:THR:HB	1:F:470:MET:HE3	1.76	0.67
1:H:312:GLU:OE1	1:H:411:LYS:HG3	1.95	0.67
1:C:280:ASP:O	1:C:434:LYS:HD2	1.94	0.67
1:E:366:LYS:HD3	1:E:368:LEU:HD21	1.77	0.67
1:H:358:ASN:O	1:H:362:GLN:HG2	1.94	0.67
1:H:111:GLY:O	1:H:343:PRO:HD2	1.95	0.67
1:C:38:PRO:HG2	1:E:351:LYS:HB3	1.75	0.67
1:C:464:PRO:HG2	1:D:490:THR:OG1	1.95	0.67
1:E:60:ASP:O	1:E:64:LYS:HG3	1.95	0.67
1:F:59:VAL:O	1:F:63:VAL:HG23	1.94	0.67
1:E:490:THR:OG1	1:F:464:PRO:HG2	1.95	0.67
1:G:12:ASN:O	1:G:15:PRO:HD3	1.95	0.67
1:A:251:ARG:HG2	1:B:262:LEU:HD21	1.77	0.66
1:C:300:GLN:HE22	1:C:345:VAL:H	1.43	0.66
1:G:77:ARG:HA	2:G:8877:HOH:O	1.95	0.66
1:E:261:ASN:HA	1:F:251:ARG:HH22	1.59	0.66
1:G:463:SER:HB3	2:G:9569:HOH:O	1.95	0.66
1:H:245:GLY:O	1:H:269:LEU:HA	1.95	0.66
1:A:206:ASN:O	1:A:209:LYS:HB3	1.96	0.66
1:G:350:PHE:O	1:G:354:LEU:HG	1.95	0.66
1:G:361:LYS:HG2	2:G:9353:HOH:O	1.95	0.66
1:E:247:THR:HG23	1:E:269:LEU:CD1	2.25	0.66
1:G:470:MET:SD	1:H:262:LEU:HD12	2.36	0.66
1:H:461:ALA:HA	1:H:477:LEU:HD22	1.77	0.66
1:F:280:ASP:O	1:F:434:LYS:HG3	1.94	0.66
1:D:284:ASP:HB2	2:D:9470:HOH:O	1.96	0.66
1:E:294:LEU:HD12	1:E:306:SER:HA	1.78	0.66
1:A:32:VAL:HG23	1:A:58:ASP:OD1	1.96	0.66
1:D:109:ASP:OD2	1:D:197:THR:HA	1.96	0.66
1:C:462:GLN:O	1:D:144:ILE:HG21	1.96	0.65
1:G:244:THR:OG1	1:G:268:GLU:HB2	1.95	0.65
1:A:15:PRO:HD2	1:A:108:LEU:HD13	1.77	0.65
1:C:103:ALA:HB2	1:C:122:LEU:HD13	1.79	0.65
1:G:361:LYS:HA	2:G:9353:HOH:O	1.95	0.65
1:A:36:THR:OG1	1:A:50:GLN:HG3	1.96	0.65
1:A:146:ILE:HG22	2:A:8700:HOH:O	1.97	0.65
1:C:134:GLY:O	1:C:138:LYS:HD2	1.96	0.65
1:E:251:ARG:HA	1:F:262:LEU:HD21	1.79	0.65
1:G:195:GLU:HA	2:G:8776:HOH:O	1.97	0.65
1:D:306:SER:O	1:D:406:GLN:HB2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ALA:HA	1:B:71:GLN:HG2	1.79	0.65
1:E:124:MET:HE3	1:E:173:LEU:HD22	1.77	0.65
1:D:155:ARG:HD3	1:D:489:LYS:HD2	1.78	0.64
1:E:347:GLU:O	1:E:351:LYS:HG3	1.97	0.64
1:F:358:ASN:O	1:F:362:GLN:HG2	1.96	0.64
1:G:247:THR:HA	1:G:269:LEU:HD22	1.78	0.64
1:G:431:VAL:HG21	1:G:442:LEU:HB3	1.79	0.64
1:F:161:VAL:HG13	2:F:8853:HOH:O	1.97	0.64
1:F:315:TYR:O	1:F:319:VAL:HG23	1.98	0.64
1:H:106:GLU:OE2	1:H:200:THR:HG21	1.97	0.64
1:H:196:GLN:H	1:H:196:GLN:NE2	1.95	0.64
1:C:13:GLN:NE2	1:C:335:PHE:HB3	2.13	0.64
1:A:55:ASP:O	1:A:59:VAL:HG23	1.98	0.64
1:B:271:GLY:HA2	1:B:425:TYR:CG	2.33	0.64
1:D:134:GLY:O	1:D:138:LYS:HD2	1.97	0.64
1:A:393:MET:O	1:A:397:LYS:HG3	1.97	0.64
1:H:37:PHE:HD2	1:H:53:GLU:HB2	1.63	0.64
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.33	0.64
1:E:247:THR:CA	1:E:269:LEU:HB3	2.27	0.64
1:H:356:TYR:CG	1:H:400:ILE:HG12	2.33	0.63
1:H:408:LEU:HB3	2:H:8635:HOH:O	1.97	0.63
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.80	0.63
1:D:155:ARG:HB2	1:D:489:LYS:HB3	1.80	0.63
1:G:156:HIS:CD2	1:G:488:VAL:HG22	2.33	0.63
1:G:315:TYR:CG	1:G:409:LYS:HE2	2.33	0.63
1:G:391:ASP:OD2	1:G:419:ARG:HG2	1.98	0.63
1:E:424:THR:CG2	1:E:470:MET:CE	2.76	0.63
1:G:47:VAL:HG13	2:G:8768:HOH:O	1.97	0.63
1:G:365:ALA:HB2	1:G:393:MET:SD	2.38	0.63
1:E:344:GLN:HG3	1:E:353:ILE:HD12	1.79	0.63
1:G:32:VAL:HG23	1:G:58:ASP:OD1	1.98	0.63
1:A:480:TYR:OH	1:B:142:LYS:HG3	1.98	0.63
1:E:424:THR:CG2	1:E:470:MET:CB	2.73	0.63
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.33	0.63
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.33	0.63
1:A:24:ILE:HG22	1:A:25:ASN:OD1	1.99	0.62
1:C:50:GLN:HG2	1:E:358:ASN:OD1	1.99	0.62
1:H:418:GLY:HA3	2:H:8803:HOH:O	1.98	0.62
1:A:350:PHE:CZ	1:A:373:ILE:HD13	2.35	0.62
1:E:464:PRO:HA	1:E:476:GLU:O	1.99	0.62
1:G:348:THR:O	1:G:352:LYS:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LYS:HE2	1:E:297:ASN:OD1	1.99	0.62
1:B:59:VAL:O	1:B:63:VAL:HG23	1.98	0.62
1:F:353:ILE:O	1:F:357:ILE:HG13	2.00	0.62
1:H:87:LEU:HB3	1:H:213:PHE:CZ	2.34	0.62
1:C:315:TYR:CD1	1:C:409:LYS:HE2	2.34	0.62
1:F:44:THR:HA	1:F:377:ARG:HD3	1.80	0.62
1:G:461:ALA:HA	1:G:477:LEU:HD22	1.82	0.62
1:F:413:ILE:O	1:F:417:VAL:HG23	1.99	0.62
1:E:424:THR:CG2	1:E:470:MET:HB2	2.12	0.62
1:E:175:GLN:HE22	1:E:201:ALA:HA	1.64	0.62
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.34	0.62
1:F:359:THR:O	1:F:363:GLU:HG3	2.00	0.62
1:G:248:GLU:O	1:G:252:VAL:HG23	2.00	0.62
1:H:12:ASN:O	1:H:15:PRO:HD3	2.00	0.62
1:C:475:GLN:OE1	1:C:480:TYR:HB3	1.99	0.61
1:E:241:VAL:HG13	1:E:265:VAL:HG13	1.82	0.61
1:E:41:ASN:ND2	1:E:43:SER:HB2	2.16	0.61
1:F:460:GLY:O	1:F:477:LEU:HD13	2.00	0.61
1:B:347:GLU:O	1:B:351:LYS:HG3	1.99	0.61
1:D:23:PHE:HB2	1:D:28:TRP:CZ3	2.36	0.61
1:D:95:ILE:HG22	1:D:126:LEU:HD21	1.82	0.61
1:E:424:THR:HG23	1:E:470:MET:CE	2.29	0.61
1:A:271:GLY:O	1:A:399:GLU:HB2	2.01	0.61
1:D:366:LYS:HD3	1:D:368:LEU:HD21	1.82	0.61
1:H:41:ASN:HD22	1:H:43:SER:H	1.47	0.61
1:B:203:TYR:HB2	2:B:8930:HOH:O	2.00	0.61
1:E:31:ALA:HA	2:E:8812:HOH:O	2.01	0.61
1:C:30:ASP:HB2	1:C:34:ARG:NH2	2.16	0.61
1:D:435:ASP:HB3	1:D:438:LYS:HB2	1.81	0.60
1:F:422:ASN:HB3	2:F:9339:HOH:O	2.01	0.60
1:G:375:ALA:HB3	1:G:380:PHE:HB2	1.82	0.60
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.36	0.60
1:A:70:PHE:CD1	1:A:77:ARG:HD3	2.36	0.60
1:D:11:PRO:HB3	1:D:114:TYR:CE1	2.36	0.60
1:D:99:ARG:HG3	1:D:122:LEU:HD22	1.82	0.60
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.36	0.60
1:E:246:SER:HG	1:E:249:ILE:H	1.49	0.60
1:A:237:ASP:HA	2:A:9067:HOH:O	2.01	0.60
1:H:393:MET:O	1:H:397:LYS:HG3	2.02	0.60
1:H:429:ALA:HB1	1:H:446:LEU:HD13	1.84	0.60
1:B:464:PRO:HG3	1:B:480:TYR:CE1	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:LYS:HB2	1:D:468:TYR:OH	2.01	0.60
1:F:298:GLN:HE21	1:F:300:GLN:NE2	1.99	0.60
1:B:347:GLU:HA	1:B:350:PHE:HB3	1.83	0.60
1:C:251:ARG:HG2	1:D:262:LEU:HD11	1.82	0.60
1:C:196:GLN:HE21	1:C:196:GLN:H	1.48	0.60
1:F:8:VAL:HG13	1:F:118:TYR:CD2	2.36	0.60
1:B:12:ASN:O	1:B:15:PRO:HD3	2.01	0.60
1:B:94:LEU:HD13	1:B:210:GLU:OE2	2.01	0.60
1:D:294:LEU:HD13	1:D:405:MET:HA	1.83	0.60
1:F:11:PRO:HB3	1:F:114:TYR:CE1	2.36	0.60
1:F:294:LEU:O	1:F:299:GLY:HA2	2.02	0.60
1:G:468:TYR:O	1:G:471:SER:HB2	2.02	0.60
1:H:107:THR:HG23	1:H:334:PRO:HB2	1.83	0.60
1:A:424:THR:HG22	1:A:470:MET:HB2	1.84	0.59
1:B:390:GLN:HG2	1:B:393:MET:HE3	1.83	0.59
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.83	0.59
1:E:435:ASP:OD1	1:E:438:LYS:HG3	2.01	0.59
1:F:298:GLN:HB2	1:F:300:GLN:NE2	2.15	0.59
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.37	0.59
1:G:36:THR:OG1	1:G:50:GLN:HG3	2.02	0.59
1:A:45:GLY:HA3	2:A:9090:HOH:O	2.01	0.59
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.84	0.59
1:H:244:THR:OG1	1:H:268:GLU:HG3	2.02	0.59
1:C:388:ASP:HA	2:C:8979:HOH:O	2.02	0.59
1:E:146:ILE:HG13	1:F:460:GLY:HA3	1.84	0.59
1:F:347:GLU:O	1:F:351:LYS:HG3	2.01	0.59
1:C:135:TRP:CZ2	1:C:479:GLU:HB2	2.38	0.59
1:C:247:THR:HA	1:C:269:LEU:HB3	1.84	0.59
1:D:468:TYR:O	1:D:471:SER:HB2	2.02	0.59
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.37	0.59
1:E:240:LYS:HZ3	1:E:242:ALA:HB2	1.67	0.59
1:B:331:VAL:HG13	1:B:341:GLN:O	2.03	0.59
1:B:461:ALA:O	1:B:477:LEU:HB3	2.01	0.59
1:A:109:ASP:OD2	1:A:198:PRO:HD2	2.03	0.59
1:F:209:LYS:HD3	2:F:8843:HOH:O	2.02	0.59
1:G:413:ILE:O	1:G:417:VAL:HG23	2.03	0.59
1:B:418:GLY:O	1:B:422:ASN:HB2	2.03	0.59
1:B:424:THR:HG21	1:B:470:MET:HE3	1.84	0.59
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.38	0.59
1:A:21:GLN:OE1	1:A:28:TRP:HB3	2.03	0.58
