



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2018 – 02:10 PM EST

PDB ID : 5VSW
Title : X-ray crystal structure of Escherichia coli RNA polymerase and DksA/ppGpp complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-05-12
Resolution : 4.29 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

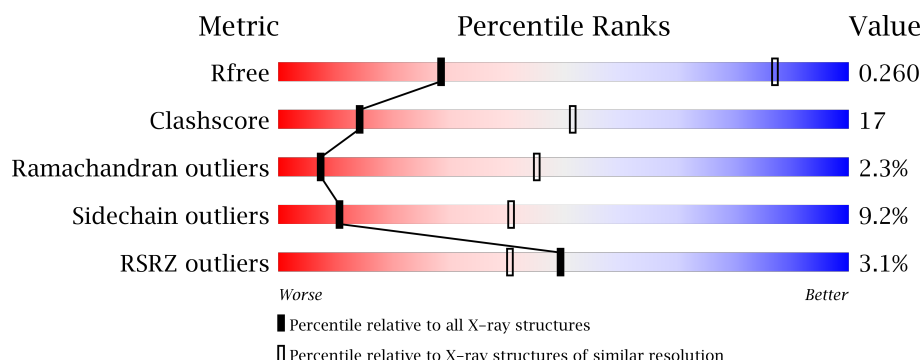
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.29 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}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>13%</div> <div> <div></div> <div>50%</div> <div>36%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	329	<div> <div>4%</div> <div> <div></div> <div>43%</div> <div>38%</div> <div>7%</div> <div>• 10%</div> </div> </div>
1	G	329	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>24%</div> <div>•</div> <div>31%</div> </div> </div>
1	H	329	<div> <div>5%</div> <div> <div></div> <div>40%</div> <div>24%</div> <div>•</div> <div>34%</div> </div> </div>
2	C	1342	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>36%</div> <div>•</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	1342	<div><div></div><div>3%</div><div>61%</div><div>35%</div><div></div></div>
3	D	1407	<div><div></div><div>%</div><div>49%</div><div>30%</div><div>•</div><div>17%</div><div></div></div>
3	J	1407	<div><div></div><div>%</div><div>48%</div><div>31%</div><div>•</div><div>18%</div><div></div></div>
4	E	91	<div><div></div><div>%</div><div>60%</div><div>33%</div><div>•</div><div></div><div></div></div>
4	K	91	<div><div>12%</div><div></div><div>52%</div><div>27%</div><div>7%</div><div>•</div><div>13%</div><div></div></div>
5	F	613	<div><div>3%</div><div></div><div>49%</div><div>25%</div><div>•</div><div>24%</div><div></div></div>
5	L	613	<div><div>2%</div><div></div><div>47%</div><div>27%</div><div>•</div><div>23%</div><div></div></div>
6	M	151	<div><div>7%</div><div></div><div>44%</div><div>46%</div><div>•</div><div>7%</div><div></div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57643 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	297	Total	C	N	O	S	0	0	0
			2297	1439	403	447	8			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called RNA polymerase-binding transcription factor DksA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			

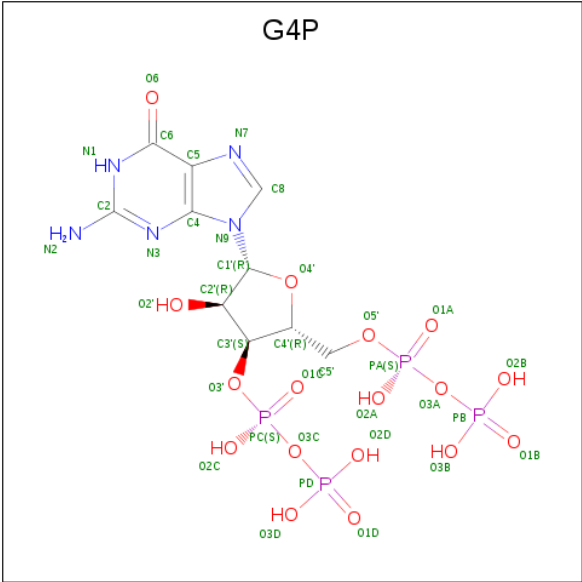
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		
8	M	1	Total	Zn	0	0
			1	1		

- Molecule 9 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).

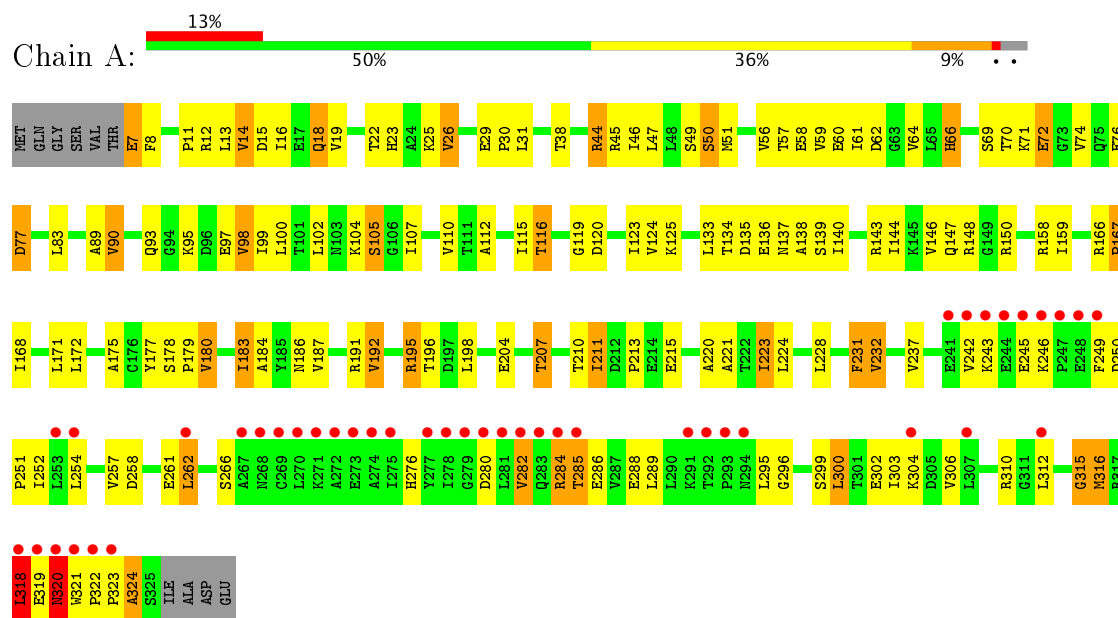


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
9	J	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
9	M	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

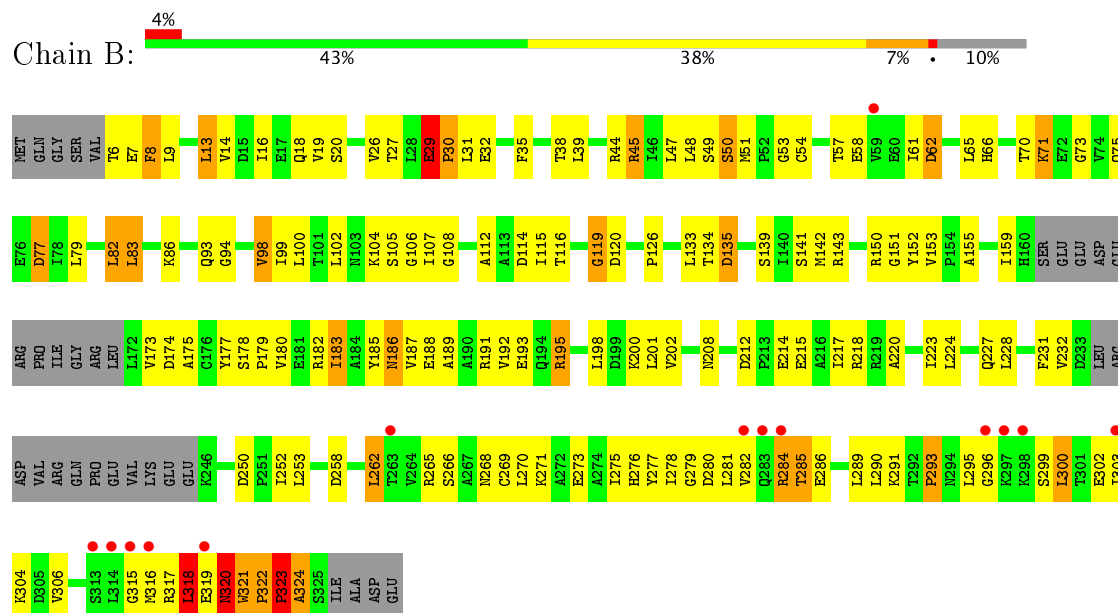
3 Residue-property plots

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

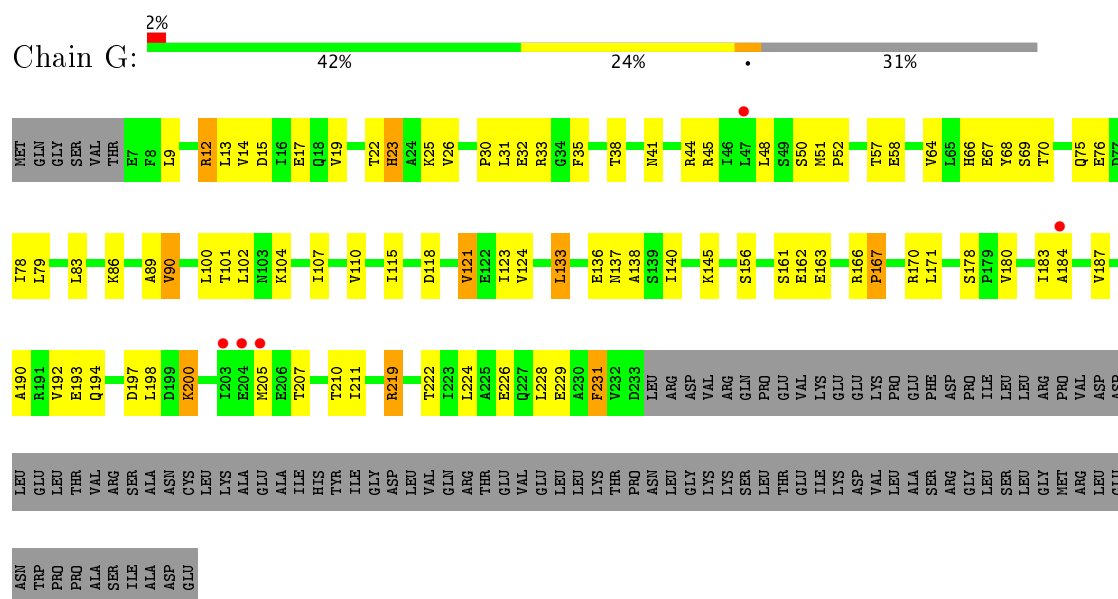
• Molecule 1: DNA-directed RNA polymerase subunit alpha