1:A:155:ARG:CZ	1:B:444:GLN:HG3	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:GLN:HG2	1:D:393:MET:HE3	1.85	0.58
1:F:311:GLN:OE1	1:F:313:ASP:HB2	2.02	0.58
1:B:348:THR:O	1:B:352:LYS:HB2	2.04	0.58
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.38	0.58
1:C:247:THR:HG23	1:C:269:LEU:CB	2.33	0.58
1:C:261:ASN:HD21	1:C:263:LYS:HE3	1.68	0.58
1:E:240:LYS:NZ	1:E:242:ALA:HB2	2.18	0.58
1:A:39:THR:HG23	1:A:48:ILE:HB	1.85	0.58
1:D:196:GLN:HE21	1:D:196:GLN:N	1.95	0.58
1:G:31:ALA:O	1:G:34:ARG:NE	2.37	0.58
1:G:205:ALA:HB2	1:G:220:ILE:CD1	2.34	0.58
1:A:76:TRP:O	1:A:79:MET:HB3	2.04	0.58
1:A:366:LYS:HE2	1:A:368:LEU:HD21	1.84	0.58
1:F:497:GLN:HG2	1:F:499:ASN:ND2	2.19	0.58
1:E:115:VAL:HG13	1:E:119:LEU:HD12	1.86	0.58
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.39	0.58
1:H:269:LEU:HD12	1:H:472:GLY:N	2.19	0.58
1:E:41:ASN:ND2	1:E:43:SER:H	2.01	0.58
1:A:200:THR:O	1:A:204:VAL:HG23	2.03	0.58
1:B:300:GLN:HE22	1:B:345:VAL:H	1.52	0.58
1:A:116:ILE:HG22	1:A:121:ASP:OD2	2.04	0.57
1:B:135:TRP:CZ2	1:B:479:GLU:HB2	2.39	0.57
1:D:280:ASP:O	1:D:434:LYS:HG3	2.03	0.57
1:A:241:VAL:HG12	1:A:265:VAL:HG22	1.86	0.57
1:F:294:LEU:HD11	1:F:404:VAL:O	2.04	0.57
1:H:300:GLN:HE22	1:H:345:VAL:N	2.01	0.57
1:A:363:GLU:HB2	2:A:9084:HOH:O	2.03	0.57
1:D:291:HIS:HE1	1:D:326:ALA:HA	1.69	0.57
1:E:294:LEU:HD11	1:E:404:VAL:O	2.04	0.57
1:A:149:ASP:HA	1:A:498:LYS:HB2	1.85	0.57
1:A:366:LYS:HG2	1:A:368:LEU:HD21	1.85	0.57
1:C:34:ARG:HD2	1:C:34:ARG:N	2.18	0.57
1:D:449:GLY:HA3	1:D:466:GLY:O	2.05	0.57
1:G:11:PRO:HB3	1:G:114:TYR:CE1	2.39	0.57
1:C:106:GLU:O	1:C:110:ASN:HB3	2.03	0.57
1:D:68:ALA:HA	1:D:71:GLN:HG2	1.87	0.57
1:E:109:ASP:OD2	1:E:198:PRO:HD2	2.04	0.57
1:F:292:PHE:CD2	1:F:296:PHE:HB2	2.40	0.57
1:G:41:ASN:ND2	1:G:43:SER:HB2	2.18	0.57
1:G:146:ILE:HG13	1:H:460:GLY:HA3	1.85	0.57
1:B:366:LYS:HG2	1:B:368:LEU:HD21	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:390:GLN:HG2	1:H:393:MET:HE3	1.86	0.57
1:A:8:VAL:HG21	1:A:115:VAL:HG22	1.85	0.57
1:A:20:ASN:HA	1:A:202:LEU:HD12	1.87	0.57
1:A:146:ILE:HG13	1:B:460:GLY:HA3	1.87	0.57
1:A:363:GLU:CG	2:A:9084:HOH:O	2.51	0.57
1:G:304:ALA:HA	2:G:9554:HOH:O	2.04	0.57
1:G:489:LYS:HB2	1:H:468:TYR:HH	1.67	0.57
1:H:477:LEU:HD21	2:H:8838:HOH:O	2.05	0.57
1:C:12:ASN:O	1:C:15:PRO:HD3	2.04	0.57
1:D:44:THR:HB	1:D:46:GLU:HG2	1.87	0.57
1:G:86:ARG:HG3	2:G:9545:HOH:O	2.04	0.57
1:A:366:LYS:HG2	1:A:368:LEU:CD2	2.35	0.57
1:G:468:TYR:OH	1:H:489:LYS:HB2	2.04	0.57
1:C:39:THR:HG23	1:C:48:ILE:HB	1.87	0.57
1:D:262:LEU:HB3	2:D:9469:HOH:O	2.05	0.57
1:E:275:ASN:ND2	1:E:430:ALA:HB3	2.20	0.57
2:E:8837:HOH:O	1:H:436:LEU:HB2	2.04	0.57
1:F:41:ASN:HD22	1:F:43:SER:H	1.51	0.57
1:H:390:GLN:CG	1:H:393:MET:HE3	2.35	0.57
1:A:12:ASN:O	1:A:15:PRO:HD3	2.04	0.56
1:A:37:PHE:HD2	1:A:53:GLU:HB2	1.70	0.56
1:E:234:SER:HA	1:E:260:SER:HB3	1.87	0.56
1:F:142:LYS:NZ	2:F:8849:HOH:O	2.37	0.56
1:A:117:SER:O	1:A:122:LEU:HD12	2.05	0.56
1:F:245:GLY:O	1:F:269:LEU:HA	2.04	0.56
1:H:329:ARG:HA	1:H:340:GLU:OE2	2.05	0.56
1:B:201:ALA:HB2	2:B:8940:HOH:O	2.04	0.56
1:D:246:SER:HG	1:D:248:GLU:HB3	1.69	0.56
1:D:392:GLY:O	1:D:397:LYS:HE2	2.05	0.56
1:F:167:PRO:HD3	1:F:244:THR:HB	1.85	0.56
1:G:131:TYR:CZ	1:G:462:GLN:HA	2.40	0.56
1:H:394:THR:HG23	1:H:398:GLU:HG3	1.88	0.56
1:C:30:ASP:HB2	1:C:34:ARG:HH21	1.70	0.56
1:E:464:PRO:HG2	1:F:490:THR:OG1	2.05	0.56
1:H:476:GLU:O	1:H:477:LEU:HB2	2.05	0.56
1:E:358:ASN:O	1:E:362:GLN:HG2	2.05	0.56
1:A:22:ILE:CD1	1:A:221:VAL:HG13	2.36	0.56
1:A:63:VAL:HG11	1:A:235:HIS:CE1	2.41	0.56
1:E:102:LEU:HD21	1:E:203:TYR:HD2	1.70	0.56
1:G:127:LYS:HE2	2:H:9549:HOH:O	2.05	0.56
1:G:156:HIS:HD2	1:G:488:VAL:HG22	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:TYR:CD1	1:G:409:LYS:HE2	2.40	0.56
1:A:131:TYR:CZ	1:A:462:GLN:HA	2.41	0.56
1:B:16:GLU:HB3	1:B:18:PHE:CZ	2.41	0.56
1:D:418:GLY:O	1:D:422:ASN:HB2	2.06	0.56
1:A:302:CYS:HB2	1:A:427:LEU:CD2	2.35	0.56
1:F:196:GLN:HE21	1:F:196:GLN:N	2.00	0.56
1:G:70:PHE:CZ	1:G:160:GLY:HA2	2.40	0.56
1:A:13:GLN:HG2	1:A:335:PHE:CG	2.41	0.56
1:D:276:ILE:HG23	1:D:416:VAL:HG21	1.86	0.56
1:E:61:LYS:HD2	2:E:9482:HOH:O	2.05	0.56
1:E:132:TYR:OH	1:E:477:LEU:HA	2.06	0.56
1:G:294:LEU:CD1	1:G:405:MET:HA	2.36	0.56
1:H:294:LEU:CD1	1:H:306:SER:HA	2.34	0.56
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.41	0.55
1:D:36:THR:OG1	1:D:50:GLN:HG3	2.05	0.55
1:E:22:ILE:CD1	1:E:222:PRO:HD2	2.35	0.55
1:F:63:VAL:HG11	1:F:235:HIS:CE1	2.41	0.55
1:G:16:GLU:HB3	1:G:18:PHE:CZ	2.41	0.55
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.41	0.55
1:C:392:GLY:O	1:C:397:LYS:HE2	2.06	0.55
1:E:251:ARG:HB3	1:F:258:GLY:O	2.06	0.55
1:H:240:LYS:HD2	1:H:264:ARG:HB3	1.88	0.55
1:C:36:THR:OG1	1:C:50:GLN:HG3	2.06	0.55
1:C:123:ASP:O	1:C:127:LYS:HG3	2.05	0.55
1:B:366:LYS:HG2	1:B:368:LEU:CD2	2.35	0.55
1:D:172:LEU:CD2	1:D:200:THR:HB	2.36	0.55
1:D:196:GLN:H	1:D:196:GLN:NE2	1.96	0.55
1:F:344:GLN:OE1	1:F:403:PRO:HD3	2.06	0.55
1:G:11:PRO:HB3	1:G:114:TYR:CD1	2.40	0.55
1:G:134:GLY:O	1:G:138:LYS:HD2	2.06	0.55
1:A:195:GLU:HG2	1:A:196:GLN:NE2	2.20	0.55
1:A:489:LYS:HB2	1:B:468:TYR:OH	2.06	0.55
1:B:131:TYR:CZ	1:B:462:GLN:HA	2.41	0.55
1:G:292:PHE:CE1	1:G:457:ASP:HB2	2.41	0.55
1:G:427:LEU:HD11	1:G:465:PHE:CZ	2.42	0.55
1:E:350:PHE:O	1:E:354:LEU:HG	2.07	0.55
1:H:461:ALA:O	1:H:477:LEU:HD22	2.06	0.55
1:H:477:LEU:HD11	2:H:8838:HOH:O	2.05	0.55
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.37	0.55
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.42	0.55
1:E:248:GLU:O	1:E:251:ARG:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:VAL:HA	2:H:8766:HOH:O	2.06	0.55
1:G:172:LEU:HG	1:G:200:THR:HB	1.89	0.55
1:A:271:GLY:HA2	1:A:425:TYR:CD2	2.41	0.55
1:B:113:PRO:HB2	1:B:116:ILE:HG12	1.88	0.55
1:B:294:LEU:HD11	1:B:404:VAL:O	2.07	0.55
1:G:106:GLU:O	1:G:110:ASN:HB3	2.07	0.55
1:G:124:MET:HE3	1:G:173:LEU:HD22	1.89	0.55
1:G:255:VAL:CG2	1:H:255:VAL:HG13	2.36	0.55
1:B:32:VAL:HG21	1:B:57:GLU:HB3	1.89	0.55
1:B:90:ARG:CZ	1:B:94:LEU:HD21	2.37	0.55
1:C:404:VAL:HG12	1:C:406:GLN:OE1	2.06	0.55
1:E:107:THR:HG23	1:E:112:LYS:O	2.07	0.55
1:G:192:LYS:HB2	1:G:232:ILE:CD1	2.37	0.55
1:B:461:ALA:HA	1:B:477:LEU:HD22	1.89	0.55
1:C:63:VAL:HG11	1:C:235:HIS:CE1	2.42	0.55
1:E:254:GLN:OE1	1:F:262:LEU:HD22	2.07	0.55
1:E:300:GLN:HE22	1:E:345:VAL:N	2.05	0.55
1:E:390:GLN:HG2	1:E:393:MET:HE3	1.87	0.55
1:C:395:ILE:HD12	1:C:406:GLN:HG3	1.88	0.54
1:E:390:GLN:HG2	1:E:393:MET:CE	2.37	0.54
1:H:109:ASP:OD2	1:H:199:LEU:HG	2.07	0.54
1:C:351:LYS:HB3	1:E:38:PRO:CG	2.35	0.54
1:G:443:SER:HA	1:G:451:VAL:HG11	1.89	0.54
1:A:8:VAL:HG13	1:A:118:TYR:CD2	2.43	0.54
1:B:95:ILE:HG22	1:B:126:LEU:HD21	1.90	0.54
1:B:317:GLU:O	1:B:321:ARG:HG3	2.07	0.54
1:D:258:GLY:HA2	1:D:262:LEU:HD23	1.88	0.54
1:D:311:GLN:OE1	1:D:313:ASP:HB2	2.06	0.54
1:F:167:PRO:CG	1:F:174:MET:HE3	2.38	0.54
1:G:255:VAL:HG13	1:H:255:VAL:HG22	1.89	0.54
1:G:292:PHE:HE1	1:G:457:ASP:HB2	1.73	0.54
1:G:372:GLY:O	1:G:382:GLN:HG3	2.07	0.54
1:A:22:ILE:HD13	1:A:221:VAL:HG13	1.89	0.54
1:A:146:ILE:CG1	1:B:460:GLY:HA3	2.38	0.54
1:B:82:SER:HB3	2:B:9159:HOH:O	2.08	0.54
1:D:424:THR:O	1:D:470:MET:HB2	2.07	0.54
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.43	0.54
1:A:100:THR:HG23	1:A:114:TYR:OH	2.08	0.54
1:A:162:CYS:HB3	2:A:9063:HOH:O	2.07	0.54
1:D:63:VAL:HG11	1:D:235:HIS:CE1	2.43	0.54
1:F:404:VAL:HG12	1:F:406:GLN:OE1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.43	0.54
1:D:276:ILE:CG2	1:D:416:VAL:HG21	2.38	0.54
1:B:329:ARG:NE	1:B:341:GLN:HB2	2.22	0.54
1:C:36:THR:CB	1:C:50:GLN:HG3	2.38	0.54
1:D:41:ASN:HD22	1:D:43:SER:H	1.55	0.54
1:D:106:GLU:O	1:D:110:ASN:HB3	2.07	0.54
1:F:23:PHE:CD2	1:F:205:ALA:HB1	2.43	0.54
1:H:99:ARG:HG3	1:H:122:LEU:HD22	1.90	0.54
1:A:303:CYS:SG	1:A:459:PHE:HZ	2.31	0.54
1:A:442:LEU:O	1:A:446:LEU:HG	2.08	0.54
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.08	0.54
1:B:56:LYS:HE2	1:B:60:ASP:OD1	2.07	0.54
1:B:269:LEU:HD12	1:B:470:MET:O	2.08	0.54
1:B:302:CYS:HB2	1:B:427:LEU:CD2	2.37	0.54
1:C:493:VAL:HG13	1:D:453:VAL:HB	1.90	0.54
1:D:393:MET:O	1:D:397:LYS:HG3	2.07	0.54
1:E:135:TRP:CG	1:E:482:LEU:HD11	2.43	0.54
1:E:240:LYS:HG3	1:E:264:ARG:HB3	1.90	0.54
1:G:107:THR:HG23	1:G:112:LYS:O	2.07	0.54
1:H:33:SER:O	1:H:34:ARG:HB2	2.08	0.54
1:A:366:LYS:HB2	2:A:9086:HOH:O	2.08	0.53
1:B:435:ASP:HB3	1:B:438:LYS:HB2	1.90	0.53
1:D:247:THR:HA	1:D:269:LEU:HD22	1.91	0.53
1:E:154:THR:HA	1:E:489:LYS:O	2.09	0.53
1:F:294:LEU:HD13	1:F:405:MET:HA	1.90	0.53
1:G:238:VAL:O	1:G:263:LYS:HE3	2.08	0.53
1:H:11:PRO:HB3	1:H:114:TYR:CE2	2.43	0.53
1:H:271:GLY:O	1:H:399:GLU:HB2	2.08	0.53
1:C:33:SER:O	1:C:34:ARG:HB2	2.08	0.53
1:E:21:GLN:HB3	1:E:29:HIS:O	2.08	0.53
1:G:170:PHE:HB3	1:G:173:LEU:HB3	1.89	0.53
1:A:148:GLY:O	1:A:498:LYS:HD3	2.08	0.53
1:B:33:SER:O	1:B:34:ARG:HB2	2.09	0.53
1:D:294:LEU:HD11	1:D:404:VAL:O	2.07	0.53
1:F:276:ILE:HG12	1:F:416:VAL:HG21	1.89	0.53
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.73	0.53
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.90	0.53
1:B:109:ASP:OD2	1:B:199:LEU:HG	2.09	0.53
1:C:254:GLN:OE1	1:D:262:LEU:HD22	2.08	0.53
1:D:464:PRO:HA	1:D:476:GLU:O	2.09	0.53
1:F:247:THR:CG2	1:F:269:LEU:HD13	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:449:GLY:HA2	1:H:468:TYR:CE1	2.44	0.53
1:A:33:SER:O	1:A:34:ARG:HB2	2.08	0.53
1:B:202:LEU:O	1:B:205:ALA:HB3	2.08	0.53
1:C:251:ARG:HA	1:D:262:LEU:HD21	1.90	0.53
1:E:175:GLN:HG3	1:E:191:MET:HE1	1.89	0.53
1:F:240:LYS:HG2	1:F:241:VAL:N	2.23	0.53
1:H:274:PRO:HA	1:H:307:ARG:O	2.08	0.53
1:D:473:SER:HA	2:D:9478:HOH:O	2.07	0.53
1:A:107:THR:HG23	1:A:112:LYS:O	2.09	0.53
1:E:146:ILE:CG1	1:F:460:GLY:HA3	2.39	0.53
1:F:36:THR:OG1	1:F:50:GLN:HG3	2.07	0.53
1:H:39:THR:HG23	1:H:48:ILE:HB	1.91	0.53
1:H:120:VAL:HG12	1:H:124:MET:CE	2.39	0.53
1:A:8:VAL:HG21	1:A:115:VAL:CG2	2.38	0.53
1:A:460:GLY:HA3	1:B:146:ILE:HG13	1.90	0.53
1:C:99:ARG:HG2	1:C:118:TYR:CE1	2.43	0.53
1:F:63:VAL:HG21	1:F:235:HIS:CD2	2.44	0.53
1:H:317:GLU:CG	1:H:321:ARG:HE	2.21	0.53
1:A:187:ASN:HD21	1:A:485:TYR:HB3	1.74	0.53
1:C:257:ALA:HA	1:C:260:SER:OG	2.09	0.53
1:D:139:TYR:CD1	1:D:482:LEU:HD12	2.43	0.53
1:F:424:THR:O	1:F:470:MET:HB2	2.09	0.53
1:H:243:PHE:CG	1:H:253:ILE:HG13	2.44	0.53
1:A:135:TRP:CG	1:A:482:LEU:HD11	2.44	0.52
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.44	0.52
1:B:460:GLY:HA3	1:B:462:GLN:HE21	1.72	0.52
1:E:247:THR:CB	1:E:269:LEU:HB3	2.39	0.52
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.90	0.52
1:G:271:GLY:HA2	1:G:425:TYR:CG	2.44	0.52
1:H:336:ASP:HB3	1:H:339:THR:OG1	2.08	0.52
1:B:26:ASN:O	1:B:209:LYS:HE3	2.10	0.52
1:D:90:ARG:NH1	1:D:94:LEU:HD21	2.24	0.52
1:E:22:ILE:HG22	1:E:24:ILE:HG13	1.89	0.52
1:F:247:THR:HA	1:F:269:LEU:CD2	2.37	0.52
1:F:497:GLN:HG2	1:F:499:ASN:HD21	1.74	0.52
1:C:240:LYS:HG2	1:C:241:VAL:N	2.23	0.52
1:C:247:THR:HG23	1:C:269:LEU:HB3	1.90	0.52
1:D:33:SER:O	1:D:34:ARG:HB2	2.08	0.52
1:A:13:GLN:HE22	1:A:333:ASN:HD21	1.57	0.52
1:A:185:THR:CG2	1:A:482:LEU:HD22	2.39	0.52
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:ASN:ND2	1:F:215:PRO:HA	2.25	0.52
1:H:94:LEU:HB3	1:H:207:LEU:HD22	1.91	0.52
1:D:11:PRO:HB3	1:D:114:TYR:CD1	2.45	0.52
1:G:470:MET:HG2	1:H:261:ASN:O	2.10	0.52
1:C:398:GLU:HA	2:C:8720:HOH:O	2.09	0.52
1:D:327:LYS:HE2	1:D:369:CYS:CB	2.40	0.52
1:E:247:THR:HA	1:E:269:LEU:CD2	2.36	0.52
1:F:21:GLN:HB3	1:F:29:HIS:O	2.09	0.52
1:F:131:TYR:CE1	1:F:462:GLN:HB3	2.45	0.52
1:B:311:GLN:NE2	1:B:312:GLU:HG2	2.25	0.52
1:D:22:ILE:HG22	1:D:24:ILE:HG13	1.91	0.52
1:A:40:VAL:HG22	1:A:47:VAL:HA	1.92	0.52
1:C:358:ASN:O	1:C:362:GLN:HG2	2.09	0.52
1:A:235:HIS:HB3	1:A:238:VAL:CG2	2.37	0.52
1:B:244:THR:HG23	1:B:268:GLU:CB	2.40	0.52
1:B:410:PHE:CD1	1:B:416:VAL:HB	2.45	0.52
1:D:271:GLY:HA2	1:D:425:TYR:CD2	2.45	0.52
1:D:323:VAL:CG1	1:D:327:LYS:HE3	2.40	0.52
1:F:26:ASN:N	1:F:26:ASN:HD22	2.07	0.52
1:H:244:THR:HG23	1:H:268:GLU:CB	2.37	0.52
1:H:257:ALA:HA	1:H:260:SER:OG	2.09	0.52
1:A:89:ASN:ND2	1:A:133:ALA:HB1	2.25	0.52
1:B:116:ILE:O	1:B:120:VAL:HB	2.10	0.52
1:C:53:GLU:HG3	2:C:8714:HOH:O	2.09	0.52
1:G:453:VAL:HB	1:H:493:VAL:HG13	1.92	0.52
1:C:315:TYR:CE1	1:C:409:LYS:HE2	2.45	0.51
1:E:247:THR:OG1	1:E:269:LEU:HB3	2.10	0.51
1:F:175:GLN:NE2	1:F:204:VAL:HG21	2.25	0.51
1:G:463:SER:O	1:G:477:LEU:HB2	2.10	0.51
1:E:240:LYS:HG2	1:E:241:VAL:N	2.23	0.51
1:E:244:THR:HG23	1:E:268:GLU:CB	2.40	0.51
1:E:247:THR:CG2	1:E:269:LEU:HD13	2.34	0.51
1:F:40:VAL:HG13	1:F:46:GLU:O	2.10	0.51
1:H:458:VAL:HA	2:H:8806:HOH:O	2.10	0.51
1:A:254:GLN:HG2	1:B:258:GLY:HA3	1.91	0.51
1:E:18:PHE:HA	2:E:9287:HOH:O	2.10	0.51
1:F:258:GLY:HA2	1:F:262:LEU:HD23	1.91	0.51
1:A:461:ALA:HA	1:A:477:LEU:CD2	2.34	0.51
1:A:487:GLU:HG3	1:B:468:TYR:CE1	2.46	0.51
1:B:291:HIS:HE1	1:B:326:ALA:HA	1.75	0.51
1:F:121:ASP:O	1:F:125:VAL:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:GLN:OE1	1:H:262:LEU:HD22	2.10	0.51
1:H:431:VAL:HG21	1:H:442:LEU:HB3	1.93	0.51
1:C:498:LYS:HD3	2:C:8984:HOH:O	2.11	0.51
1:D:100:THR:HG23	1:D:114:TYR:OH	2.11	0.51
1:D:167:PRO:HD3	1:D:244:THR:HB	1.92	0.51
1:E:268:GLU:OE2	1:E:476:GLU:OE1	2.28	0.51
1:F:39:THR:HG23	1:F:48:ILE:HB	1.93	0.51
1:F:291:HIS:NE2	1:F:329:ARG:HD2	2.25	0.51
1:D:327:LYS:HE2	1:D:369:CYS:HB3	1.91	0.51
1:G:63:VAL:HG11	1:G:235:HIS:CE1	2.46	0.51
1:G:244:THR:OG1	1:G:268:GLU:OE1	2.29	0.51
1:H:266:THR:O	1:H:267:LEU:HD23	2.11	0.51
1:D:99:ARG:HD3	1:D:118:TYR:CZ	2.46	0.51
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.45	0.51
1:E:250:GLY:HA2	1:E:253:ILE:HG12	1.92	0.51
1:H:36:THR:OG1	1:H:50:GLN:HG3	2.10	0.51
1:B:431:VAL:CG1	1:B:442:LEU:HD12	2.41	0.51
1:A:39:THR:OG1	1:A:109:ASP:OD1	2.29	0.51
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.92	0.51
1:D:235:HIS:HB3	1:D:238:VAL:CG2	2.41	0.51
1:E:312:GLU:OE1	1:E:411:LYS:HG3	2.10	0.51
1:F:315:TYR:CD1	1:F:409:LYS:HE2	2.46	0.51
1:H:409:LYS:HG2	2:H:8802:HOH:O	2.10	0.51
1:C:355:GLY:HA2	1:E:50:GLN:NE2	2.25	0.51
1:C:358:ASN:OD1	1:E:50:GLN:HG3	2.11	0.51
1:E:262:LEU:HD13	1:F:269:LEU:HD11	1.92	0.51
1:A:496:PRO:HG2	1:C:441:TYR:HB2	1.93	0.50
1:B:468:TYR:O	1:B:471:SER:HB2	2.10	0.50
1:C:15:PRO:HG2	1:C:108:LEU:HD22	1.93	0.50
1:H:178:LYS:HD3	1:H:476:GLU:OE2	2.11	0.50
1:C:313:ASP:HB3	2:C:9454:HOH:O	2.11	0.50
1:C:487:GLU:HG3	1:D:468:TYR:CZ	2.46	0.50
1:F:199:LEU:HB2	2:F:8749:HOH:O	2.10	0.50
1:A:366:LYS:HE2	1:A:368:LEU:CD2	2.40	0.50
1:D:123:ASP:CG	1:D:127:LYS:HE3	2.37	0.50
1:E:142:LYS:HG3	1:F:480:TYR:OH	2.12	0.50
1:E:350:PHE:CE2	1:E:354:LEU:HD11	2.46	0.50
1:F:294:LEU:CD1	1:F:405:MET:HA	2.42	0.50
1:H:413:ILE:O	1:H:417:VAL:HG23	2.11	0.50
1:B:8:VAL:HG13	1:B:118:TYR:CD2	2.46	0.50
1:B:311:GLN:OE1	1:B:313:ASP:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.46	0.50
1:G:246:SER:HG	1:G:249:ILE:H	1.58	0.50