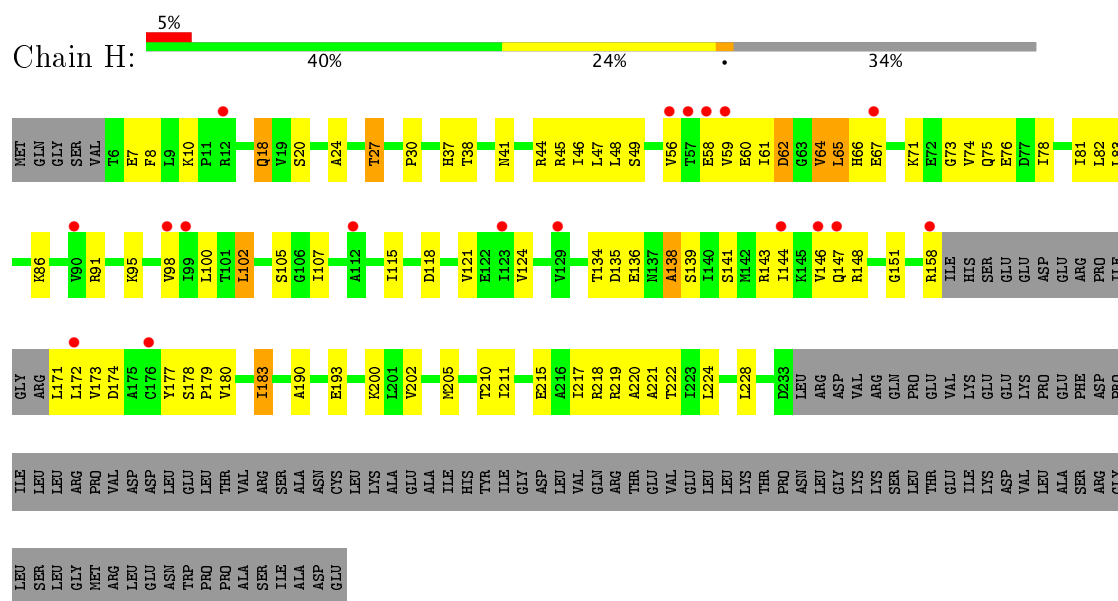
• Molecule 1: DNA-directed RNA polymerase subunit alpha



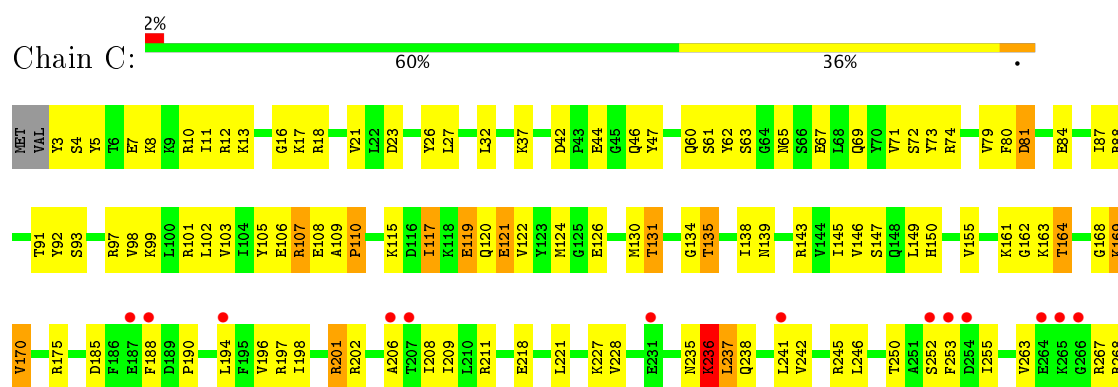
• Molecule 1: DNA-directed RNA polymerase subunit alpha

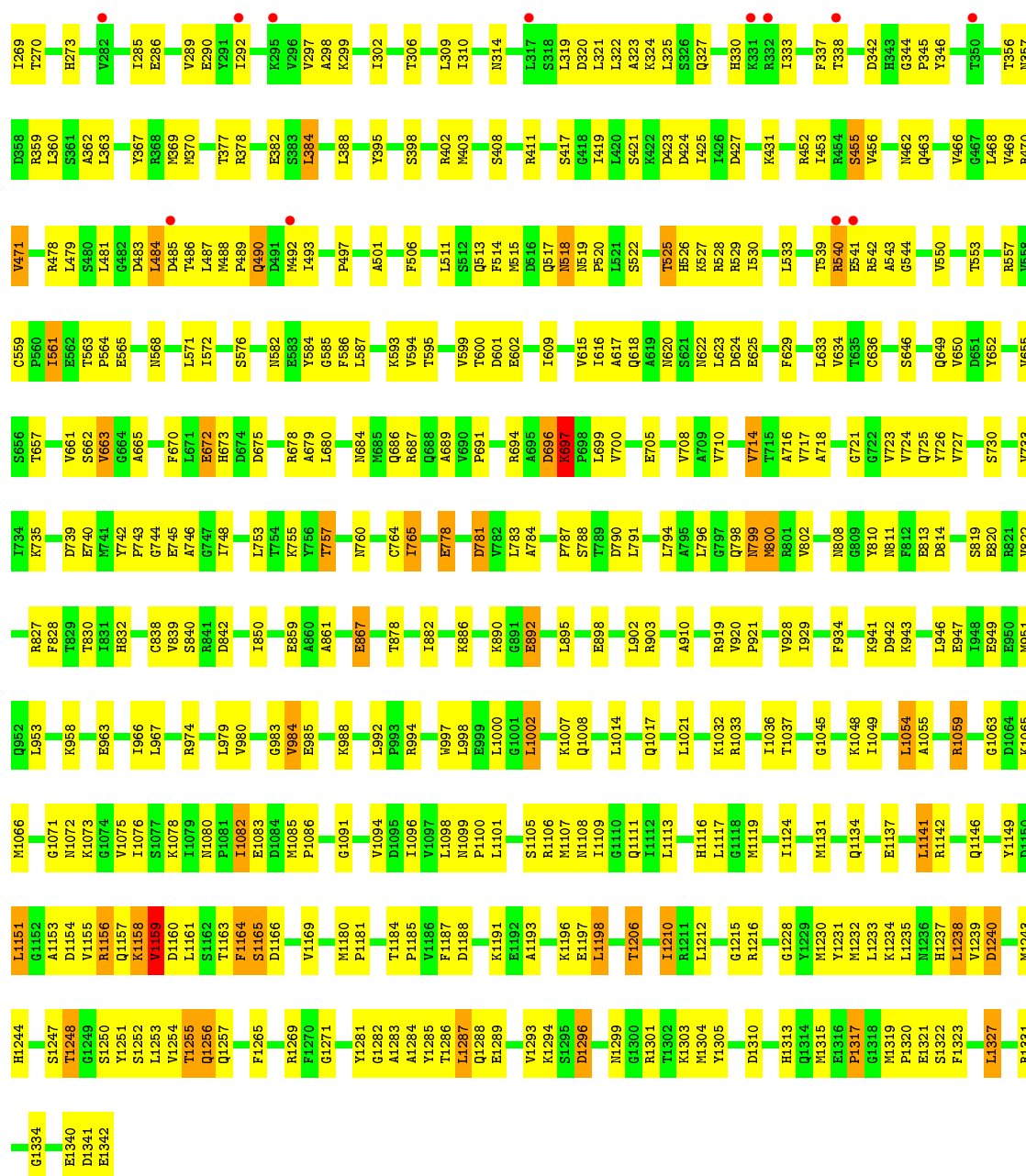


• Molecule 1: DNA-directed RNA polymerase subunit alpha

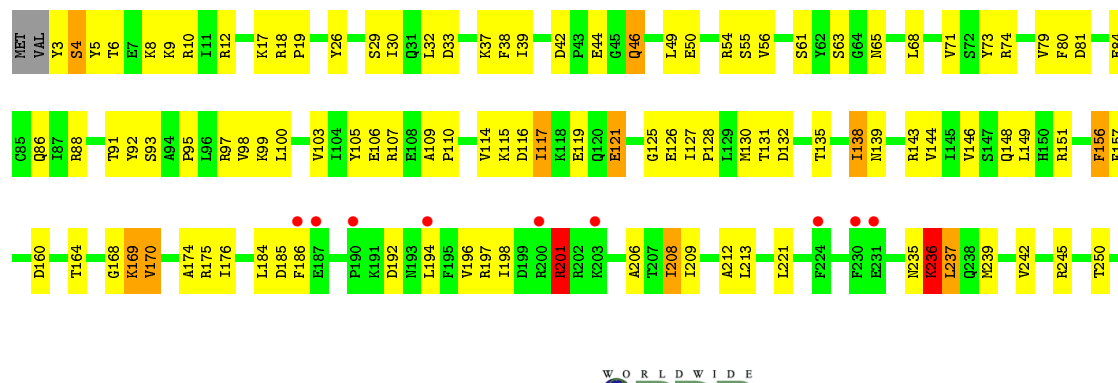


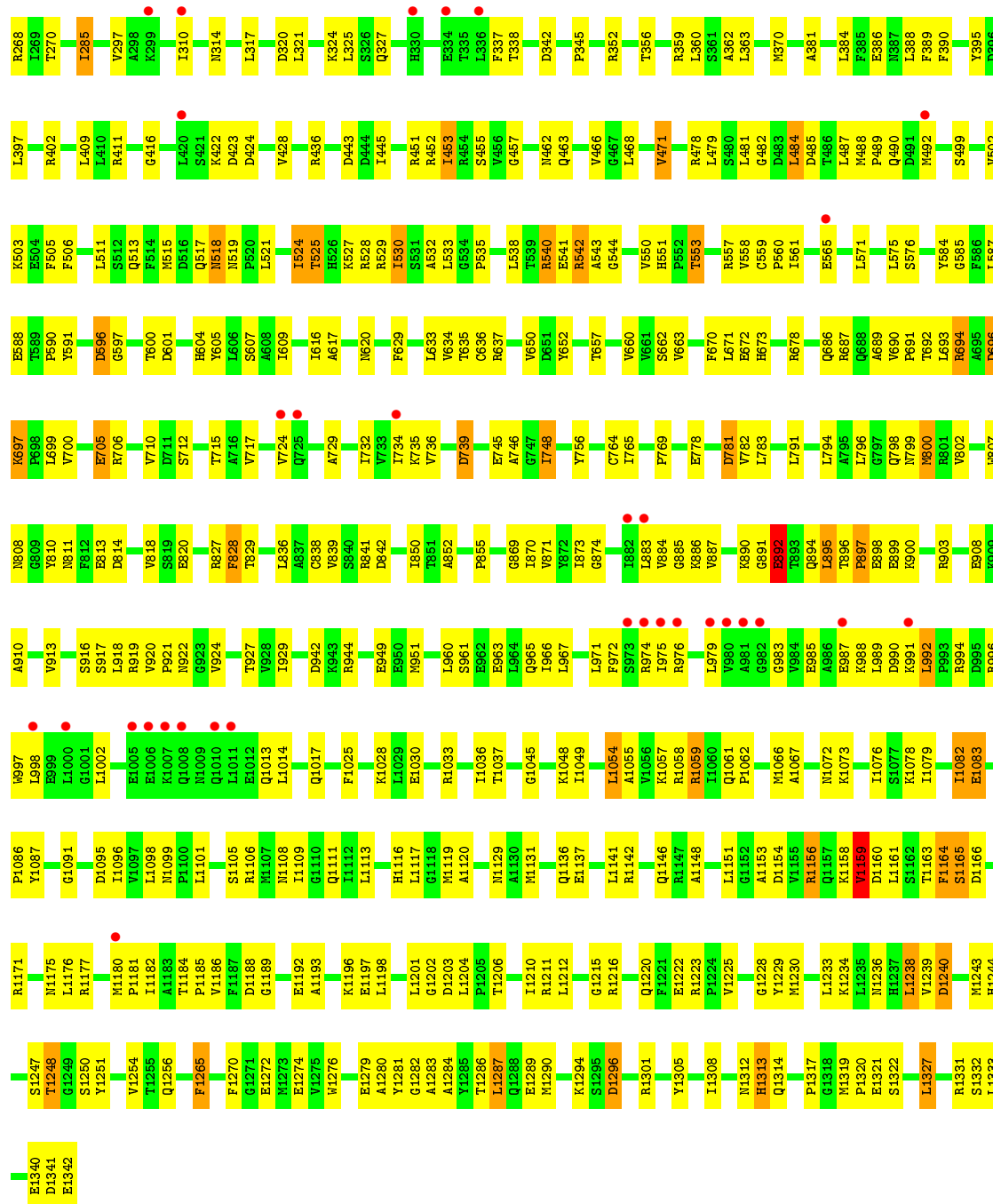
• Molecule 2: DNA-directed RNA polymerase subunit beta



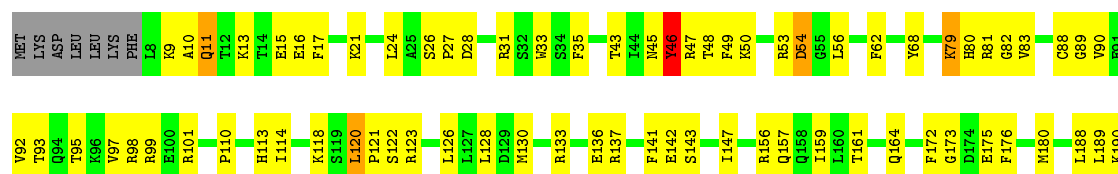


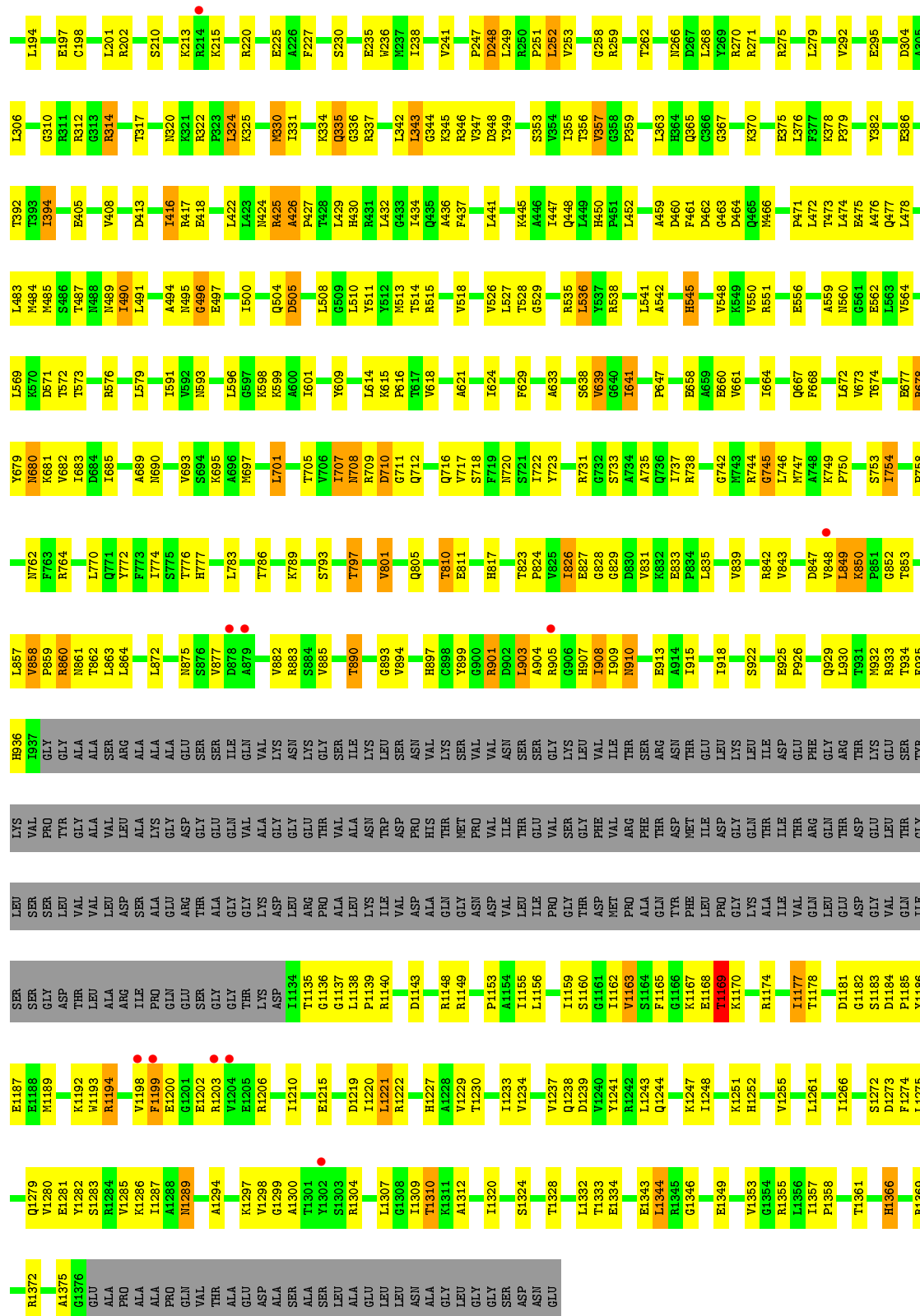
• Molecule 2: DNA-directed RNA polymerase subunit beta





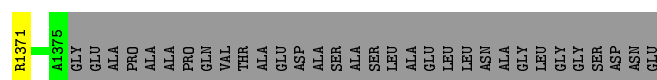
• Molecule 3: DNA-directed RNA polymerase subunit beta'



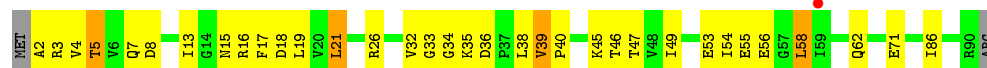


• Molecule 3: DNA-directed RNA polymerase subunit beta'

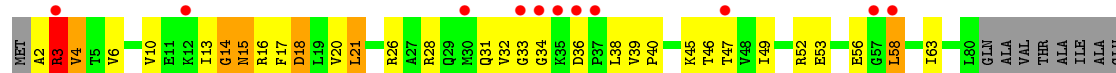
V1280	P1185	LEU	GLN	THR	GLY	P926	D847	G745	S655	V548	Q448	R362	R278	V90	MET
E1281	Y1186	GLU	THR	ASP	ARG	THR	V948	L746	E656	V549	L449	L363	R279	E91	LYS
S1282	K1182	ASP	GLU	THR	LYS	THR	K850	L747	E657	K851	A456	H364	A287	V92	ASP
R1284	W1193	VAL	GLU	THR	LYS	THR	P851	M748	E658	K852	A457	H365	P288	T93	LEU
V1285	R1194	GLN	THR	THR	SER	THR	G852	K749	A659	N560	H458	C366	L291	Q94	LEU
K1286		ILE	GLY	GLY	TVR	PHE	T853	P750	E660	N561	A459	G367	L292	T95	LYS
I1287	V1198	SER	LEU	THR	LYS	HIS	T854		A662	T567	D460	L368	V292	K96	PHE
N1288	F1199	SER	SER	SER	VAL	ILE	T754		E663	S568	F461	A373	R298	V97	LEU
R1289		GLY	SER	LEU	PRO	GLY	T755		E664	L569	D462	L374	R299	R98	LYS
E1290	E1202	ASP	THR	VAL	THR	GLY	E756		K570	D571	M466	L376	R300	E100	ALA
E1291	R1203	THR	VAL	GLY	GLY	ALA	T757		F668	T572			D304	E195	GLN
L1292	V1204	LEU	VAL	ALA	VAL	SER	P758		T674	T573	P471		H104	R101	THR
E1293	E1205	ALA	LEU	VAL	VAL	SER	A761		A675	V574	L472		L205		LYS
A1294	G1207	ARG	ASP	LEU	ALA	ARG	R764		G676	G575	L473		M206	E16	GLU
N1295	R1208	PRO	ALA	SER	ALA	ALA	L764		E677	R576	L474		R214	W115	F17
G1296	V1209	GLN	GLY	GLY	ALA	ALA	R678		R678	L579	E475		R311	F116	
K1297	I1210	GLU	ASP	THR	GLY	GLY	L770		H680	L579	A476		R312	I117	
V1298	E1215	SER	THR	THR	GLY	SER	Q771		K681	L587	Q477		R313	K118	
		GLY	ALA	ALA	GLY	SER	T772		V682	L588	L478		G313	S119	
		THR	GLY	GLY	VAL	ILE	T773		L683	I591	E479		R314	L120	
		GLY	GLY	GLY	VAL	ILE	T774				A480			P121	
		GLY	GLY	GLY	VAL	ILE	T775				R481			S26	
		GLY	GLY	GLY	VAL	ILE	T776				A482			P27	
		GLY	GLY	GLY	VAL	ILE	H777				L483			D28	
		GLY	GLY	GLY	VAL	ILE	R780				M484			R31	
		GLY	GLY	GLY	VAL	ILE	S793				S486			S32	
		GLY	GLY	GLY	VAL	ILE	T797				K598			N33	
		GLY	GLY	GLY	VAL	ILE	S884				A600			S34	
		GLY	GLY	GLY	VAL	ILE	S885				I601			P35	
		GLY	GLY	GLY	VAL	ILE	F892				M604			G36	
		GLY	GLY	GLY	VAL	ILE	G893				S492			E37	
		GLY	GLY	GLY	VAL	ILE	V894				Y609			R137	
		GLY	GLY	GLY	VAL	ILE	H897				L612			Y140	
		GLY	GLY	GLY	VAL	ILE	C898				G613			F141	
		GLY	GLY	GLY	VAL	ILE	R901				L614			E142	
		GLY	GLY	GLY	VAL	ILE	L902				K615			I147	
		GLY	GLY	GLY	VAL	ILE	A904				P616			L154	
		GLY	GLY	GLY	VAL	ILE	L903				T617			E155	
		GLY	GLY	GLY	VAL	ILE	S905				D505			D54	
		GLY	GLY	GLY	VAL	ILE	G906				L510			A65	
		GLY	GLY	GLY	VAL	ILE	H907				Y511			Q157	
		GLY	GLY	GLY	VAL	ILE	I908				V512			Q158	
		GLY	GLY	GLY	VAL	ILE	I909				G640			I159	
		GLY	GLY	GLY	VAL	ILE	N910				T514			L160	
		GLY	GLY	GLY	VAL	ILE	A914				R515			T161	
		GLY	GLY	GLY	VAL	ILE	I915				D516			G257	
		GLY	GLY	GLY	VAL	ILE	R918				L432			Q164	
		GLY	GLY	GLY	VAL	ILE	I923				G433			F172	
		GLY	GLY	GLY	VAL	ILE	G924				V518			G173	
		GLY	GLY	GLY	VAL	ILE	E925				P647			D174	
		GLY	GLY	GLY	VAL	ILE					R536			E175	
		GLY	GLY	GLY	VAL	ILE					K649			F176	
		GLY	GLY	GLY	VAL	ILE					K650			K179	
		GLY	GLY	GLY	VAL	ILE					I653				
		GLY	GLY	GLY	VAL	ILE					I654				