1:G:298:GLN:HG3	1:G:341:GLN:HG3	1.92	0.50
1:H:247:THR:OG1	1:H:269:LEU:HB3	2.11	0.50
1:H:356:TYR:CB	1:H:400:ILE:HG12	2.42	0.50
1:A:464:PRO:HG3	1:A:480:TYR:CE1	2.46	0.50
1:B:444:GLN:NE2	1:D:499:ASN:HB2	2.26	0.50
1:D:13:GLN:HA	1:D:335:PHE:CE1	2.46	0.50
1:D:190:VAL:HG22	1:D:219:ASN:HB2	1.94	0.50
1:G:195:GLU:HG2	1:G:196:GLN:NE2	2.26	0.50
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.50
1:H:44:THR:O	1:H:377:ARG:NH1	2.44	0.50
1:H:344:GLN:HG3	1:H:353:ILE:HD12	1.94	0.50
1:A:363:GLU:HG3	2:A:9084:HOH:O	2.10	0.50
1:A:465:PHE:HB2	1:A:477:LEU:HD12	1.94	0.50
1:B:268:GLU:OE1	1:B:476:GLU:OE1	2.30	0.50
1:C:185:THR:HG23	1:C:482:LEU:HD22	1.94	0.50
1:F:130:ARG:HD3	1:H:86:ARG:CZ	2.42	0.50
2:A:8696:HOH:O	1:D:498:LYS:HE3	2.12	0.50
1:E:487:GLU:HG3	1:F:468:TYR:CE1	2.46	0.50
1:F:94:LEU:HD22	1:F:97:ARG:NH2	2.27	0.50
1:H:68:ALA:HA	1:H:71:GLN:HG2	1.93	0.50
1:H:132:TYR:CE2	1:H:181:PRO:HB3	2.46	0.50
1:H:373:ILE:HG22	1:H:375:ALA:H	1.77	0.50
1:A:126:LEU:O	1:A:130:ARG:HG3	2.11	0.50
1:A:140:HIS:ND1	1:D:142:LYS:HD3	2.27	0.50
1:A:294:LEU:HD12	1:A:306:SER:HA	1.93	0.50
1:B:424:THR:HG23	1:B:470:MET:HE3	1.94	0.50
1:E:131:TYR:CZ	1:E:462:GLN:HA	2.47	0.50
1:F:247:THR:CA	1:F:269:LEU:HB3	2.41	0.50
1:H:425:TYR:O	1:H:469:LYS:HD2	2.11	0.50
1:A:251:ARG:CG	1:B:262:LEU:HD21	2.42	0.50
1:C:347:GLU:OE1	1:E:347:GLU:OE1	2.30	0.50
1:E:257:ALA:HA	1:E:260:SER:OG	2.12	0.50
1:F:315:TYR:CD2	1:F:409:LYS:HG3	2.46	0.50
1:F:350:PHE:HZ	1:F:373:ILE:HG12	1.77	0.50
1:G:467:GLY:O	1:G:472:GLY:O	2.30	0.50
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.11	0.50
1:A:25:ASN:HA	1:A:216:GLY:N	2.27	0.49
1:D:351:LYS:HD3	1:F:347:GLU:CD	2.37	0.49
1:E:251:ARG:O	1:E:255:VAL:HG23	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:424:THR:HG21	1:E:470:MET:CE	2.39	0.49
1:G:79:MET:SD	1:G:83:HIS:HD2	2.35	0.49
1:E:79:MET:SD	1:E:83:HIS:HD2	2.35	0.49
1:F:175:GLN:HE22	1:F:204:VAL:HG21	1.76	0.49
1:A:11:PRO:HD3	2:A:8905:HOH:O	2.12	0.49
1:A:36:THR:HB	1:A:51:VAL:O	2.13	0.49
1:A:280:ASP:O	1:A:434:LYS:HG3	2.11	0.49
1:C:476:GLU:O	1:C:477:LEU:HB2	2.12	0.49
1:E:363:GLU:CD	1:E:394:THR:H	2.20	0.49
1:A:236:GLU:OE2	1:A:260:SER:HB2	2.13	0.49
1:A:374:ALA:HB2	1:A:382:GLN:CG	2.43	0.49
1:A:413:ILE:HD11	1:A:442:LEU:HG	1.94	0.49
1:D:106:GLU:OE2	1:D:171:PRO:HB2	2.12	0.49
1:D:323:VAL:HG13	1:D:327:LYS:HE3	1.95	0.49
1:E:264:ARG:HH22	1:F:474:GLY:N	2.11	0.49
1:G:275:ASN:HD22	1:G:430:ALA:HB3	1.75	0.49
1:G:487:GLU:HG3	1:H:468:TYR:CE1	2.47	0.49
1:A:431:VAL:HG21	1:A:442:LEU:HB3	1.94	0.49
1:B:370:GLY:HA2	1:B:382:GLN:OE1	2.13	0.49
1:D:425:TYR:O	1:D:469:LYS:HD2	2.11	0.49
1:F:361:LYS:HD2	1:F:367:LEU:HD22	1.94	0.49
1:A:300:GLN:HE22	1:A:345:VAL:H	1.61	0.49
1:F:294:LEU:HD12	1:F:306:SER:HA	1.93	0.49
1:G:344:GLN:HG3	1:G:353:ILE:HD12	1.94	0.49
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.94	0.49
1:G:272:LYS:HE2	1:G:396:ALA:C	2.38	0.49
1:G:483:GLN:NE2	2:G:8808:HOH:O	2.45	0.49
1:H:21:GLN:HB3	1:H:29:HIS:O	2.12	0.49
1:H:27:GLU:O	1:H:29:HIS:HD2	1.96	0.49
1:A:173:LEU:HD11	1:A:177:TRP:NE1	2.27	0.49
1:B:465:PHE:O	1:B:476:GLU:N	2.44	0.49
1:C:424:THR:CG2	1:C:470:MET:HB2	2.34	0.49
1:D:249:ILE:O	1:D:252:VAL:HB	2.13	0.49
1:D:363:GLU:CD	1:D:394:THR:H	2.20	0.49
1:B:41:ASN:HD22	1:B:42:PRO:HD2	1.77	0.49
1:B:413:ILE:HG12	1:B:441:TYR:CE2	2.47	0.49
1:B:462:GLN:HB2	2:D:9062:HOH:O	2.13	0.49
1:E:410:PHE:CD1	1:E:416:VAL:HB	2.48	0.49
1:E:489:LYS:HB2	1:F:468:TYR:OH	2.13	0.49
1:A:21:GLN:O	1:A:28:TRP:HZ3	1.95	0.48
1:B:235:HIS:HB3	1:B:238:VAL:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:PHE:CZ	1:F:373:ILE:HG12	2.48	0.48
1:G:300:GLN:HE22	1:G:345:VAL:H	1.61	0.48
1:A:79:MET:SD	1:A:83:HIS:HD2	2.36	0.48
1:A:374:ALA:HB2	1:A:382:GLN:HG2	1.94	0.48
1:D:99:ARG:HG2	1:D:118:TYR:CE1	2.48	0.48
1:F:276:ILE:HG12	1:F:416:VAL:CG2	2.43	0.48
1:H:168:TRP:O	1:H:171:PRO:HD3	2.13	0.48
1:A:468:TYR:O	1:A:471:SER:HB2	2.14	0.48
1:C:154:THR:HA	1:C:489:LYS:O	2.13	0.48
1:D:155:ARG:HD2	2:D:8727:HOH:O	2.13	0.48
1:D:240:LYS:HE3	1:D:484:ALA:O	2.11	0.48
1:D:460:GLY:O	1:D:477:LEU:HD13	2.13	0.48
1:E:330:VAL:HG21	2:E:9316:HOH:O	2.13	0.48
1:F:167:PRO:HG2	1:F:174:MET:HE3	1.94	0.48
1:G:365:ALA:CA	1:G:393:MET:HE1	2.43	0.48
1:A:241:VAL:CG1	1:A:265:VAL:HG22	2.43	0.48
1:B:302:CYS:HB2	1:B:427:LEU:HD21	1.95	0.48
1:C:25:ASN:HA	1:C:216:GLY:N	2.29	0.48
1:C:37:PHE:HD2	1:C:53:GLU:HB2	1.78	0.48
1:D:22:ILE:HG12	1:D:222:PRO:HD2	1.94	0.48
1:E:302:CYS:HB2	1:E:427:LEU:CD2	2.44	0.48
1:F:107:THR:CG2	1:F:334:PRO:HB2	2.44	0.48
1:G:294:LEU:HD21	1:G:404:VAL:C	2.38	0.48
1:A:255:VAL:HG22	1:B:255:VAL:HG13	1.95	0.48
1:B:394:THR:HG23	1:B:398:GLU:OE1	2.14	0.48
1:C:366:LYS:HE2	1:C:368:LEU:HD21	1.95	0.48
1:D:249:ILE:HD12	1:D:249:ILE:H	1.78	0.48
1:D:424:THR:HB	1:D:470:MET:HE3	1.96	0.48
1:E:241:VAL:CG1	1:E:265:VAL:HG13	2.43	0.48
1:G:33:SER:O	1:G:34:ARG:HB2	2.12	0.48
1:G:269:LEU:CD1	1:H:262:LEU:HD13	2.44	0.48
1:G:392:GLY:O	1:G:397:LYS:HE2	2.14	0.48
1:H:276:ILE:CD1	1:H:446:LEU:HD11	2.37	0.48
1:B:11:PRO:HB3	1:B:114:TYR:CE2	2.49	0.48
1:B:413:ILE:HG12	1:B:441:TYR:HE2	1.78	0.48
1:B:449:GLY:HA2	1:B:468:TYR:CE1	2.49	0.48
1:C:344:GLN:HG3	1:C:353:ILE:HD12	1.95	0.48
1:C:356:TYR:CG	1:C:400:ILE:HG12	2.48	0.48
1:D:294:LEU:CD1	1:D:405:MET:HA	2.43	0.48
1:E:33:SER:O	1:E:34:ARG:HB2	2.13	0.48
1:G:366:LYS:HE2	1:G:368:LEU:CD2	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TYR:CE1	1:A:319:VAL:HG21	2.49	0.48
1:B:79:MET:HG3	1:B:83:HIS:HB3	1.95	0.48
1:C:131:TYR:CZ	1:C:462:GLN:HA	2.49	0.48
1:D:240:LYS:HG2	1:D:241:VAL:N	2.28	0.48
1:E:123:ASP:O	1:E:127:LYS:HG3	2.14	0.48
1:E:145:PRO:HG3	2:H:9581:HOH:O	2.14	0.48
1:F:39:THR:HG22	1:F:49:CYS:O	2.13	0.48
1:F:464:PRO:HA	1:F:476:GLU:O	2.13	0.48
1:G:23:PHE:CE1	1:G:26:ASN:HA	2.49	0.48
1:A:353:ILE:O	1:A:357:ILE:HG13	2.13	0.48
1:B:441:TYR:CD2	1:B:442:LEU:HD23	2.48	0.48
1:D:123:ASP:OD2	1:D:127:LYS:HE3	2.14	0.48
1:D:315:TYR:CE1	1:D:409:LYS:HE2	2.49	0.48
1:G:235:HIS:HB3	1:G:238:VAL:HG23	1.95	0.48
1:H:356:TYR:CD1	1:H:400:ILE:HG12	2.49	0.48
1:A:298:GLN:HG3	1:A:341:GLN:HG3	1.96	0.48
1:C:280:ASP:HB3	2:C:9447:HOH:O	2.14	0.48
1:C:465:PHE:C	1:C:475:GLN:HB3	2.39	0.48
1:G:244:THR:HA	1:G:268:GLU:O	2.14	0.48
1:H:310:VAL:HG21	1:H:318:PHE:CD2	2.49	0.48
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.48	0.47
1:B:353:ILE:O	1:B:357:ILE:HG13	2.13	0.47
1:D:163:GLY:O	1:D:241:VAL:HA	2.13	0.47
1:E:80:ASP:OD1	1:H:498:LYS:NZ	2.47	0.47
1:A:172:LEU:CD2	1:A:200:THR:HB	2.39	0.47
1:A:281:ALA:HB2	1:A:432:PHE:O	2.14	0.47
1:D:291:HIS:CE1	1:D:326:ALA:HA	2.48	0.47
1:E:263:LYS:O	1:E:265:VAL:HG23	2.14	0.47
1:F:44:THR:HA	1:F:377:ARG:CD	2.42	0.47
1:G:345:VAL:HG12	1:G:349:GLN:HG3	1.97	0.47
1:B:257:ALA:HB1	1:B:263:LYS:CG	2.43	0.47
1:C:32:VAL:HA	1:C:34:ARG:NH1	2.28	0.47
1:C:100:THR:HG22	2:C:8954:HOH:O	2.14	0.47
1:C:347:GLU:OE1	1:E:379:TYR:OH	2.30	0.47
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.50	0.47
1:F:107:THR:HG23	1:F:334:PRO:HB2	1.95	0.47
1:F:395:ILE:HD12	1:F:406:GLN:HG3	1.96	0.47
1:G:44:THR:HA	1:G:377:ARG:HD3	1.95	0.47
1:G:120:VAL:HG12	1:G:124:MET:CE	2.40	0.47
1:H:71:GLN:HA	1:H:71:GLN:NE2	2.30	0.47
1:A:17:VAL:HG13	2:A:9055:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HB3	1:B:207:LEU:HD22	1.96	0.47
1:E:15:PRO:HD2	1:E:108:LEU:HD13	1.96	0.47
1:A:367:LEU:HD11	1:A:369:CYS:O	2.13	0.47
1:B:452:TRP:HB3	1:B:455:CYS:O	2.14	0.47