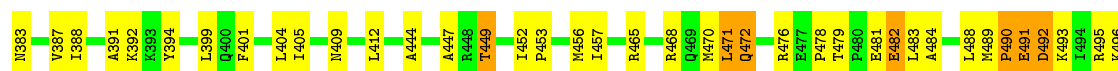
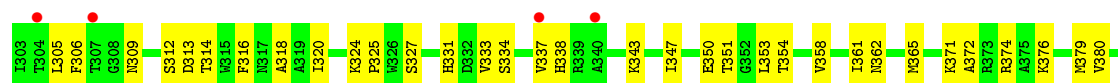
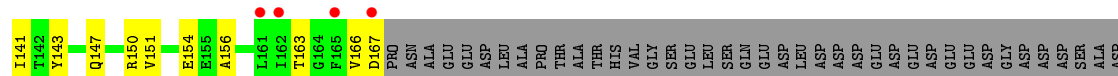
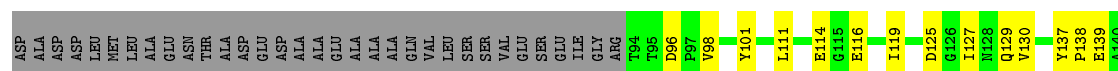
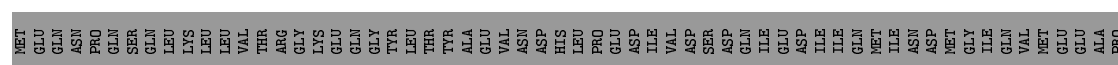
- Molecule 4: DNA-directed RNA polymerase subunit omega



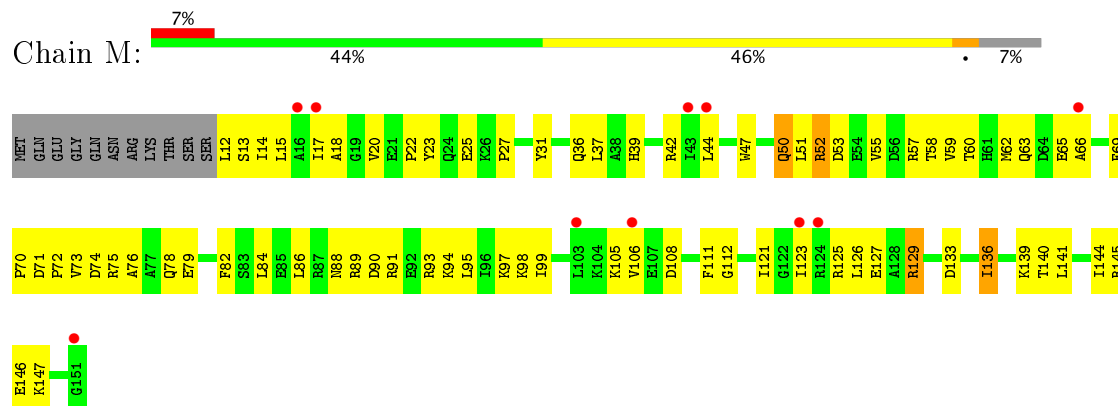
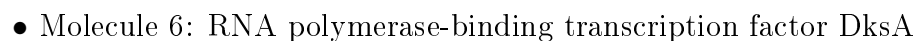
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.27Å 205.26Å 311.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.82 – 4.29 49.55 – 4.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (46.82-4.29) 81.4 (49.55-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.221 , 0.259 0.222 , 0.260	Depositor DCC
R_{free} test set	1783 reflections (2.52%)	DCC
Wilson B-factor (Å ²)	187.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 225.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	57643	wwPDB-VP
Average B, all atoms (Å ²)	279.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, ZN, MG

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	0.29	0/2524	0.62	1/3421 (0.0%)
1	B	0.31	0/2326	0.77	2/3153 (0.1%)
1	G	0.27	0/1777	0.56	0/2408
1	H	0.27	0/1681	0.61	1/2278 (0.0%)
2	C	0.29	0/10739	0.56	1/14489 (0.0%)
2	I	0.28	0/10735	0.54	1/14484 (0.0%)
3	D	0.29	0/9235	0.57	0/12472
3	J	0.28	0/9140	0.57	1/12341 (0.0%)
4	E	0.28	0/693	0.49	0/935
4	K	0.26	0/629	0.58	1/847 (0.1%)
5	F	0.26	0/3864	0.53	1/5194 (0.0%)
5	L	0.27	0/3872	0.51	0/5205
6	M	0.36	0/1155	0.65	1/1549 (0.1%)
All	All	0.29	0/58370	0.57	10/78776 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	3	ARG	N-CA-C	-6.51	93.41	111.00
1	A	318	LEU	CA-CB-CG	6.18	129.50	115.30
3	J	1221	LEU	CA-CB-CG	5.99	129.08	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	236	LYS	N-CA-C	5.86	126.82	111.00
1	B	318	LEU	CA-CB-CG	5.77	128.56	115.30
1	H	65	LEU	CA-CB-CG	5.56	128.09	115.30
2	I	236	LYS	N-CA-C	5.46	125.76	111.00
5	F	608	ARG	NE-CZ-NH1	5.43	123.01	120.30
6	M	95	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	82	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	323	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2542	123	0
1	B	2297	0	2350	144	1
1	G	1755	0	1773	60	0
1	H	1662	0	1687	57	0
2	C	10570	0	10582	390	0
2	I	10566	0	10576	362	0
3	D	9095	0	9222	376	0
3	J	9001	0	9167	366	1
4	E	691	0	695	25	0
4	K	627	0	634	28	0
5	F	3813	0	3880	125	0
5	L	3821	0	3884	119	0
6	M	1140	0	1119	63	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
9	E	36	0	11	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	36	0	11	4	0
9	M	36	0	11	7	0
All	All	57643	0	58144	2018	1

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 17.