1:C:11:PRO:HB3	1:C:114:TYR:CE2	2.49	0.47
1:C:100:THR:HG23	1:C:114:TYR:OH	2.15	0.47
1:C:164:GLN:CD	1:C:178:LYS:HB3	2.39	0.47
1:F:435:ASP:HB3	1:F:438:LYS:HB2	1.94	0.47
1:G:195:GLU:OE1	1:G:224:PHE:HD2	1.97	0.47
1:G:249:ILE:HA	1:G:252:VAL:CG2	2.44	0.47
1:A:124:MET:HE3	1:A:173:LEU:HD22	1.97	0.47
1:E:257:ALA:HB1	1:E:263:LYS:HG3	1.97	0.47
1:F:28:TRP:CZ3	1:F:202:LEU:HD22	2.50	0.47
1:F:327:LYS:HE3	1:F:369:CYS:HB3	1.96	0.47
1:G:255:VAL:HG13	1:H:255:VAL:CG2	2.44	0.47
1:A:174:MET:HE1	1:A:177:TRP:CZ3	2.49	0.47
1:A:215:PRO:HG3	2:A:8907:HOH:O	2.15	0.47
1:C:414:GLU:HG3	1:C:441:TYR:OH	2.14	0.47
1:D:498:LYS:HE2	1:D:498:LYS:HB3	1.70	0.47
1:E:436:LEU:N	2:E:8837:HOH:O	2.48	0.47
1:F:60:ASP:O	1:F:64:LYS:HG3	2.14	0.47
1:F:247:THR:HG23	1:F:269:LEU:CB	2.45	0.47
1:A:116:ILE:O	1:A:120:VAL:HB	2.15	0.47
1:A:196:GLN:H	1:A:196:GLN:NE2	1.93	0.47
1:A:272:LYS:HE3	1:A:306:SER:CB	2.32	0.47
1:B:132:TYR:OH	1:B:477:LEU:HA	2.15	0.47
1:D:73:GLY:HA2	1:D:78:ARG:HD2	1.97	0.47
1:E:271:GLY:HA2	1:E:425:TYR:HB3	1.97	0.47
1:G:347:GLU:O	1:G:351:LYS:HE2	2.15	0.47
1:D:161:VAL:N	1:D:239:ASP:OD2	2.44	0.47
1:D:246:SER:OG	1:D:249:ILE:CD1	2.59	0.47
1:D:449:GLY:HA2	1:D:468:TYR:CE1	2.50	0.47
1:E:70:PHE:CZ	1:E:160:GLY:HA2	2.50	0.47
1:E:79:MET:HE3	1:E:79:MET:HB2	1.72	0.47
1:E:440:ASN:HD22	1:G:495:VAL:HG12	1.79	0.47
1:G:40:VAL:HG13	1:G:46:GLU:O	2.14	0.47
1:H:75:PRO:HG2	2:H:9364:HOH:O	2.15	0.47
1:A:48:ILE:HG21	1:A:199:LEU:HD11	1.96	0.47
1:A:240:LYS:HG3	1:A:241:VAL:N	2.28	0.47
1:B:106:GLU:O	1:B:110:ASN:HB3	2.15	0.47
1:B:246:SER:HG	1:B:249:ILE:H	1.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:MET:N	2:E:8830:HOH:O	2.48	0.47
2:E:8837:HOH:O	1:H:436:LEU:N	2.47	0.47
1:G:96:GLU:O	1:G:99:ARG:HB2	2.14	0.47
1:G:240:LYS:HG3	1:G:241:VAL:N	2.30	0.47
1:B:241:VAL:HG13	1:B:265:VAL:HG13	1.96	0.46
1:C:487:GLU:HG3	1:D:468:TYR:CE1	2.51	0.46
1:D:126:LEU:HD12	2:D:9168:HOH:O	2.14	0.46
1:D:302:CYS:HB2	1:D:427:LEU:CD2	2.45	0.46
1:G:315:TYR:CD2	1:G:409:LYS:HG3	2.49	0.46
1:H:40:VAL:HG13	1:H:46:GLU:O	2.15	0.46
1:A:187:ASN:ND2	1:A:485:TYR:HB3	2.29	0.46
1:A:312:GLU:HB3	2:A:9097:HOH:O	2.15	0.46
1:B:359:THR:O	1:B:363:GLU:HG3	2.15	0.46
1:B:363:GLU:CD	1:B:394:THR:H	2.22	0.46
1:B:431:VAL:HG21	1:B:442:LEU:HB3	1.97	0.46
1:D:356:TYR:CG	1:D:400:ILE:HG12	2.51	0.46
1:E:264:ARG:HH22	1:F:474:GLY:H	1.63	0.46
1:E:271:GLY:HA2	1:E:425:TYR:CG	2.51	0.46
1:G:370:GLY:HA2	2:G:8782:HOH:O	2.15	0.46
1:A:164:GLN:OE1	1:A:191:MET:HE3	2.16	0.46
1:A:260:SER:O	1:B:251:ARG:NH2	2.49	0.46
1:C:41:ASN:HD22	1:C:43:SER:H	1.62	0.46
1:C:198:PRO:O	1:C:202:LEU:HG	2.16	0.46
1:D:251:ARG:O	1:D:255:VAL:HG23	2.15	0.46
1:A:106:GLU:O	1:A:110:ASN:HB3	2.16	0.46
1:F:87:LEU:HB3	1:F:213:PHE:CZ	2.50	0.46
1:F:208:ILE:CD1	1:F:218:VAL:HG11	2.46	0.46
1:H:344:GLN:HG3	1:H:353:ILE:CD1	2.46	0.46
1:B:107:THR:CG2	1:B:334:PRO:HB2	2.46	0.46
1:E:307:ARG:NH1	2:E:9314:HOH:O	2.48	0.46
1:F:24:ILE:O	1:F:27:GLU:HB2	2.16	0.46
1:G:74:SER:OG	1:G:77:ARG:HG2	2.15	0.46
1:H:435:ASP:HB3	1:H:438:LYS:HB2	1.98	0.46
1:A:56:LYS:HE2	1:A:60:ASP:OD2	2.15	0.46
1:A:476:GLU:O	1:A:477:LEU:HB2	2.16	0.46
1:B:167:PRO:HD3	1:B:244:THR:HB	1.97	0.46
1:B:255:VAL:O	1:B:259:SER:OG	2.23	0.46
1:C:107:THR:OG1	1:C:112:LYS:O	2.30	0.46
1:D:25:ASN:C	1:D:215:PRO:HB3	2.41	0.46
1:E:356:TYR:CG	1:E:400:ILE:HG12	2.50	0.46
1:G:424:THR:HG22	1:G:424:THR:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:120:VAL:C	1:H:124:MET:HE2	2.41	0.46
1:A:18:PHE:HD1	1:A:101:TYR:HH	1.63	0.46
1:A:350:PHE:HE1	1:A:380:PHE:O	1.98	0.46
1:B:312:GLU:HG3	1:B:313:ASP:N	2.31	0.46
1:B:369:CYS:SG	1:B:385:VAL:HG23	2.56	0.46
1:C:241:VAL:HG13	1:C:265:VAL:HG13	1.98	0.46
1:C:424:THR:HG22	1:C:424:THR:O	2.15	0.46
1:H:33:SER:HB2	1:H:35:LYS:HD3	1.97	0.46
1:A:241:VAL:HG13	1:A:241:VAL:O	2.15	0.46
1:D:132:TYR:OH	1:D:477:LEU:HA	2.16	0.46
1:D:347:GLU:O	1:D:350:PHE:HB3	2.15	0.46
1:E:76:TRP:CH2	1:E:84:ARG:HD2	2.51	0.46
1:E:283:MET:HE3	1:E:317:GLU:CD	2.40	0.46
1:E:306:SER:O	1:E:406:GLN:HB2	2.15	0.46
1:E:428:ALA:HB1	1:E:452:TRP:CZ3	2.51	0.46
1:F:348:THR:HA	1:F:351:LYS:HE3	1.97	0.46
1:G:294:LEU:HD11	1:G:405:MET:HA	1.98	0.46
1:B:413:ILE:CG1	1:B:442:LEU:HD21	2.46	0.46
1:C:144:ILE:CG2	1:D:462:GLN:HB2	2.45	0.46
1:D:374:ALA:HB3	1:D:380:PHE:HB3	1.97	0.46
1:F:164:GLN:CD	1:F:178:LYS:HB3	2.41	0.46
1:F:323:VAL:HG21	1:F:368:LEU:HB3	1.98	0.46
1:H:132:TYR:OH	1:H:477:LEU:HA	2.16	0.46
1:A:170:PHE:HB3	1:A:173:LEU:HB3	1.98	0.46
1:A:376:ASP:OD1	1:A:376:ASP:N	2.49	0.46
1:B:109:ASP:OD2	1:B:199:LEU:HB2	2.16	0.46
1:F:246:SER:HB3	2:F:8646:HOH:O	2.15	0.46
1:H:131:TYR:CZ	1:H:462:GLN:HA	2.51	0.46
1:A:363:GLU:CB	2:A:9084:HOH:O	2.60	0.45
1:C:32:VAL:HA	1:C:34:ARG:HH11	1.80	0.45
1:F:23:PHE:CG	1:F:205:ALA:HB1	2.51	0.45
1:F:464:PRO:HG3	1:F:480:TYR:CE1	2.51	0.45
1:G:466:GLY:HA3	2:G:8784:HOH:O	2.16	0.45
1:C:350:PHE:CD1	1:C:379:TYR:HB3	2.52	0.45
2:C:9206:HOH:O	1:E:352:LYS:HE2	2.16	0.45
1:D:167:PRO:HB2	2:D:9259:HOH:O	2.17	0.45
1:D:302:CYS:HB2	1:D:427:LEU:HD21	1.98	0.45
1:A:388:ASP:O	1:A:390:GLN:NE2	2.50	0.45
1:A:413:ILE:O	1:A:416:VAL:HG12	2.16	0.45
1:B:413:ILE:HG12	1:B:442:LEU:HD21	1.97	0.45
1:B:463:SER:O	1:B:477:LEU:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:THR:HB	1:D:407:ILE:HA	1.98	0.45
1:E:43:SER:HA	1:E:343:PRO:HG3	1.99	0.45
1:E:131:TYR:CE1	1:E:462:GLN:HB3	2.51	0.45
1:H:43:SER:OG	1:H:334:PRO:HG3	2.16	0.45
1:H:317:GLU:HG2	1:H:321:ARG:HE	1.80	0.45
1:A:173:LEU:HD11	1:A:177:TRP:HE1	1.82	0.45
1:D:185:THR:OG1	1:D:187:ASN:ND2	2.50	0.45
1:E:155:ARG:NE	1:E:157:GLU:OE2	2.44	0.45
1:E:344:GLN:HG3	1:E:353:ILE:CD1	2.46	0.45
1:E:381:ILE:HG22	1:E:403:PRO:HG2	1.97	0.45
1:G:275:ASN:ND2	1:G:430:ALA:HB3	2.32	0.45
1:H:159:VAL:N	1:H:187:ASN:OD1	2.49	0.45
1:H:460:GLY:HA3	1:H:462:GLN:HE21	1.81	0.45
1:A:317:GLU:OE1	1:A:321:ARG:NH2	2.47	0.45
1:A:323:VAL:HG12	1:A:327:LYS:HD2	1.98	0.45
1:A:356:TYR:HE2	1:A:398:GLU:OE2	2.00	0.45
1:A:424:THR:HG22	1:A:424:THR:O	2.16	0.45
1:A:483:GLN:NE2	1:B:483:GLN:OE1	2.50	0.45
1:B:315:TYR:CD1	1:B:409:LYS:HE2	2.51	0.45
1:B:465:PHE:N	1:B:476:GLU:O	2.50	0.45
1:D:8:VAL:HG13	1:D:118:TYR:CD2	2.52	0.45
1:D:192:LYS:NZ	2:D:9260:HOH:O	2.50	0.45
1:D:476:GLU:O	1:D:477:LEU:HB2	2.17	0.45
1:E:100:THR:HG22	2:E:9298:HOH:O	2.15	0.45
1:E:281:ALA:HB2	1:E:432:PHE:O	2.16	0.45
1:C:465:PHE:N	1:C:476:GLU:O	2.50	0.45
1:D:421:ASN:ND2	1:D:445:ALA:O	2.50	0.45
1:E:217:VAL:HG12	1:E:218:VAL:HG23	1.99	0.45
1:E:440:ASN:ND2	2:E:9358:HOH:O	2.50	0.45
1:F:23:PHE:HA	1:F:27:GLU:O	2.16	0.45
1:G:103:ALA:HB2	1:G:122:LEU:HD13	1.98	0.45
1:G:408:LEU:HD23	1:G:419:ARG:HH11	1.80	0.45
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.40	0.45
1:A:32:VAL:HG23	1:A:61:LYS:HZ3	1.82	0.45
1:A:59:VAL:HG21	1:A:231:ALA:HB3	1.98	0.45
1:B:32:VAL:HG11	1:B:57:GLU:OE1	2.17	0.45
1:B:107:THR:HG23	1:B:112:LYS:O	2.16	0.45
1:B:185:THR:OG1	1:B:187:ASN:ND2	2.50	0.45
1:D:300:GLN:HB3	1:D:401:PHE:CE2	2.52	0.45
1:F:476:GLU:O	1:F:477:LEU:HB2	2.16	0.45
1:F:498:LYS:HG2	1:F:499:ASN:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:LYS:HG2	2:G:9550:HOH:O	2.16	0.45
1:H:244:THR:HG23	1:H:268:GLU:HG3	1.99	0.45
1:A:90:ARG:HH21	1:A:94:LEU:CD2	2.25	0.45
1:A:290:ALA:N	2:A:9077:HOH:O	2.50	0.45
1:B:431:VAL:HG11	1:B:442:LEU:HD12	1.99	0.45
1:E:358:ASN:HD22	1:E:361:LYS:NZ	2.15	0.45
1:G:260:SER:O	1:H:251:ARG:NH2	2.50	0.45
1:G:294:LEU:O	1:G:299:GLY:HA2	2.17	0.45
1:H:257:ALA:HB1	1:H:263:LYS:CG	2.46	0.45
1:A:22:ILE:HD11	1:A:54:GLY:CA	2.47	0.45
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.16	0.45
1:A:260:SER:OG	1:A:263:LYS:NZ	2.50	0.45
1:B:117:SER:HA	1:B:121:ASP:HB2	1.98	0.45
1:B:462:GLN:CD	1:B:462:GLN:H	2.25	0.45
1:C:294:LEU:HD11	1:C:404:VAL:O	2.16	0.45
1:D:144:ILE:HD11	1:D:154:THR:HG23	1.99	0.45
1:D:159:VAL:N	1:D:187:ASN:OD1	2.50	0.45
1:F:170:PHE:HZ	1:F:301:CYS:HG	1.64	0.45
1:F:315:TYR:CG	1:F:409:LYS:HE2	2.51	0.45
1:G:76:TRP:CH2	1:G:84:ARG:HD2	2.52	0.45
1:G:254:GLN:OE1	1:H:262:LEU:CD2	2.64	0.45
1:G:315:TYR:CE1	1:G:319:VAL:HG21	2.52	0.45
1:H:41:ASN:ND2	2:H:8792:HOH:O	2.49	0.45
1:C:449:GLY:HA2	1:C:468:TYR:CE1	2.51	0.45
1:E:70:PHE:CZ	1:E:158:PRO:HB2	2.52	0.45
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.52	0.45
1:H:444:GLN:NE2	2:H:8804:HOH:O	2.50	0.45
1:C:272:LYS:NZ	1:C:395:ILE:O	2.50	0.44
1:C:462:GLN:CD	1:C:462:GLN:H	2.24	0.44
1:D:71:GLN:O	1:D:74:SER:HB3	2.17	0.44
1:F:247:THR:HG23	1:F:269:LEU:CD1	2.43	0.44
1:A:267:LEU:O	1:A:473:SER:N	2.50	0.44
1:B:99:ARG:HD3	1:B:118:TYR:CZ	2.52	0.44
1:B:124:MET:HE2	1:B:173:LEU:HD21	1.98	0.44
1:C:260:SER:OG	1:C:263:LYS:NZ	2.49	0.44
1:D:260:SER:OG	1:D:263:LYS:NZ	2.50	0.44
1:D:417:VAL:HG11	1:D:445:ALA:HB1	1.99	0.44
1:E:79:MET:HB3	2:E:8814:HOH:O	2.17	0.44
1:E:273:SER:HB2	1:E:304:ALA:O	2.17	0.44
1:F:465:PHE:N	1:F:476:GLU:O	2.50	0.44
1:A:48:ILE:HD11	1:A:109:ASP:HA	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:MET:HE3	1:A:79:MET:HB2	1.76	0.44
1:A:344:GLN:HG3	1:A:353:ILE:HD12	2.00	0.44
1:E:159:VAL:N	1:E:187:ASN:OD1	2.50	0.44
1:E:208:ILE:HG23	1:E:213:PHE:CD1	2.52	0.44
1:E:294:LEU:HD13	1:E:405:MET:HA	2.00	0.44
1:F:208:ILE:HD13	1:F:218:VAL:HG11	2.00	0.44
1:H:465:PHE:N	1:H:476:GLU:O	2.49	0.44
1:A:272:LYS:HA	1:A:306:SER:OG	2.17	0.44
1:A:332:GLY:HA3	2:A:9079:HOH:O	2.17	0.44
1:A:373:ILE:HG22	1:A:375:ALA:H	1.82	0.44
1:B:253:ILE:HD13	1:B:253:ILE:N	2.32	0.44
1:D:39:THR:OG1	1:D:109:ASP:OD1	2.35	0.44
1:E:251:ARG:CA	1:F:262:LEU:HD21	2.46	0.44
1:E:498:LYS:HE2	1:E:498:LYS:HB3	1.81	0.44
1:F:8:VAL:HG13	1:F:118:TYR:CG	2.51	0.44
1:F:26:ASN:N	2:F:8842:HOH:O	2.50	0.44
1:F:135:TRP:CE2	1:H:138:LYS:HD3	2.52	0.44
1:F:333:ASN:O	1:F:339:THR:OG1	2.36	0.44
1:F:498:LYS:NZ	1:G:80:ASP:OD1	2.46	0.44
1:A:291:HIS:O	1:A:295:PHE:HB2	2.17	0.44
1:B:257:ALA:HA	1:B:260:SER:OG	2.17	0.44
1:C:99:ARG:HA	1:C:122:LEU:HD22	2.00	0.44
1:C:118:TYR:HD2	1:C:119:LEU:HD23	1.83	0.44
1:C:262:LEU:HD21	1:D:251:ARG:HG2	1.99	0.44
1:G:172:LEU:CG	1:G:200:THR:HB	2.48	0.44
1:A:112:LYS:HE2	1:A:112:LYS:HB3	1.69	0.44
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.52	0.44
1:C:21:GLN:HB3	1:C:29:HIS:O	2.17	0.44
1:C:142:LYS:NZ	2:C:8658:HOH:O	2.50	0.44
1:E:138:LYS:HD3	1:G:135:TRP:CE2	2.53	0.44
1:E:363:GLU:OE2	1:E:394:THR:N	2.50	0.44
1:F:60:ASP:OD1	1:F:235:HIS:NE2	2.50	0.44
1:F:159:VAL:N	1:F:187:ASN:OD1	2.50	0.44
1:G:476:GLU:O	1:G:477:LEU:HB2	2.18	0.44
1:A:13:GLN:HB3	2:A:8906:HOH:O	2.17	0.44
1:A:273:SER:N	2:A:9073:HOH:O	2.50	0.44
1:A:468:TYR:CE1	1:B:487:GLU:HG3	2.52	0.44
1:B:308:THR:HB	1:B:407:ILE:HA	1.99	0.44
1:C:297:ASN:ND2	1:C:300:GLN:O	2.50	0.44
1:F:102:LEU:HD21	1:F:203:TYR:HD2	1.81	0.44
1:G:357:ILE:HG22	1:G:361:LYS:HE2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLY:HA3	1:A:463:SER:HB2	1.98	0.44
1:D:160:GLY:HA3	1:D:239:ASP:OD2	2.17	0.44
1:D:198:PRO:O	1:D:202:LEU:HG	2.18	0.44
1:D:246:SER:HG	1:D:249:ILE:HD12	1.82	0.44
1:D:417:VAL:HG22	1:D:442:LEU:HD23	1.99	0.44
1:E:170:PHE:O	1:E:174:MET:HG2	2.18	0.44
1:E:247:THR:HG21	1:E:425:TYR:HE2	1.82	0.44
1:E:260:SER:OG	1:E:263:LYS:NZ	2.50	0.44
1:E:291:HIS:ND1	1:E:325:ARG:HG3	2.32	0.44
1:A:142:LYS:O	1:A:153:TYR:HA	2.18	0.44
1:C:106:GLU:OE2	1:C:171:PRO:HB2	2.17	0.44
1:D:138:LYS:NZ	2:D:9467:HOH:O	2.50	0.44
1:E:233:ALA:O	1:E:263:LYS:NZ	2.50	0.44
1:G:462:GLN:CD	1:G:462:GLN:H	2.26	0.44
1:H:77:ARG:HG3	1:H:77:ARG:HH11	1.83	0.44
1:H:241:VAL:O	1:H:241:VAL:HG13	2.17	0.44
1:A:453:VAL:HB	1:B:493:VAL:HG13	2.00	0.43
1:D:22:ILE:HD13	1:D:58:ASP:HB3	2.00	0.43
1:E:348:THR:O	1:E:352:LYS:HB2	2.18	0.43
1:E:452:TRP:HB3	1:E:455:CYS:O	2.18	0.43
1:F:33:SER:O	1:F:34:ARG:HB2	2.17	0.43
1:G:159:VAL:HG12	1:G:187:ASN:OD1	2.17	0.43
1:B:122:LEU:O	1:B:126:LEU:HG	2.18	0.43
1:C:196:GLN:H	1:C:196:GLN:NE2	2.14	0.43
1:E:253:ILE:HD13	1:E:253:ILE:N	2.33	0.43
1:A:55:ASP:N	1:A:58:ASP:OD2	2.49	0.43
1:B:193:VAL:HG22	1:B:222:PRO:HA	1.99	0.43
1:D:94:LEU:O	1:D:97:ARG:HB3	2.18	0.43
1:D:103:ALA:HB2	1:D:122:LEU:HD13	1.99	0.43
1:D:390:GLN:CG	1:D:393:MET:HE3	2.47	0.43
1:D:404:VAL:HG12	1:D:406:GLN:OE1	2.17	0.43
1:E:275:ASN:HD22	1:E:430:ALA:HB3	1.82	0.43
1:E:444:GLN:HG3	1:F:155:ARG:CZ	2.48	0.43
1:F:95:ILE:HG23	1:F:102:LEU:HD13	2.00	0.43
1:H:135:TRP:CG	1:H:482:LEU:HD11	2.53	0.43
1:B:346:ASP:OD1	1:B:349:GLN:HB2	2.18	0.43
1:E:61:LYS:NZ	2:E:8811:HOH:O	2.50	0.43
1:E:67:ARG:O	1:E:71:GLN:NE2	2.50	0.43
1:E:432:PHE:HA	1:E:454:ASN:OD1	2.18	0.43
1:F:302:CYS:O	1:F:427:LEU:HD23	2.18	0.43
1:G:249:ILE:O	1:G:252:VAL:HB	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:LEU:CD1	1:G:306:SER:HA	2.43	0.43
1:H:28:TRP:HH2	1:H:202:LEU:O	2.01	0.43
1:B:330:VAL:HG12	1:B:339:THR:HA	2.00	0.43
1:E:264:ARG:NH2	1:F:474:GLY:H	2.16	0.43
1:H:461:ALA:CA	1:H:477:LEU:HD22	2.47	0.43
1:A:245:GLY:HA3	2:A:9070:HOH:O	2.18	0.43
1:A:399:GLU:HG3	2:A:9095:HOH:O	2.17	0.43
1:D:112:LYS:HB3	1:D:112:LYS:HE2	1.77	0.43
1:D:168:TRP:CZ2	1:D:345:VAL:HG11	2.54	0.43
1:E:241:VAL:HG12	1:E:265:VAL:HG22	1.99	0.43
1:A:27:GLU:O	1:A:29:HIS:HD2	2.01	0.43
1:E:418:GLY:O	1:E:422:ASN:HB2	2.18	0.43
1:E:424:THR:O	1:E:470:MET:HB2	2.18	0.43
1:F:315:TYR:CE1	1:F:319:VAL:HG21	2.53	0.43
1:G:460:GLY:HA3	1:H:146:ILE:HG13	2.00	0.43
1:H:42:PRO:HD2	2:H:8792:HOH:O	2.18	0.43
1:H:102:LEU:HD21	1:H:203:TYR:CD2	2.53	0.43
1:B:235:HIS:O	1:B:263:LYS:NZ	2.50	0.43
1:B:294:LEU:O	1:B:299:GLY:HA2	2.19	0.43
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.19	0.43
1:D:208:ILE:HD13	1:D:218:VAL:HG11	2.00	0.43
1:G:31:ALA:O	1:G:34:ARG:NH1	2.52	0.43
1:G:161:VAL:HA	1:G:188:VAL:CG2	2.49	0.43
1:H:71:GLN:O	1:H:74:SER:HB3	2.19	0.43
1:B:71:GLN:O	1:B:74:SER:HB3	2.18	0.43
1:D:361:LYS:HD2	1:D:367:LEU:HD22	2.01	0.43
1:G:269:LEU:HD13	1:H:262:LEU:HD13	2.01	0.43
1:H:178:LYS:NZ	1:H:476:GLU:OE2	2.50	0.43
1:H:235:HIS:HB3	1:H:238:VAL:HG23	2.00	0.43
1:A:175:GLN:HE22	1:A:201:ALA:HA	1.84	0.43
1:A:198:PRO:O	1:A:202:LEU:HG	2.19	0.43
1:A:258:GLY:HA3	1:B:254:GLN:HG2	2.00	0.43
1:B:459:PHE:HE2	1:B:465:PHE:CD1	2.37	0.43
1:D:81:ALA:O	1:D:136:ALA:HB1	2.19	0.43
1:D:123:ASP:OD1	1:D:127:LYS:HE3	2.19	0.43
1:E:23:PHE:CG	1:E:205:ALA:HB1	2.54	0.43
1:H:334:PRO:HG2	2:H:8787:HOH:O	2.19	0.43
1:A:350:PHE:CE1	1:A:381:ILE:HG13	2.54	0.42
1:B:82:SER:N	2:B:9159:HOH:O	2.50	0.42
1:E:102:LEU:HD21	1:E:203:TYR:CD2	2.52	0.42
1:E:437:ASP:HB3	1:G:496:PRO:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:389:VAL:HG11	1:G:396:ALA:HB2	2.00	0.42
1:H:247:THR:HA	1:H:269:LEU:CD2	2.32	0.42
1:H:317:GLU:OE1	1:H:321:ARG:NH2	2.50	0.42
1:A:13:GLN:HE21	1:A:335:PHE:HD1	1.60	0.42
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.92	0.42
1:B:171:PRO:HG3	1:B:197:THR:HG21	2.01	0.42
1:B:443:SER:HA	1:B:451:VAL:HG11	2.01	0.42
1:C:346:ASP:O	1:C:350:PHE:HB2	2.19	0.42
1:C:366:LYS:HE2	1:C:368:LEU:CD2	2.49	0.42
1:E:28:TRP:CH2	1:E:202:LEU:HB3	2.54	0.42
1:E:106:GLU:O	1:E:110:ASN:HB3	2.19	0.42