All (2018) 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:B:29:GLU:HB3	1:B:30:PRO:CD	1.26	1.46
1:B:29:GLU:CB	1:B:30:PRO:HD2	1.35	1.45
1:B:279:GLY:HA3	1:B:321:TRP:CZ2	1.55	1.41
5:F:600:HIS:O	5:F:604:SER:HB3	1.33	1.29
1:B:253:LEU:O	1:B:321:TRP:HZ2	0.98	1.26
1:B:253:LEU:O	1:B:321:TRP:CZ2	1.88	1.24
2:C:106:GLU:CB	2:C:109:ALA:HB2	1.67	1.24
1:B:29:GLU:O	1:B:31:LEU:HD22	1.36	1.20
5:F:600:HIS:O	5:F:604:SER:CB	1.93	1.16
1:B:29:GLU:CB	1:B:30:PRO:CD	2.02	1.13
5:F:600:HIS:CD2	5:F:601:PRO:HD3	1.86	1.09
2:C:106:GLU:HB3	2:C:109:ALA:CB	1.82	1.09
3:J:863:LEU:HD11	3:J:901:ARG:HG2	1.24	1.09
2:C:236:LYS:O	2:C:237:LEU:HB2	1.29	1.08
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.14	1.05
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.36	1.04
1:B:29:GLU:O	1:B:31:LEU:CD2	2.05	1.03
1:B:279:GLY:HA3	1:B:321:TRP:CH2	1.93	1.02
2:I:236:LYS:O	2:I:237:LEU:CB	2.01	1.02
3:D:1372:ARG:HA	3:J:853:THR:HG21	1.39	1.00
6:M:23:TYR:N	6:M:127:GLU:OE2	1.94	1.00
2:C:236:LYS:O	2:C:237:LEU:CB	2.10	0.97
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.47	0.96
2:C:106:GLU:HB3	2:C:109:ALA:HB2	0.96	0.95
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.48	0.94
2:I:236:LYS:O	2:I:237:LEU:HB2	1.17	0.94
1:B:279:GLY:CA	1:B:321:TRP:CZ2	2.50	0.93
3:D:929:GLN:NE2	6:M:66:ALA:O	2.02	0.92
1:A:316:MET:SD	5:F:600:HIS:HE1	1.92	0.92
1:A:316:MET:SD	5:F:600:HIS:CE1	2.63	0.92
4:K:3:ARG:O	4:K:4:VAL:HB	1.70	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:863:LEU:HD11	3:D:901:ARG:HG2	1.53	0.91
3:J:863:LEU:CD1	3:J:901:ARG:HG2	2.03	0.89
3:J:863:LEU:HD11	3:J:901:ARG:CG	2.01	0.89
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.06	0.89
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.52	0.88
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.37	0.88
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.54	0.88
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.52	0.88
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.56	0.87
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.54	0.86
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.40	0.86
1:B:29:GLU:CG	1:B:30:PRO:HD3	2.06	0.86
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.57	0.86
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.57	0.86
1:A:296:GLY:H	1:A:299:SER:HB2	1.38	0.85
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.59	0.85
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	1.57	0.85
1:B:296:GLY:H	1:B:299:SER:HB2	1.43	0.84
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.59	0.84
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.42	0.84
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.60	0.84
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.42	0.83
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.44	0.83
2:C:235:ASN:O	2:C:236:LYS:HB2	1.78	0.83
1:B:323:PRO:HA	1:B:324:ALA:HB2	1.60	0.83
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.11	0.82
3:D:936:HIS:HA	3:D:1135:THR:HA	1.61	0.82
2:I:235:ASN:O	2:I:236:LYS:HB2	1.76	0.82
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.24	0.82
1:B:29:GLU:CG	1:B:30:PRO:CD	2.57	0.82
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.59	0.82
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.62	0.82
6:M:121:ILE:HG23	6:M:125:ARG:HH11	1.45	0.81
3:J:853:THR:HG22	3:J:854:ALA:H	1.44	0.81
1:G:45:ARG:HG2	1:H:38:THR:HB	1.62	0.81
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.62	0.81
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.62	0.81
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.14	0.80
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.62	0.80
6:M:105:LYS:NZ	6:M:133:ASP:OD2	2.14	0.80
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.62	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.27	0.79
2:C:106:GLU:C	2:C:109:ALA:H	1.86	0.79
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.64	0.79
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.47	0.79
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.64	0.78
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.66	0.78
3:D:1372:ARG:HA	3:J:853:THR:CG2	2.13	0.78
2:I:268:ARG:HH21	2:I:270:THR:HG22	1.48	0.78
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.66	0.78
1:A:224:LEU:HD23	1:B:228:LEU:HD11	1.64	0.77
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.66	0.77
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.66	0.77
1:B:279:GLY:HA3	1:B:321:TRP:CE2	2.19	0.77
3:J:362:ARG:NH2	9:J:2004:G4P:O4'	2.17	0.77
1:A:150:ARG:NH1	1:B:7:GLU:O	2.17	0.77
1:B:83:LEU:HD21	3:D:526:VAL:HB	1.65	0.77
3:J:901:ARG:HB2	3:J:908:ILE:HA	1.66	0.77
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.50	0.77
4:K:40:PRO:O	4:K:52:ARG:NH2	2.18	0.77
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.65	0.77
6:M:121:ILE:HG23	6:M:125:ARG:NH1	2.00	0.77
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.65	0.76
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.50	0.76
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.67	0.76
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.66	0.76
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.66	0.76
5:L:573:LEU:HD12	5:L:588:ARG:HE	1.49	0.76
2:C:106:GLU:H	2:C:109:ALA:HB3	1.51	0.76
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.04	0.76
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.68	0.76
3:J:709:ARG:O	3:J:711:GLY:N	2.19	0.76
2:I:705:GLU:HB2	2:I:794:LEU:H	1.50	0.76
1:B:29:GLU:CB	1:B:30:PRO:HD3	2.14	0.76
9:J:2004:G4P:O3D	4:K:2:ALA:N	2.18	0.76
3:J:901:ARG:CB	3:J:908:ILE:HA	2.15	0.75
1:B:119:GLY:HA3	1:B:271:LYS:HG2	1.68	0.75
1:B:27:THR:HG23	1:B:202:VAL:HG22	1.66	0.75
3:D:1136:GLY:HA2	3:D:1140:ARG:HG2	1.69	0.75
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.69	0.75
3:D:660:GLU:HG3	6:M:12:LEU:HD23	1.68	0.75
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.67	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.69	0.74
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.19	0.74
5:L:573:LEU:H	5:L:573:LEU:HD23	1.53	0.74
2:I:30:ILE:HD12	2:I:30:ILE:H	1.50	0.74
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.52	0.74
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.70	0.74
3:J:48:THR:O	3:J:50:LYS:N	2.20	0.74
1:B:119:GLY:H	1:B:271:LYS:HE3	1.51	0.74
3:D:490:ILE:HD13	3:D:490:ILE:H	1.52	0.74
1:H:134:THR:HG23	1:H:135:ASP:H	1.53	0.74
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.53	0.74
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.69	0.74
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.20	0.73
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.70	0.73
3:D:615:LYS:NZ	9:E:101:G4P:O1C	2.20	0.73
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.69	0.73
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.70	0.73
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.70	0.73
3:D:709:ARG:O	3:D:711:GLY:N	2.21	0.73
6:M:91:ARG:NH1	9:M:202:G4P:O1D	2.19	0.73
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.22	0.73
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.21	0.73
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.53	0.73
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.21	0.73
6:M:94:LYS:NZ	9:M:202:G4P:O1C	2.21	0.73
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.70	0.73
4:K:32:VAL:O	4:K:34:GLY:N	2.21	0.73
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.70	0.72
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.53	0.72
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.70	0.72
1:A:191:ARG:NH1	1:A:198:LEU:O	2.21	0.72
2:C:705:GLU:HB2	2:C:794:LEU:H	1.53	0.72
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.70	0.72
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.71	0.72
1:A:252:ILE:HG21	1:A:312:LEU:HD11	1.70	0.72
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.70	0.72
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.72	0.72
4:K:14:GLY:O	4:K:16:ARG:N	2.22	0.72
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.54	0.72
2:C:678:ARG:NH1	2:C:1071:GLY:O	2.23	0.72
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.53	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.72	0.71
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.53	0.71
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.25	0.71
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.72	0.71
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.22	0.71
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.72	0.71
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.73	0.71
3:J:853:THR:O	3:J:855:ASP:N	2.24	0.71
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.73	0.71
5:F:600:HIS:O	5:F:604:SER:HB2	1.87	0.71
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.71	0.70
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.72	0.70
3:J:844:THR:OG1	3:J:860:ARG:O	2.08	0.70
1:B:279:GLY:CA	1:B:321:TRP:CH2	2.72	0.70
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.24	0.70
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.73	0.70
2:I:533:LEU:HD13	2:I:540:ARG:HE	1.57	0.70
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.74	0.70
3:D:48:THR:O	3:D:50:LYS:N	2.25	0.70
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.74	0.70
2:C:106:GLU:N	2:C:109:ALA:HB3	2.07	0.70
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.74	0.70
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.25	0.69
2:I:739:ASP:N	2:I:739:ASP:OD1	2.26	0.69
3:D:495:ASN:O	3:D:497:GLU:N	2.25	0.69
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.72	0.69
5:F:600:HIS:CD2	5:F:601:PRO:CD	2.71	0.69
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.57	0.69
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.75	0.69
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.75	0.69
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.75	0.69
2:I:4:SER:OG	2:I:5:TYR:N	2.26	0.69
3:D:674:THR:HG21	6:M:139:LYS:HG2	1.74	0.69
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.24	0.69
3:D:418:GLU:HG3	4:E:45:LYS:H	1.57	0.69
1:B:79:LEU:HD11	3:D:526:VAL:HG11	1.74	0.69
3:D:673:VAL:HB	6:M:129:ARG:NH1	2.08	0.69
1:B:289:LEU:HD13	1:B:300:LEU:HD21	1.75	0.69
2:I:151:ARG:HH22	2:I:175:ARG:HH11	1.41	0.69
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.74	0.69
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.69
3:D:679:TYR:OH	3:D:754:ILE:O	2.09	0.68
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.28	0.68
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.75	0.68
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.57	0.68
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.74	0.68
1:A:14:VAL:HG22	1:A:15:ASP:H	1.58	0.68
1:A:7:GLU:HB3	1:B:150:ARG:HH12	1.56	0.68
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.75	0.68
3:D:1244:GLN:O	6:M:66:ALA:HB3	1.94	0.68
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.22	0.68
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.25	0.68
3:J:1365:TYR:OH	3:J:1369:ARG:NH1	2.26	0.68
1:B:77:ASP:OD1	1:B:77:ASP:N	2.26	0.68
2:C:168:GLY:O	2:C:170:VAL:N	2.22	0.68
3:D:1178:THR:HG23	3:D:1184:ASP:HB3	1.75	0.68
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.25	0.68
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.74	0.68
3:J:853:THR:C	3:J:855:ASP:H	1.97	0.68
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.94	0.68
4:E:4:VAL:HG13	4:E:5:THR:H	1.59	0.68
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.75	0.68
2:I:560:PRO:O	3:J:780:ARG:NH2	2.26	0.68
2:I:17:LYS:NZ	2:I:1154:ASP:OD1	2.27	0.68
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.76	0.68
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.75	0.68
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.76	0.68
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.94	0.67
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.76	0.67
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.75	0.67
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.76	0.67
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.76	0.67
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.76	0.67
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.10	0.67
2:C:197:ARG:NH1	2:C:201:ARG:O	2.27	0.67
2:I:798:GLN:OE1	2:I:827:ARG:HB2	1.94	0.67
2:C:324:LYS:O	2:C:327:GLN:NE2	2.26	0.67
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.77	0.67
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.75	0.67
6:M:37:LEU:HD22	6:M:106:VAL:HG13	1.76	0.67
1:A:47:LEU:HD23	1:A:51:MET:HE2	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.76	0.67
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.29	0.67
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.75	0.67
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.77	0.67
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.67
1:A:77:ASP:N	1:A:77:ASP:OD1	2.28	0.67
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.59	0.67
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.77	0.66
1:B:253:LEU:HB3	1:B:321:TRP:NE1	2.09	0.66
2:I:596:ASP:CG	2:I:597:GLY:H	1.97	0.66
5:L:561:MET:HA	5:L:567:MET:HE1	1.77	0.66
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.77	0.66
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.59	0.66
3:D:935:PHE:O	3:D:1136:GLY:N	2.29	0.66