1:F:298:GLN:NE2	2:F:8848:HOH:O	2.52	0.42
1:H:315:TYR:O	1:H:319:VAL:HG23	2.19	0.42
1:B:131:TYR:O	1:D:138:LYS:NZ	2.52	0.42
1:B:331:VAL:HA	1:B:341:GLN:O	2.19	0.42
1:C:287:VAL:HG22	1:C:318:PHE:CD1	2.54	0.42
1:D:76:TRP:HA	1:D:79:MET:HE3	2.00	0.42
1:D:421:ASN:O	1:D:469:LYS:NZ	2.52	0.42
1:D:431:VAL:HG21	1:D:442:LEU:HB3	2.01	0.42
1:E:358:ASN:HD22	1:E:361:LYS:HZ2	1.66	0.42
1:G:70:PHE:CE2	1:G:160:GLY:HA2	2.54	0.42
1:H:95:ILE:HG22	1:H:126:LEU:HD21	2.01	0.42
1:H:408:LEU:HD12	1:H:408:LEU:N	2.34	0.42
1:H:462:GLN:CD	1:H:462:GLN:H	2.28	0.42
1:A:42:PRO:HG3	1:A:110:ASN:O	2.19	0.42
1:A:283:MET:HE1	1:A:314:ILE:HB	2.02	0.42
1:B:330:VAL:O	1:B:340:GLU:N	2.46	0.42
1:B:389:VAL:HB	1:B:408:LEU:HG	2.01	0.42
1:D:353:ILE:O	1:D:357:ILE:HG13	2.20	0.42
1:F:41:ASN:ND2	1:F:43:SER:H	2.16	0.42
1:G:23:PHE:HB2	1:G:28:TRP:CZ3	2.54	0.42
1:H:177:TRP:NE1	2:H:8838:HOH:O	2.51	0.42
1:A:275:ASN:ND2	2:A:9074:HOH:O	2.51	0.42
1:B:246:SER:OG	1:B:249:ILE:HG12	2.19	0.42
1:C:107:THR:CG2	1:C:334:PRO:HB2	2.49	0.42
1:C:241:VAL:HG13	1:C:241:VAL:O	2.19	0.42
1:C:435:ASP:HB3	1:C:438:LYS:HD2	2.01	0.42
1:D:71:GLN:HA	1:D:71:GLN:NE2	2.35	0.42
1:F:498:LYS:HE2	1:F:498:LYS:HB3	1.67	0.42
1:G:371:GLY:N	1:G:384:THR:OG1	2.53	0.42
1:H:120:VAL:O	1:H:124:MET:HE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:GLY:O	1:H:253:ILE:HB	2.20	0.42
1:H:256:ALA:O	1:H:260:SER:HB3	2.19	0.42
1:B:167:PRO:HG2	1:B:174:MET:HG3	2.01	0.42
1:C:283:MET:HE1	1:C:314:ILE:HB	2.02	0.42
1:E:78:ARG:HD2	1:H:497:GLN:CD	2.44	0.42
1:E:494:LYS:NZ	2:E:8642:HOH:O	2.48	0.42
1:F:475:GLN:OE1	1:F:480:TYR:HB3	2.20	0.42
1:G:49:CYS:N	2:G:8768:HOH:O	2.49	0.42
1:G:248:GLU:CG	1:G:249:ILE:HD13	2.40	0.42
1:H:79:MET:HE3	1:H:79:MET:HB2	1.68	0.42
1:H:216:GLY:HA2	1:H:219:ASN:OD1	2.19	0.42
1:A:465:PHE:N	1:A:476:GLU:O	2.49	0.42
1:B:26:ASN:N	2:B:8933:HOH:O	2.50	0.42
1:C:240:LYS:HG3	1:C:264:ARG:HB3	2.02	0.42
1:E:350:PHE:HZ	1:E:373:ILE:HG23	1.84	0.42
1:F:332:GLY:O	1:F:380:PHE:HE2	2.03	0.42
1:H:347:GLU:O	1:H:350:PHE:HB3	2.19	0.42
1:H:347:GLU:O	1:H:351:LYS:HG3	2.20	0.42
1:A:496:PRO:HD2	2:A:9139:HOH:O	2.19	0.42
1:B:185:THR:HG23	1:B:482:LEU:HD22	2.01	0.42
1:D:246:SER:OG	1:D:248:GLU:HB3	2.19	0.42
1:D:415:GLU:OE2	1:D:419:ARG:NH2	2.50	0.42
1:F:132:TYR:OH	1:F:477:LEU:HA	2.20	0.42
1:A:22:ILE:HD11	1:A:54:GLY:HA3	2.02	0.42
1:A:464:PRO:HB3	1:A:480:TYR:HD1	1.85	0.42
1:D:362:GLN:NE2	2:D:8631:HOH:O	2.53	0.42
1:H:243:PHE:CB	1:H:253:ILE:HG13	2.50	0.42
1:A:25:ASN:C	1:A:215:PRO:HB3	2.44	0.42
1:B:170:PHE:HB3	1:B:173:LEU:HB3	2.01	0.42
1:B:346:ASP:O	1:B:350:PHE:HB2	2.20	0.42
1:C:273:SER:HA	1:C:274:PRO:HD3	1.95	0.42
1:E:464:PRO:HG2	1:F:490:THR:HG1	1.83	0.42
1:E:465:PHE:N	1:E:476:GLU:O	2.50	0.42
1:E:468:TYR:O	1:E:471:SER:HB2	2.19	0.42
1:G:112:LYS:HB3	1:G:112:LYS:HE2	1.70	0.42
1:G:238:VAL:HB	1:G:263:LYS:HE2	2.02	0.42
1:A:142:LYS:HD2	1:B:480:TYR:CZ	2.54	0.41
1:A:473:SER:HA	2:A:8661:HOH:O	2.19	0.41
1:C:50:GLN:NE2	1:E:355:GLY:HA2	2.34	0.41
1:A:347:GLU:O	1:A:351:LYS:HG3	2.20	0.41
1:B:112:LYS:HE2	1:B:112:LYS:HB3	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:PHE:O	1:B:475:GLN:HA	2.20	0.41
1:B:465:PHE:C	1:B:476:GLU:H	2.28	0.41
1:C:125:VAL:HG22	1:C:173:LEU:HA	2.01	0.41
1:E:124:MET:CE	1:E:173:LEU:HD22	2.46	0.41
1:E:244:THR:HA	1:E:268:GLU:HB2	2.02	0.41
1:G:185:THR:OG1	1:G:187:ASN:ND2	2.53	0.41
1:G:294:LEU:HD13	2:G:8881:HOH:O	2.19	0.41
1:H:113:PRO:O	1:H:116:ILE:HB	2.20	0.41
1:A:199:LEU:HB2	2:A:8636:HOH:O	2.19	0.41
1:B:96:GLU:OE2	1:B:130:ARG:NH1	2.50	0.41
1:H:175:GLN:O	1:H:179:LEU:HG	2.20	0.41
1:A:35:LYS:HE2	2:A:8909:HOH:O	2.20	0.41
1:A:131:TYR:CE1	1:A:462:GLN:HB3	2.55	0.41
1:A:274:PRO:HA	1:A:307:ARG:O	2.21	0.41
1:A:307:ARG:HD3	1:A:396:ALA:O	2.20	0.41
1:B:134:GLY:HA3	2:D:9467:HOH:O	2.21	0.41
1:C:21:GLN:O	1:C:28:TRP:HZ3	2.03	0.41
1:D:20:ASN:O	1:D:51:VAL:HA	2.21	0.41
1:D:44:THR:CB	1:D:46:GLU:HG2	2.50	0.41
1:D:226:PRO:O	1:D:230:ALA:HB3	2.20	0.41
1:E:350:PHE:CE1	1:E:381:ILE:HG13	2.55	0.41
1:E:393:MET:O	1:E:397:LYS:HG3	2.20	0.41
1:F:28:TRP:HZ3	1:F:202:LEU:HD22	1.85	0.41
1:F:44:THR:HA	1:F:377:ARG:NE	2.36	0.41
1:F:473:SER:HA	2:F:8764:HOH:O	2.20	0.41
1:G:82:SER:O	1:G:86:ARG:HG2	2.20	0.41
1:H:346:ASP:HA	1:H:379:TYR:CE1	2.55	0.41
1:H:435:ASP:OD1	1:H:438:LYS:HG3	2.20	0.41
1:A:464:PRO:HB3	1:A:480:TYR:CD1	2.56	0.41
1:B:435:ASP:HB3	1:B:438:LYS:HD2	2.02	0.41
1:B:460:GLY:CA	1:B:462:GLN:HE21	2.34	0.41
1:C:258:GLY:HA2	1:D:254:GLN:CD	2.46	0.41
1:D:131:TYR:CZ	1:D:462:GLN:HA	2.56	0.41
1:F:48:ILE:HD13	1:F:108:LEU:HD23	2.02	0.41
1:F:146:ILE:HG21	1:F:150:PHE:HB2	2.01	0.41
1:F:166:ILE:HG22	1:F:178:LYS:HE2	2.01	0.41
1:G:31:ALA:C	1:G:34:ARG:HH11	2.28	0.41
1:H:24:ILE:HD13	1:H:61:LYS:HB3	2.02	0.41
1:H:375:ALA:HB3	1:H:380:PHE:HB2	2.01	0.41
1:A:13:GLN:NE2	1:A:335:PHE:HB2	2.36	0.41
1:B:294:LEU:CD1	1:B:306:SER:HA	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:PHE:HB3	1:B:476:GLU:HB2	2.03	0.41
1:C:142:LYS:HD2	1:D:480:TYR:OH	2.21	0.41
1:E:243:PHE:HD2	1:E:267:LEU:HD22	1.85	0.41
1:E:462:GLN:H	1:E:462:GLN:CD	2.27	0.41
1:F:243:PHE:HB3	1:F:267:LEU:HD22	2.01	0.41
1:G:8:VAL:HA	1:G:9:PRO:HD3	1.95	0.41
1:G:249:ILE:HD13	1:G:249:ILE:N	2.35	0.41
1:G:449:GLY:HA2	1:G:468:TYR:CE1	2.54	0.41
1:H:87:LEU:HB3	1:H:213:PHE:CE1	2.56	0.41
1:A:370:GLY:HA3	1:A:383:PRO:O	2.21	0.41
1:A:498:LYS:HE2	1:A:498:LYS:HB3	1.90	0.41
1:B:249:ILE:HD13	1:B:249:ILE:N	2.35	0.41
1:E:56:LYS:O	1:E:60:ASP:OD1	2.39	0.41
1:F:106:GLU:O	1:F:110:ASN:HB3	2.20	0.41
1:F:249:ILE:N	1:F:249:ILE:HD13	2.36	0.41
1:G:333:ASN:HA	1:G:334:PRO:HD2	1.91	0.41
1:H:131:TYR:CE1	1:H:462:GLN:HB3	2.56	0.41
1:H:249:ILE:HD13	1:H:249:ILE:N	2.36	0.41
1:A:253:ILE:HG22	1:A:265:VAL:HG11	2.02	0.41
1:A:350:PHE:HZ	1:A:373:ILE:HD13	1.80	0.41
1:B:323:VAL:CG1	1:B:327:LYS:HE3	2.50	0.41
1:C:124:MET:CE	1:C:173:LEU:HD22	2.50	0.41
1:D:275:ASN:HD21	1:D:432:PHE:HE1	1.66	0.41
1:E:166:ILE:CG2	1:E:178:LYS:HG3	2.51	0.41
1:F:415:GLU:O	1:F:419:ARG:HG3	2.21	0.41
1:G:87:LEU:HB3	1:G:213:PHE:CZ	2.56	0.41
1:G:89:ASN:OD1	1:G:130:ARG:HG2	2.21	0.41
1:A:87:LEU:HB3	1:A:213:PHE:CZ	2.56	0.41
1:B:24:ILE:CD1	1:B:61:LYS:HB3	2.50	0.41
1:B:67:ARG:NH2	1:B:161:VAL:HG23	2.36	0.41
1:B:498:LYS:HD2	2:B:8938:HOH:O	2.21	0.41
1:B:498:LYS:HE2	1:B:498:LYS:HB3	1.93	0.41
1:C:34:ARG:NH2	2:C:9202:HOH:O	2.51	0.41
1:C:79:MET:HG2	1:C:84:ARG:HG2	2.02	0.41
1:C:148:GLY:O	1:C:498:LYS:HE2	2.21	0.41
1:C:175:GLN:HE22	1:C:201:ALA:HA	1.86	0.41
1:C:261:ASN:OD1	1:C:263:LYS:HG2	2.21	0.41
1:C:288:GLU:CD	1:C:325:ARG:HE	2.29	0.41
1:E:78:ARG:HD2	1:H:497:GLN:NE2	2.36	0.41
1:E:431:VAL:HG21	1:E:442:LEU:HB3	2.03	0.41
1:F:141:GLY:HA3	1:G:143:THR:OG1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:GLN:HE22	1:F:204:VAL:CG2	2.34	0.41
1:G:11:PRO:HB3	1:G:114:TYR:CG	2.56	0.41
1:G:444:GLN:HG3	1:H:155:ARG:CZ	2.51	0.41
1:G:466:GLY:N	2:G:8892:HOH:O	2.45	0.41
1:H:113:PRO:HA	1:H:334:PRO:O	2.21	0.41
1:H:311:GLN:CD	1:H:312:GLU:HG2	2.46	0.41
1:B:331:VAL:HG22	1:B:341:GLN:HB3	2.03	0.41
1:C:23:PHE:CG	1:C:205:ALA:HB1	2.56	0.41
1:C:27:GLU:HB3	1:C:29:HIS:NE2	2.36	0.41
1:C:344:GLN:CG	1:C:381:ILE:HD12	2.51	0.41
1:D:331:VAL:HG21	1:D:383:PRO:HD3	2.02	0.41
1:D:365:ALA:HB2	1:D:393:MET:SD	2.61	0.41
1:E:245:GLY:O	1:E:269:LEU:HA	2.21	0.41
1:F:169:ASN:OD1	1:F:169:ASN:N	2.53	0.41
1:G:315:TYR:O	1:G:319:VAL:HG23	2.21	0.41
1:H:329:ARG:HE	1:H:341:GLN:HB2	1.85	0.41