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.27	0.66
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.78	0.66
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.61	0.66
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.77	0.66
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.11	0.66
5:F:465:ARG:HD2	5:F:468:ARG:HH22	1.60	0.66
2:C:1106:ARG:HG3	6:M:74:ASP:OD1	1.96	0.66
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.27	0.66
1:B:94:GLY:H	1:B:276:HIS:CD2	2.13	0.66
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.61	0.66
2:C:861:ALA:HB1	2:C:882:ILE:HD13	1.76	0.66
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.26	0.66
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.61	0.66
3:J:495:ASN:O	3:J:497:GLU:N	2.29	0.65
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.60	0.65
2:I:1243:MET:HA	3:J:353:SER:HB3	1.79	0.65
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.78	0.65
1:B:100:LEU:HD23	1:B:115:ILE:HG21	1.79	0.65
3:D:932:MET:HA	3:D:1139:PRO:HD3	1.77	0.65
2:I:1244:HIS:HD2	2:I:1265:PHE:HB2	1.60	0.65
6:M:44:LEU:HD22	6:M:99:ILE:HG23	1.78	0.65
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.78	0.65
2:I:452:ARG:NH1	2:I:584:TYR:O	2.30	0.65
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.78	0.65
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.78	0.65
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.77	0.65
2:C:106:GLU:CB	2:C:109:ALA:CB	2.57	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.79	0.65
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.29	0.65
1:A:59:VAL:HG22	1:A:144:ILE:HA	1.79	0.65
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.77	0.65
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.77	0.65
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.27	0.65
4:E:32:VAL:O	4:E:34:GLY:N	2.30	0.65
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.79	0.65
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.30	0.65
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	1.79	0.65
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.61	0.65
3:J:259:ARG:HD3	5:L:502:LYS:HD2	1.78	0.65
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.79	0.64
5:L:493:LYS:HG2	5:L:496:LYS:HE2	1.77	0.64
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.31	0.64
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.62	0.64
1:B:94:GLY:HA3	1:B:276:HIS:HB3	1.79	0.64
2:I:206:ALA:O	2:I:209:ILE:HG22	1.97	0.64
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.62	0.64
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.79	0.64
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.79	0.64
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.79	0.64
3:D:863:LEU:HD11	3:D:901:ARG:CG	2.25	0.64
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.80	0.64
2:I:168:GLY:O	2:I:170:VAL:N	2.30	0.64
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.79	0.64
3:J:364:HIS:CE1	4:K:3:ARG:HH21	2.16	0.64
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.80	0.64
3:D:793:SER:O	3:D:797:THR:HG23	1.98	0.64
2:I:1116:HIS:HE1	3:J:641:ILE:N	1.94	0.64
3:J:853:THR:HG22	3:J:854:ALA:N	2.12	0.64
3:D:473:THR:HG23	3:D:476:ALA:H	1.63	0.64
1:G:14:VAL:HG13	1:G:15:ASP:H	1.62	0.64
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.80	0.64
1:A:134:THR:HG21	2:C:727:VAL:O	1.98	0.64
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.78	0.64
1:B:253:LEU:CB	1:B:321:TRP:HE1	2.11	0.63
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.80	0.63
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.78	0.63
3:D:789:LYS:HD2	6:M:79:GLU:OE2	1.97	0.63
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.31	0.63
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.63	0.63
3:J:473:THR:HG23	3:J:476:ALA:H	1.63	0.63
1:B:119:GLY:N	1:B:271:LYS:HE3	2.13	0.63
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.30	0.63
3:D:658:GLU:O	3:D:661:VAL:HG22	1.97	0.63
3:D:668:PHE:HB2	3:D:678:ARG:HG3	1.80	0.63
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.80	0.63
2:C:106:GLU:O	2:C:109:ALA:N	2.31	0.63
2:C:211:ARG:NH1	2:C:357:ASN:O	2.32	0.63
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.80	0.63
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.80	0.63
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.64	0.63
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.81	0.63
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.81	0.63
1:A:22:THR:O	1:A:207:THR:N	2.27	0.62
5:F:479:THR:HG23	5:F:481:GLU:H	1.63	0.62
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.62
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.80	0.62
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.81	0.62
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.81	0.62
3:D:677:GLU:HG2	6:M:129:ARG:NH1	2.14	0.62
1:A:237:VAL:HG13	1:B:13:LEU:H	1.62	0.62
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.81	0.62
2:I:842:ASP:N	2:I:1045:GLY:O	2.30	0.62
3:D:1206:ARG:NH2	3:J:1295:ASN:OD1	2.32	0.62
6:M:94:LYS:O	6:M:98:LYS:HD2	1.98	0.62
1:B:253:LEU:HB3	1:B:321:TRP:HE1	1.65	0.62
1:G:161:SER:O	1:G:163:GLU:N	2.32	0.62
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.35	0.62
1:A:97:GLU:HB3	1:A:147:GLN:HG2	1.81	0.62
3:D:1198:VAL:HB	3:D:1210:ILE:HG23	1.80	0.62
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.32	0.62
2:I:149:LEU:O	2:I:532:ALA:HA	1.99	0.62
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.80	0.62
6:M:59:VAL:O	6:M:63:GLN:HG3	2.00	0.62
1:A:23:HIS:HE1	1:A:204:GLU:HG2	1.64	0.62
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.81	0.62
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.82	0.62
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.82	0.62
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.35	0.62
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.81	0.62
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.80	0.62
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.82	0.62
2:I:81:ASP:HA	2:I:92:TYR:HE1	1.63	0.62
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.81	0.62
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.15	0.62
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.64	0.62
2:C:360:LEU:HD22	2:C:378:ARG:HH21	1.65	0.61
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.81	0.61
6:M:55:VAL:HG22	6:M:89:ARG:HG3	1.82	0.61
1:B:102:LEU:HD23	1:B:115:ILE:HG12	1.82	0.61
3:D:137:ARG:HD3	3:D:143:SER:HB2	1.83	0.61
3:D:252:LEU:HD23	3:D:262:THR:HB	1.81	0.61
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.82	0.61
3:D:678:ARG:HA	6:M:129:ARG:NH2	2.15	0.61
2:I:808:ASN:H	3:J:633:ALA:HB2	1.65	0.61
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.00	0.61
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.80	0.61
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.35	0.61
2:C:778:GLU:O	2:C:781:ASP:HB2	2.01	0.61
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.82	0.61
1:A:45:ARG:HG2	1:B:38:THR:OG1	2.00	0.61
3:D:614:LEU:HD23	4:E:5:THR:HB	1.82	0.61
2:I:208:ILE:HG12	2:I:362:ALA:HB1	1.82	0.61
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.66	0.61
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.16	0.61
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.82	0.61
2:C:1244:HIS:HD2	2:C:1265:PHE:HB2	1.66	0.61
3:D:935:PHE:HA	6:M:86:LEU:HD11	1.82	0.61
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.83	0.61
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.83	0.60
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.83	0.60
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.00	0.60
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.30	0.60
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.82	0.60
3:J:418:GLU:HG3	4:K:45:LYS:H	1.65	0.60
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.35	0.60
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.82	0.60
5:L:379:MET:O	5:L:383:ASN:ND2	2.34	0.60
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.82	0.60
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.83	0.60
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.37	0.60
3:D:901:ARG:HB2	3:D:908:ILE:HA	1.84	0.60
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.82	0.60
3:J:853:THR:C	3:J:855:ASP:N	2.54	0.60
1:A:135:ASP:O	1:A:137:ASN:N	2.34	0.60
2:I:1294:LYS:HB3	3:J:347:VAL:HG13	1.82	0.60
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.83	0.60
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.83	0.60
2:I:37:LYS:HD2	2:I:46:GLN:HE21	1.66	0.60
1:A:211:ILE:HD12	1:A:215:GLU:HG2	1.84	0.60
1:A:316:MET:CE	5:F:600:HIS:NE2	2.65	0.60
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.82	0.60
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.82	0.60
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.35	0.60
5:F:561:MET:HA	5:F:567:MET:HE1	1.84	0.60
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.84	0.60
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.82	0.60
3:J:674:THR:O	3:J:678:ARG:HB3	2.02	0.60
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.84	0.60
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.16	0.60
2:C:1119:MET:HE1	2:C:1210:ILE:HD11	1.84	0.60
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.84	0.60
3:J:1290:ARG:HD2	3:J:1298:VAL:HG12	1.84	0.60
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.35	0.59
1:B:47:LEU:HD23	1:B:51:MET:HE2	1.84	0.59
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.83	0.59
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.84	0.59
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.84	0.59
2:C:408:SER:O	2:C:431:LYS:NZ	2.35	0.59
2:I:268:ARG:NH2	2:I:270:THR:HG22	2.17	0.59
3:D:325:LYS:HE2	3:D:330:MET:HG3	1.83	0.59
3:D:355:ILE:HG12	3:D:464:ASP:O	2.02	0.59
3:D:515:ARG:O	3:D:545:HIS:HB3	2.02	0.59
3:D:849:LEU:HD22	3:D:849:LEU:H	1.68	0.59
1:G:12:ARG:H	1:G:30:PRO:HD2	1.67	0.59
3:J:678:ARG:HA	3:J:681:LYS:HB3	1.84	0.59
1:B:93:GLN:HB2	1:B:276:HIS:CD2	2.38	0.59
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.83	0.59
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLU:H	2:C:109:ALA:CB	2.14	0.59
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.84	0.59
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.84	0.59
1:B:175:ALA:HB1	1:B:177:TYR:CE1	2.37	0.59
1:B:53:GLY:HA3	1:B:177:TYR:O	2.02	0.59
1:B:321:TRP:H	1:B:322:PRO:HD3	1.67	0.59
2:C:356:THR:HG21	2:C:362:ALA:HA	1.84	0.59
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.84	0.59
1:B:57:THR:HG22	1:B:58:GLU:HG3	1.84	0.59
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.02	0.59
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.84	0.59
1:A:45:ARG:NE	2:C:1083:GLU:HB3	2.17	0.59
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.85	0.59
3:D:505:ASP:HB3	3:D:629:PHE:HE1	1.67	0.59
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.85	0.59
1:H:102:LEU:HG	1:H:115:ILE:HG12	1.83	0.59
3:J:140:TYR:O	3:J:297:ARG:NH1	2.36	0.59
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.02	0.59
2:C:723:VAL:O	2:C:735:LYS:N	2.33	0.59
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.85	0.59
1:B:119:GLY:HA3	1:B:271:LYS:CG	2.33	0.58
2:C:814:ASP:CG	2:C:1106:ARG:HH12	2.05	0.58
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.85	0.58
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.85	0.58
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.85	0.58
3:J:492:SER:HB2	3:J:499:ILE:HB	1.84	0.58
3:D:1165:PHE:HE1	3:D:1200:GLU:HB2	1.66	0.58
5:F:279:ARG:HB3	5:F:347:ILE:HD11	1.85	0.58
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.85	0.58
2:I:1240:ASP:N	2:I:1240:ASP:OD1	2.27	0.58
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.03	0.58
3:D:317:THR:HG22	3:D:322:ARG:O	2.03	0.58
3:D:673:VAL:HB	6:M:129:ARG:HH12	1.67	0.58
5:F:314:THR:HA	5:F:318:ALA:HB3	1.85	0.58
1:G:228:LEU:HG	1:H:221:ALA:HB1	1.85	0.58
2:I:106:GLU:HB3	2:I:109:ALA:HB2	1.83	0.58
2:I:524:ILE:HD12	2:I:712:SER:HB2	1.85	0.58
2:I:998:LEU:HD12	2:I:998:LEU:H	1.67	0.58
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.67	0.58
1:A:223:ILE:HD13	1:B:8:PHE:CE2	2.37	0.58
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.02	0.58
3:J:385:LEU:HD23	3:J:411:ILE:HG13	1.85	0.58
3:D:88:CYS:O	3:D:90:VAL:N	2.36	0.58
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.17	0.58
5:L:551:LEU:HD23	5:L:597:LYS:HD2	1.84	0.58
1:A:166:ARG:O	1:A:168:ILE:N	2.37	0.58
1:A:284:ARG:HG3	1:A:288:GLU:HG3	1.85	0.58
3:J:425:ARG:HG2	3:J:426:ALA:H	1.68	0.58
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.84	0.58
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.85	0.58
1:H:98:VAL:O	1:H:146:VAL:HG22	2.04	0.58
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.86	0.58
3:J:362:ARG:HE	9:J:2004:G4P:C2	2.17	0.58
2:C:488:MET:O	2:C:490:GLN:N	2.33	0.58
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.69	0.58
3:J:708:ASN:N	3:J:708:ASN:OD1	2.37	0.58
1:B:266:SER:HB3	1:B:303:ILE:HD11	1.86	0.58
2:C:617:ALA:HA	2:C:636:CYS:SG	2.44	0.58
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.37	0.58
2:I:324:LYS:O	2:I:327:GLN:NE2	2.37	0.58
1:B:321:TRP:H	1:B:322:PRO:CD	2.17	0.57
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.39	0.57
2:I:528:ARG:NH2	2:I:576:SER:O	2.37	0.57
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.69	0.57