1:A:21:GLN:HB2	1:A:28:TRP:HE3	1.87	0.40
1:A:289:GLN:HB2	2:A:9077:HOH:O	2.21	0.40
1:C:214:PRO:O	1:C:217:VAL:HG23	2.21	0.40
1:C:221:VAL:HA	1:C:222:PRO:HD2	1.93	0.40
1:D:17:VAL:CG1	1:D:199:LEU:HD22	2.51	0.40
1:D:427:LEU:HD11	1:D:465:PHE:CZ	2.56	0.40
1:G:389:VAL:CG1	1:G:396:ALA:HB2	2.50	0.40
1:H:18:PHE:HD1	1:H:101:TYR:HH	1.64	0.40
1:H:333:ASN:O	1:H:339:THR:OG1	2.30	0.40
1:C:70:PHE:CZ	1:C:160:GLY:HA2	2.56	0.40
1:C:376:ASP:OD1	1:C:376:ASP:N	2.50	0.40
1:D:107:THR:HG23	1:D:334:PRO:HB2	2.04	0.40
1:D:169:ASN:HD22	1:D:401:PHE:HZ	1.69	0.40
1:F:246:SER:OG	1:F:249:ILE:HG12	2.22	0.40
1:H:67:ARG:HD2	2:H:8896:HOH:O	2.21	0.40
1:C:247:THR:HG23	1:C:269:LEU:HB2	2.01	0.40
1:D:430:ALA:HA	1:D:452:TRP:O	2.21	0.40
1:E:444:GLN:HG3	1:F:155:ARG:NH2	2.36	0.40
1:G:99:ARG:HD2	2:G:8772:HOH:O	2.20	0.40
1:G:113:PRO:HB2	1:G:116:ILE:HG12	2.03	0.40
1:G:200:THR:O	1:G:204:VAL:HG23	2.21	0.40
1:B:476:GLU:O	1:B:477:LEU:HB2	2.21	0.40
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.56	0.40
1:D:241:VAL:O	1:D:241:VAL:HG13	2.21	0.40
1:D:452:TRP:NE1	1:D:458:VAL:H	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:PHE:O	1:E:51:VAL:N	2.50	0.40
1:F:241:VAL:O	1:F:241:VAL:HG13	2.21	0.40
2:F:9536:HOH:O	1:G:72:LEU:HD23	2.21	0.40
1:G:101:TYR:N	2:G:9547:HOH:O	2.50	0.40
1:H:443:SER:HA	1:H:451:VAL:HG11	2.03	0.40
1:D:208:ILE:CD1	1:D:218:VAL:HG11	2.52	0.40
1:E:247:THR:HG23	1:E:269:LEU:CB	2.51	0.40
1:F:27:GLU:HB3	1:F:29:HIS:NE2	2.36	0.40
1:F:359:THR:HG22	1:F:363:GLU:CD	2.46	0.40
1:G:35:LYS:HB3	1:G:35:LYS:HE2	1.98	0.40
1:G:70:PHE:CE1	1:G:158:PRO:HB2	2.57	0.40
1:G:424:THR:CG2	1:G:470:MET:HB2	2.44	0.40
1:H:116:ILE:O	1:H:120:VAL:HB	2.21	0.40
1:H:149:ASP:HA	1:H:498:LYS:HB2	2.04	0.40
1:H:333:ASN:HA	1:H:334:PRO:HD2	1.91	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	492/500 (98%)	475 (96%)	16 (3%)	1 (0%)	43	44
1	B	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	C	492/500 (98%)	471 (96%)	21 (4%)	0	100	100
1	D	492/500 (98%)	473 (96%)	18 (4%)	1 (0%)	43	44
1	E	492/500 (98%)	472 (96%)	19 (4%)	1 (0%)	43	44
1	F	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	G	492/500 (98%)	472 (96%)	20 (4%)	0	100	100
1	H	492/500 (98%)	477 (97%)	14 (3%)	1 (0%)	43	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3936/4000 (98%)	3792 (96%)	140 (4%)	4 (0%)	48 50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	270	GLY
1	H	426	GLY
1	A	426	GLY
1	D	426	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	399/402 (99%)	371 (93%)	28 (7%)	14 9
1	B	399/402 (99%)	369 (92%)	30 (8%)	12 8
1	C	399/402 (99%)	376 (94%)	23 (6%)	18 14
1	D	399/402 (99%)	378 (95%)	21 (5%)	20 17
1	E	399/402 (99%)	370 (93%)	29 (7%)	13 8
1	F	399/402 (99%)	377 (94%)	22 (6%)	19 15
1	G	399/402 (99%)	377 (94%)	22 (6%)	19 15
1	H	399/402 (99%)	378 (95%)	21 (5%)	20 17
All	All	3192/3216 (99%)	2996 (94%)	196 (6%)	17 12

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	14	GLN
1	A	22	ILE
1	A	50	GLN
1	A	55	ASP
1	A	79	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	VAL
1	A	122	LEU
1	A	142	LYS
1	A	192	LYS
1	A	196	GLN
1	A	202	LEU
1	A	240	LYS
1	A	246	SER
1	A	249	ILE
1	A	264	ARG
1	A	294	LEU
1	A	302	CYS
1	A	320	GLU
1	A	338	LYS
1	A	361	LYS
1	A	373	ILE
1	A	376	ASP
1	A	377	ARG
1	A	390	GLN
1	A	463	SER
1	A	473	SER
1	A	483	GLN
1	B	13	GLN
1	B	14	GLN
1	B	50	GLN
1	B	56	LYS
1	B	79	MET
1	B	108	LEU
1	B	122	LEU
1	B	142	LYS
1	B	146	ILE
1	B	192	LYS
1	B	196	GLN
1	B	240	LYS
1	B	246	SER
1	B	249	ILE
1	B	253	ILE
1	B	264	ARG
1	B	269	LEU
1	B	273	SER
1	B	302	CYS
1	B	320	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	338	LYS
1	B	361	LYS
1	B	376	ASP
1	B	377	ARG
1	B	399	GLU
1	B	401	PHE
1	B	463	SER
1	B	470	MET
1	B	473	SER
1	B	486	THR
1	C	14	GLN
1	C	34	ARG
1	C	79	MET
1	C	87	LEU
1	C	122	LEU
1	C	142	LYS
1	C	146	ILE
1	C	159	VAL
1	C	192	LYS
1	C	196	GLN
1	C	240	LYS
1	C	246	SER
1	C	249	ILE
1	C	264	ARG
1	C	268	GLU
1	C	269	LEU
1	C	302	CYS
1	C	351	LYS
1	C	377	ARG
1	C	463	SER
1	C	470	MET
1	C	473	SER
1	C	486	THR
1	D	8	VAL
1	D	14	GLN
1	D	50	GLN
1	D	122	LEU
1	D	192	LYS
1	D	196	GLN
1	D	209	LYS
1	D	220	ILE
1	D	240	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	246	SER
1	D	264	ARG
1	D	268	GLU
1	D	302	CYS
1	D	351	LYS
1	D	358	ASN
1	D	376	ASP
1	D	377	ARG
1	D	401	PHE
1	D	463	SER
1	D	473	SER
1	D	475	GLN
1	E	14	GLN
1	E	22	ILE
1	E	41	ASN
1	E	50	GLN
1	E	122	LEU
1	E	142	LYS
1	E	159	VAL
1	E	192	LYS
1	E	196	GLN
1	E	246	SER
1	E	248	GLU
1	E	249	ILE
1	E	251	ARG
1	E	253	ILE
1	E	264	ARG
1	E	268	GLU
1	E	269	LEU
1	E	294	LEU
1	E	302	CYS
1	E	320	GLU
1	E	338	LYS
1	E	361	LYS
1	E	376	ASP
1	E	377	ARG
1	E	399	GLU
1	E	401	PHE
1	E	463	SER
1	E	473	SER
1	E	486	THR
1	F	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	34	ARG
1	F	122	LEU
1	F	146	ILE
1	F	159	VAL
1	F	192	LYS
1	F	196	GLN
1	F	246	SER
1	F	249	ILE
1	F	264	ARG
1	F	269	LEU
1	F	288	GLU
1	F	302	CYS
1	F	320	GLU
1	F	338	LYS
1	F	347	GLU
1	F	377	ARG
1	F	401	PHE
1	F	463	SER
1	F	473	SER
1	F	486	THR
1	F	498	LYS
1	G	14	GLN
1	G	41	ASN
1	G	122	LEU
1	G	192	LYS
1	G	195	GLU
1	G	196	GLN
1	G	240	LYS
1	G	246	SER
1	G	248	GLU
1	G	249	ILE
1	G	251	ARG
1	G	259	SER
1	G	264	ARG
1	G	338	LYS
1	G	351	LYS
1	G	376	ASP
1	G	377	ARG
1	G	401	PHE
1	G	463	SER
1	G	470	MET
1	G	473	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	486	THR
1	H	41	ASN
1	H	79	MET
1	H	122	LEU
1	H	146	ILE
1	H	159	VAL
1	H	192	LYS
1	H	196	GLN
1	H	220	ILE
1	H	246	SER
1	H	249	ILE
1	H	268	GLU
1	H	269	LEU
1	H	302	CYS
1	H	338	LYS
1	H	376	ASP
1	H	377	ARG
1	H	409	LYS
1	H	463	SER
1	H	470	MET
1	H	473	SER
1	H	486	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	ASN
1	A	29	HIS
1	A	41	ASN
1	A	83	HIS
1	A	89	ASN
1	A	175	GLN
1	A	196	GLN
1	A	275	ASN
1	A	300	GLN
1	B	25	ASN
1	B	26	ASN
1	B	41	ASN
1	B	175	GLN
1	B	196	GLN
1	B	206	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	275	ASN
1	B	300	GLN
1	B	344	GLN
1	B	362	GLN
1	B	406	GLN
1	B	462	GLN
1	C	13	GLN
1	C	26	ASN
1	C	41	ASN
1	C	50	GLN
1	C	140	HIS
1	C	175	GLN
1	C	196	GLN
1	C	275	ASN
1	C	300	GLN
1	C	349	GLN
1	D	13	GLN
1	D	26	ASN
1	D	41	ASN
1	D	50	GLN
1	D	71	GLN
1	D	89	ASN
1	D	164	GLN
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	289	GLN
1	D	291	HIS
1	D	300	GLN
1	D	362	GLN
1	E	13	GLN
1	E	26	ASN
1	E	29	HIS
1	E	41	ASN
1	E	50	GLN
1	E	71	GLN
1	E	89	ASN
1	E	175	GLN
1	E	196	GLN
1	E	275	ASN
1	E	289	GLN
1	E	300	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	358	ASN
1	E	440	ASN
1	F	26	ASN
1	F	41	ASN
1	F	83	HIS
1	F	175	GLN
1	F	196	GLN
1	F	300	GLN
1	F	447	GLN
1	G	26	ASN
1	G	41	ASN
1	G	140	HIS
1	G	175	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	G	406	GLN
1	G	462	GLN
1	G	483	GLN
1	H	13	GLN
1	H	26	ASN
1	H	29	HIS
1	H	41	ASN
1	H	83	HIS
1	H	196	GLN
1	H	300	GLN
1	H	444	GLN
1	H	462	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	494/500 (98%)	-1.48	0 100 100	8, 20, 44, 68	0
1	B	494/500 (98%)	-1.51	0 100 100	8, 20, 44, 68	0
1	C	494/500 (98%)	-1.51	0 100 100	9, 19, 44, 68	0
1	D	494/500 (98%)	-1.50	0 100 100	9, 20, 43, 68	0
1	E	494/500 (98%)	-1.53	0 100 100	8, 19, 43, 68	0
1	F	494/500 (98%)	-1.51	0 100 100	8, 19, 43, 68	0
1	G	494/500 (98%)	-1.49	0 100 100	8, 20, 44, 68	0
1	H	494/500 (98%)	-1.49	0 100 100	8, 20, 44, 68	0
All	All	3952/4000 (98%)	-1.50	0 100 100	8, 20, 44, 68	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.