3:J:848:VAL:HG21	3:J:880:VAL:HG22	1.86	0.57
1:B:252:ILE:HG22	1:B:278:ILE:HD11	1.84	0.57
2:C:953:LEU:CD1	2:C:1033:ARG:HG3	2.34	0.57
2:C:1247:SER:HB3	3:D:375:GLU:O	2.03	0.57
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.57
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.85	0.57
3:J:438:GLU:OE2	3:J:481:ARG:NH2	2.34	0.57
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.85	0.57
1:B:86:LYS:NZ	3:D:526:VAL:O	2.38	0.57
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.86	0.57
3:J:436:ALA:HB3	3:J:485:MET:HA	1.86	0.57
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.69	0.57
3:D:708:ASN:N	3:D:708:ASN:OD1	2.33	0.57
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.87	0.57
4:K:58:LEU:O	4:K:63:ILE:HG21	2.05	0.57
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.34	0.57
5:F:584:ARG:HH11	5:F:584:ARG:HA	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:SER:OG	1:H:139:SER:HA	2.04	0.57
2:I:841:ARG:CZ	3:J:256:ASP:HB3	2.35	0.57
1:B:273:GLU:OE2	1:B:293:PRO:HD2	2.04	0.57
2:C:842:ASP:N	2:C:1045:GLY:O	2.37	0.57
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.18	0.57
3:D:425:ARG:HG2	3:D:426:ALA:H	1.69	0.57
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.86	0.57
2:I:106:GLU:OE1	2:I:114:VAL:HG22	2.04	0.57
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.87	0.57
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.39	0.57
1:A:137:ASN:OD1	1:A:137:ASN:N	2.38	0.57
2:C:802:VAL:HG21	2:C:1098:LEU:HD22	1.85	0.57
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.85	0.57
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.87	0.57
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.87	0.57
2:C:1271:GLY:HA3	3:D:343:LEU:HD12	1.87	0.56
2:C:250:THR:HA	2:C:268:ARG:HA	1.85	0.56
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.87	0.56
5:F:245:ALA:O	5:F:249:ILE:HG13	2.04	0.56
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.85	0.56
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.87	0.56
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.39	0.56
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.86	0.56
5:L:479:THR:HG23	5:L:481:GLU:H	1.69	0.56
1:B:29:GLU:CD	1:B:30:PRO:HD3	2.24	0.56
2:C:106:GLU:O	2:C:108:GLU:HA	2.05	0.56
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.17	0.56
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.86	0.56
5:L:245:ALA:O	5:L:249:ILE:HG13	2.05	0.56
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.87	0.56
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.88	0.56
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.87	0.56
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.87	0.56
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.69	0.56
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.36	0.56
5:L:573:LEU:HD11	5:L:588:ARG:HH21	1.70	0.56
2:C:1285:TYR:CD1	3:D:475:GLU:HG2	2.40	0.56
3:D:709:ARG:HD2	3:D:710:ASP:H	1.70	0.56
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.36	0.56
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.54	0.56
2:C:102:LEU:HD23	2:C:117:ILE:HD11	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:SER:OG	2:C:126:GLU:OE1	2.17	0.56
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.36	0.56
2:I:151:ARG:HH22	2:I:175:ARG:NH1	2.04	0.56
3:J:770:LEU:HD22	3:J:770:LEU:H	1.70	0.56
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.87	0.56
3:D:194:LEU:O	3:D:198:CYS:N	2.35	0.56
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.41	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.71	0.56
6:M:141:LEU:O	6:M:145:ARG:HG3	2.05	0.56
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.86	0.56
1:A:300:LEU:HD13	1:A:304:LYS:HE2	1.86	0.56
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.39	0.56
3:D:903:LEU:HD22	3:D:909:ILE:HD12	1.87	0.56
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.87	0.56
3:J:824:PRO:HD3	3:J:835:LEU:HD13	1.86	0.56
5:L:312:SER:OG	5:L:313:ASP:N	2.39	0.56
1:B:275:ILE:HD11	1:B:284:ARG:HD3	1.86	0.56
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.87	0.56
4:E:8:ASP:HB2	4:E:55:GLU:OE2	2.06	0.56
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.70	0.56
3:J:749:LYS:HB3	3:J:755:ILE:HD11	1.87	0.56
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.88	0.56
2:I:91:THR:HG21	2:I:503:LYS:HE3	1.87	0.56
1:A:12:ARG:H	1:A:30:PRO:HD2	1.69	0.56
2:C:582:ASN:HB3	2:C:586:PHE:H	1.71	0.56
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.53	0.56
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.88	0.56
1:B:318:LEU:O	1:B:320:ASN:N	2.32	0.55
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.89	0.55
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.88	0.55
1:A:296:GLY:N	1:A:299:SER:HB2	2.15	0.55
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.06	0.55
2:C:624:ASP:OD1	2:C:625:GLU:N	2.38	0.55
3:D:48:THR:C	3:D:50:LYS:H	2.09	0.55
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.89	0.55
2:I:462:ASN:O	2:I:466:VAL:HG23	2.06	0.55
3:J:1319:PHE:HB3	3:J:1340:LYS:HD2	1.88	0.55
3:J:16:GLU:HG3	3:J:17:PHE:H	1.71	0.55
3:J:677:GLU:O	3:J:681:LYS:N	2.37	0.55
2:C:714:VAL:HB	2:C:787:PRO:HD2	1.87	0.55
2:I:93:SER:OG	2:I:126:GLU:OE1	2.15	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.42	0.55
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.21	0.55
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.42	0.55
2:C:106:GLU:HG3	2:C:107:ARG:H	1.72	0.55
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.72	0.55
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.88	0.55
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.42	0.55
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.42	0.55
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.88	0.55
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.36	0.55
5:F:312:SER:OG	5:F:313:ASP:N	2.39	0.55
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.40	0.55
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.89	0.55
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.88	0.55
3:D:681:LYS:HZ2	6:M:12:LEU:HD22	1.72	0.55
2:I:1164:PHE:O	2:I:1166:ASP:N	2.40	0.55
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.42	0.55
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.89	0.55
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.87	0.55
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.71	0.55
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.41	0.55
1:B:48:LEU:HD22	3:D:535:ARG:HD3	1.88	0.55
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.40	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.55
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.88	0.55
2:C:1164:PHE:O	2:C:1166:ASP:N	2.39	0.55
3:D:901:ARG:CB	3:D:908:ILE:HA	2.36	0.55
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.89	0.55
2:I:1131:MET:HE2	2:I:1136:GLN:HG3	1.89	0.55
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.88	0.55
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.88	0.55
3:J:658:GLU:O	3:J:661:VAL:HG22	2.06	0.55
9:M:202:G4P:O2C	9:M:202:G4P:O2'	2.23	0.55
1:B:253:LEU:HB3	1:B:321:TRP:CE2	2.42	0.55
2:C:453:ILE:HD12	2:C:587:LEU:HG	1.88	0.55
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.25	0.55
2:I:710:VAL:HA	2:I:715:THR:HG21	1.88	0.55
2:I:693:LEU:HB2	2:I:829:THR:O	2.07	0.55
3:J:549:LYS:HD3	3:J:569:LEU:HD23	1.88	0.55
5:L:595:LEU:O	5:L:599:ARG:HB2	2.06	0.55
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.07	0.54
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.88	0.54
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.89	0.54
2:C:403:MET:HG3	2:C:584:TYR:CE1	2.43	0.54
3:D:54:ASP:N	3:D:54:ASP:OD1	2.40	0.54
3:D:596:LEU:HD12	3:D:601:ILE:HG13	1.89	0.54
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.89	0.54
1:A:310:ARG:O	5:F:608:ARG:NH2	2.38	0.54
1:B:6:THR:OG1	1:B:7:GLU:N	2.40	0.54
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.22	0.54
5:F:513:ASP:C	5:F:515:GLU:H	2.11	0.54
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.89	0.54
2:I:800:MET:O	2:I:1229:TYR:HA	2.08	0.54
3:J:258:GLY:HA3	5:L:499:LYS:HE2	1.89	0.54
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.89	0.54
6:M:98:LYS:NZ	9:M:202:G4P:O4'	2.40	0.54
1:B:29:GLU:HG2	1:B:30:PRO:HD3	1.87	0.54
1:B:323:PRO:CA	1:B:324:ALA:HB2	2.35	0.54
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.39	0.54
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.88	0.54
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.90	0.54
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.41	0.54
3:J:79:LYS:HB2	5:L:569:THR:H	1.72	0.54
1:B:277:TYR:HB2	1:B:321:TRP:HH2	1.71	0.54
5:F:489:MET:O	5:F:491:GLU:N	2.40	0.54
5:F:612:ASP:N	5:F:612:ASP:OD1	2.38	0.54
3:J:274:ASN:OD1	5:L:446:GLN:NE2	2.41	0.54
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.88	0.54
3:D:1344:LEU:O	3:D:1346:GLY:N	2.39	0.54
3:D:709:ARG:HD2	3:D:710:ASP:N	2.22	0.54
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.71	0.54
5:F:316:PHE:HZ	5:F:334:SER:HA	1.72	0.54
6:M:13:SER:O	6:M:17:ILE:HG13	2.08	0.54
1:B:115:ILE:HG22	1:B:116:THR:H	1.72	0.54
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.90	0.54
5:F:536:THR:O	5:F:540:LEU:N	2.38	0.54
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.43	0.54
3:J:99:ARG:HG3	3:J:249:LEU:HD21	1.90	0.54
1:A:47:LEU:O	1:A:180:VAL:HG21	2.08	0.54
1:A:11:PRO:HD2	1:B:227:GLN:HA	1.90	0.54
2:C:1075:VAL:HG21	3:D:463:GLY:HA2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:CE	5:F:600:HIS:CE1	2.91	0.54
2:I:148:GLN:NE2	2:I:535:PRO:O	2.39	0.54
3:J:705:THR:HG21	3:J:719:PHE:H	1.71	0.54
5:L:515:GLU:HG2	5:L:516:ASP:N	2.23	0.54
1:B:228:LEU:O	1:B:232:VAL:HG23	2.08	0.53
1:B:268:ASN:O	1:B:271:LYS:HB3	2.07	0.53
2:C:72:SER:O	2:C:99:LYS:N	2.32	0.53
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.90	0.53
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.73	0.53
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.43	0.53
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.90	0.53
3:D:667:GLN:HG2	3:D:672:LEU:HD12	1.90	0.53
3:J:793:SER:O	3:J:797:THR:HG23	2.07	0.53
3:J:908:ILE:HG12	3:J:909:ILE:N	2.22	0.53
3:J:201:LEU:HB2	3:J:221:ILE:HD13	1.90	0.53
3:J:357:VAL:HG22	3:J:461:PHE:HE1	1.73	0.53
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.90	0.53
3:J:853:THR:CG2	3:J:854:ALA:H	2.10	0.53
2:C:130:MET:SD	2:C:134:GLY:HA2	2.48	0.53
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.89	0.53
2:I:138:ILE:O	2:I:139:ASN:ND2	2.41	0.53
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.90	0.53
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.90	0.53
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.73	0.53
1:H:49:SER:O	1:H:151:GLY:HA2	2.09	0.53
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.44	0.53
3:J:420:PRO:O	3:J:471:PRO:HD2	2.09	0.53
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.90	0.53
3:D:576:ARG:NH1	3:D:593:ASN:O	2.41	0.53
3:D:903:LEU:HD21	3:D:913:GLU:OE1	2.09	0.53
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.91	0.53
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.74	0.53
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.43	0.53
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.90	0.53
4:E:49:ILE:O	4:E:53:GLU:HG3	2.08	0.53
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.42	0.53
5:F:261:LEU:H	5:F:261:LEU:HD12	1.74	0.53
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.41	0.53
3:J:317:THR:HG22	3:J:322:ARG:O	2.09	0.53
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.91	0.53
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.43	0.53
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.74	0.53
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.90	0.53
3:D:678:ARG:HA	6:M:129:ARG:HH22	1.74	0.53
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.91	0.53
1:H:27:THR:HB	1:H:202:VAL:HG22	1.91	0.53
1:A:221:ALA:HB1	1:B:228:LEU:HD23	1.90	0.53
2:C:1116:HIS:HE1	3:D:641:ILE:N	2.03	0.53
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.09	0.53
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.74	0.53
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.08	0.53
2:I:1321:GLU:OE2	3:J:99:ARG:HD3	2.09	0.53
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.91	0.53
3:J:1326:GLN:HB3	3:J:1330:ARG:NH2	2.24	0.53
5:L:612:ASP:N	5:L:612:ASP:OD1	2.42	0.53
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.91	0.52
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.90	0.52
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.91	0.52
5:L:139:GLU:HG2	5:L:351:THR:HA	1.90	0.52
5:L:137:TYR:CE1	5:L:351:THR:HB	2.45	0.52
3:D:197:GLU:O	3:D:201:LEU:HG	2.09	0.52
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.90	0.52
1:G:137:ASN:N	1:G:137:ASN:OD1	2.42	0.52
3:J:268:LEU:HD11	3:J:324:LEU:HD13	1.90	0.52
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.29	0.52
3:D:932:MET:HA	3:D:1138:LEU:HB3	1.91	0.52
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.74	0.52
3:D:1372:ARG:HG3	3:J:853:THR:HB	1.91	0.52
1:A:45:ARG:HG3	1:A:46:ILE:HD13	1.90	0.52
2:C:714:VAL:HG12	2:C:765:ILE:HD12	1.91	0.52
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.92	0.52
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.45	0.52
1:A:115:ILE:HG22	1:A:116:THR:H	1.73	0.52
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.43	0.52
2:C:721:GLY:N	2:C:740:GLU:OE1	2.35	0.52
2:C:998:LEU:HD12	2:C:998:LEU:H	1.74	0.52
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.92	0.52
5:F:279:ARG:NH2	5:F:350:GLU:OE2	2.36	0.52
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.92	0.52
2:I:411:ARG:NH2	2:I:424:ASP:OD1	2.38	0.52
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:891:GLY:O	2:I:892:GLU:HG3	2.10	0.52
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.91	0.52
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.55	0.52
2:I:169:LYS:O	2:I:170:VAL:HG22	2.09	0.52
3:J:850:LYS:HE2	3:J:855:ASP:HB3	1.92	0.52
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.92	0.52
4:E:46:THR:HA	4:E:49:ILE:HB	1.91	0.52
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.92	0.52
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.09	0.52
3:J:449:LEU:HD22	3:J:466:MET:SD	2.50	0.52
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.45	0.52
1:A:14:VAL:HG22	1:A:15:ASP:N	2.25	0.52
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.92	0.52
2:C:252:SER:H	2:C:255:ILE:HD11	1.75	0.52
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.92	0.52
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.74	0.52
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.09	0.52
2:I:38:PHE:HB2	2:I:457:GLY:HA2	1.91	0.52
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.91	0.52
3:J:903:LEU:HD23	3:J:905:ARG:HD3	1.92	0.52
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.33	0.52
1:A:112:ALA:O	1:A:115:ILE:HG13	2.10	0.52
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.75	0.52
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.92	0.52
1:H:102:LEU:O	1:H:141:SER:HA	2.10	0.52
2:I:356:THR:HG21	2:I:362:ALA:HA	1.92	0.52
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.91	0.52
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.92	0.52
3:J:668:PHE:CD1	3:J:678:ARG:HG2	2.44	0.52
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.91	0.52
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.91	0.52
3:D:156:ARG:NH1	3:D:157:GLN:HE21	2.07	0.52
3:D:425:ARG:HG2	3:D:426:ALA:N	2.24	0.52
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.91	0.52
5:F:111:LEU:HD13	5:F:116:GLU:HA	1.92	0.52
1:G:75:GLN:HA	2:I:729:ALA:N	2.25	0.52
2:I:168:GLY:C	2:I:170:VAL:H	2.11	0.52
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.25	0.52
3:J:517:CYS:HB3	3:J:719:PHE:CE2	2.45	0.52
5:L:320:ILE:O	5:L:327:SER:HB3	2.10	0.52
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLU:HG3	2:C:107:ARG:N	2.25	0.51
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.38	0.51
2:I:920:VAL:HG22	2:I:1054:LEU:HD21	1.92	0.51
2:I:1142:ARG:HH11	2:I:1161:LEU:HD11	1.75	0.51
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.11	0.51
2:I:1282:GLY:O	2:I:1284:ALA:N	2.43	0.51
6:M:52:ARG:HB2	6:M:52:ARG:HH11	1.75	0.51
3:D:783:LEU:HD23	6:M:76:ALA:CB	2.40	0.51
2:C:941:LYS:HB2	2:C:946:LEU:HG	1.92	0.51
5:F:575:GLU:O	5:F:579:GLN:HG2	2.10	0.51
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.92	0.51
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.92	0.51
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.91	0.51
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.92	0.51
5:L:244:THR:O	5:L:247:GLU:HG2	2.10	0.51
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.10	0.51
1:B:44:ARG:HD2	1:B:183:ILE:HD13	1.92	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.45	0.51
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.24	0.51
2:C:1106:ARG:NE	3:D:731:ARG:HH21	2.08	0.51
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.91	0.51
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.92	0.51
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.92	0.51
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.93	0.51
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.75	0.51
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.76	0.51
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.92	0.51
3:D:26:SER:HB2	3:D:236:TRP:CZ2	2.45	0.51
3:D:322:ARG:HB2	3:D:322:ARG:NH1	2.26	0.51
5:F:151:VAL:HG22	5:F:156:ALA:HB3	1.92	0.51
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.92	0.51
5:L:316:PHE:HZ	5:L:334:SER:HA	1.76	0.51
1:A:66:HIS:HE1	1:A:69:SER:HB3	1.75	0.51
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.91	0.51
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.26	0.51
3:D:460:ASP:OD2	3:D:462:ASP:OD1	2.28	0.51
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.26	0.51
1:G:133:LEU:HD12	1:G:138:ALA:HB3	1.93	0.51
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.92	0.51
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.76	0.51
2:C:302:ILE:O	2:C:330:HIS:NE2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.93	0.51
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.93	0.51
5:F:399:LEU:HD22	5:F:447:ALA:HB2	1.93	0.51
5:L:476:ARG:NH1	5:L:476:ARG:HB3	2.26	0.51
2:C:106:GLU:N	2:C:109:ALA:CB	2.73	0.51
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.93	0.51
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.25	0.51
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.38	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.51
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.46	0.51
3:J:504:GLN:HG3	3:J:505:ASP:H	1.76	0.51
1:B:51:MET:HE2	1:B:220:ALA:HB2	1.93	0.51
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.41	0.51
2:C:80:PHE:HB3	2:C:84:GLU:HB2	1.92	0.51
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.93	0.51
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.75	0.51
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.76	0.51
1:B:186:ASN:HD22	1:B:202:VAL:HB	1.76	0.50
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.10	0.50
2:C:515:MET:HG2	2:C:517:GLN:HB2	1.93	0.50
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.20	0.50
2:I:596:ASP:CG	2:I:597:GLY:N	2.64	0.50
2:I:706:ARG:NH2	2:I:791:LEU:O	2.44	0.50
5:L:137:TYR:HE1	5:L:351:THR:HB	1.76	0.50
1:A:285:THR:OG1	1:A:286:GLU:N	2.44	0.50
3:D:110:PRO:HB3	3:D:238:ILE:CG2	2.41	0.50
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.94	0.50
3:D:528:THR:O	3:D:551:ARG:HB3	2.12	0.50
3:D:770:LEU:H	3:D:770:LEU:HD22	1.77	0.50
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.92	0.50
2:I:1061:GLN:HG3	2:I:1239:VAL:HG11	1.93	0.50
2:I:42:ASP:O	2:I:44:GLU:N	2.43	0.50
6:M:78:GLN:HG2	6:M:82:PHE:HE2	1.77	0.50
2:C:903:ARG:HE	2:C:910:ALA:HB2	1.76	0.50
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.92	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.93	0.50
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.93	0.50
2:I:921:PRO:O	2:I:924:VAL:HG22	2.11	0.50
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.92	0.50
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.94	0.50
2:C:540:ARG:HH11	2:C:540:ARG:HB2	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.94	0.50
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.30	0.50
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.93	0.50
1:G:23:HIS:HB2	1:G:205:MET:O	2.12	0.50
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.94	0.50
2:I:620:ASN:ND2	2:I:620:ASN:O	2.44	0.50
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.94	0.50
1:H:62:ASP:N	1:H:62:ASP:OD1	2.30	0.50
2:I:1247:SER:HB3	3:J:375:GLU:O	2.11	0.50
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.47	0.50
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.32	0.50
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.93	0.50
3:J:836:ARG:HD2	3:J:873:GLU:OE1	2.11	0.50
6:M:71:ASP:OD1	6:M:73:VAL:HG23	2.11	0.50
1:B:214:GLU:O	1:B:218:ARG:HG3	2.11	0.50
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.12	0.50
2:C:1282:GLY:O	2:C:1284:ALA:N	2.44	0.50
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.27	0.50
2:C:88:ARG:HH11	2:C:88:ARG:HB2	1.76	0.50
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.93	0.50
1:B:73:GLY:O	1:B:134:THR:HG22	2.12	0.50
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.93	0.50
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.94	0.50
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.93	0.50
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.76	0.50
2:I:144:VAL:HG11	2:I:527:LYS:HA	1.93	0.50
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.94	0.50
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.76	0.50
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.12	0.50
3:J:661:VAL:HG11	3:J:686:TRP:CE2	2.47	0.50
6:M:15:LEU:HD13	6:M:22:PRO:HG3	1.93	0.50
1:B:253:LEU:HB3	1:B:321:TRP:CZ2	2.47	0.50
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.52	0.50
5:F:147:GLN:HE22	5:F:150:ARG:HH11	1.58	0.50
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.94	0.50
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.92	0.50
2:I:174:ALA:N	2:I:186:PHE:O	2.44	0.50
2:I:235:ASN:O	2:I:236:LYS:CB	2.52	0.50
3:J:797:THR:O	3:J:801:VAL:HG12	2.12	0.50
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.93	0.50
2:C:1255:THR:O	2:C:1257:GLN:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:HB	2:C:138:ILE:O	2.12	0.50
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.93	0.50
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.76	0.50
3:D:317:THR:HA	3:D:324:LEU:HD23	1.93	0.50
5:F:372:ALA:O	5:F:376:LYS:HG3	2.12	0.50
2:I:445:ILE:HG23	2:I:451:ARG:HE	1.76	0.50
2:I:894:GLN:HE21	3:J:78:LEU:HD21	1.77	0.50
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.92	0.50
1:B:98:VAL:HG22	1:B:100:LEU:HD12	1.92	0.49
1:B:94:GLY:H	1:B:276:HIS:HD2	1.56	0.49
1:B:29:GLU:OE1	1:B:30:PRO:HD3	2.12	0.49
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.94	0.49
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.76	0.49
2:I:519:ASN:ND2	2:I:689:ALA:HB3	2.27	0.49
3:J:1178:THR:HA	3:J:1184:ASP:HB2	1.93	0.49
3:J:253:VAL:HG21	5:L:523:ILE:HG21	1.93	0.49
3:J:425:ARG:HG2	3:J:426:ALA:N	2.27	0.49
5:L:354:THR:O	5:L:358:VAL:HG23	2.12	0.49
2:C:13:LYS:HA	2:C:1157:GLN:OE1	2.12	0.49
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.42	0.49
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.94	0.49
2:C:730:SER:O	2:C:753:LEU:HB2	2.12	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.77	0.49
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.95	0.49
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.94	0.49
3:J:489:ASN:HA	3:J:904:ALA:CB	2.41	0.49
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.26	0.49
3:D:705:THR:OG1	3:D:718:SER:HA	2.12	0.49
5:F:453:PRO:O	5:F:456:MET:HB2	2.12	0.49
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.93	0.49
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.10	0.49
3:J:1206:ARG:NH2	3:J:1223:LEU:O	2.46	0.49
3:J:657:ALA:HA	3:J:660:GLU:HB2	1.95	0.49
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.10	0.49
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.94	0.49
2:C:1106:ARG:O	2:C:1108:ASN:N	2.44	0.49
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.12	0.49
2:C:359:ARG:NH1	2:C:382:GLU:OE2	2.46	0.49
3:D:1137:GLY:H	3:D:1140:ARG:HB3	1.77	0.49
2:I:1287:LEU:HD22	3:J:1357:ILE:HG13	1.94	0.49
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.94	0.49
2:C:563:THR:HG22	2:C:680:LEU:HD11	1.94	0.49
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.46	0.49
5:F:233:ASP:O	5:F:236:LYS:HE2	2.13	0.49
5:F:388:ILE:O	5:F:392:LYS:HG3	2.13	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.12	0.49
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.78	0.49
3:J:48:THR:C	3:J:50:LYS:H	2.11	0.49
3:J:56:LEU:HD12	3:J:56:LEU:H	1.77	0.49
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	1.95	0.49
2:C:1340:GLU:HG3	3:D:21:LYS:HB2	1.93	0.49
3:D:1243:LEU:O	6:M:63:GLN:HG2	2.12	0.49
3:D:905:ARG:NH1	4:E:16:ARG:HB2	2.27	0.49
5:F:320:ILE:HG23	5:F:327:SER:O	2.13	0.49
5:F:449:THR:OG1	5:F:503:GLU:OE1	2.31	0.49
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.13	0.49
2:C:138:ILE:O	2:C:139:ASN:ND2	2.45	0.49
3:D:1178:THR:HG23	3:D:1184:ASP:CB	2.43	0.49
3:D:16:GLU:O	3:D:1369:ARG:NH2	2.46	0.49
3:D:436:ALA:HB3	3:D:485:MET:HA	1.94	0.49
3:D:859:PRO:HD2	3:D:862:THR:HG21	1.94	0.49
3:D:1361:THR:HG22	4:E:21:LEU:HD22	1.94	0.49
5:F:316:PHE:CZ	5:F:334:SER:HA	2.48	0.49
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.95	0.49
1:G:68:TYR:HE2	2:I:927:THR:HB	1.76	0.49
1:H:151:GLY:O	1:H:177:TYR:HB2	2.12	0.49
2:I:1120:ALA:HA	2:I:1204:LEU:HD12	1.94	0.49
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.48	0.49
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.95	0.49
1:A:318:LEU:O	1:A:320:ASN:N	2.41	0.49
1:B:94:GLY:HA2	1:B:277:TYR:CE2	2.47	0.49
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.13	0.49
2:C:800:MET:HE1	2:C:822:VAL:HG13	1.94	0.49
3:D:504:GLN:HG3	3:D:505:ASP:H	1.76	0.49
4:E:3:ARG:HD2	9:E:101:G4P:H4'	1.95	0.49
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.48	0.49
3:J:115:TRP:HZ2	3:J:328:ALA:HB2	1.77	0.49
2:C:1293:VAL:HG13	2:C:1301:ARG:HA	1.95	0.49
2:C:402:ARG:NE	2:C:417:SER:O	2.46	0.49
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.13	0.49
3:D:336:GLY:HA3	3:D:1324:SER:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:460:ASP:CG	3:D:462:ASP:OD1	2.50	0.49
1:B:79:LEU:HD21	3:D:526:VAL:HG21	1.95	0.49
5:F:484:ALA:O	5:F:491:GLU:HB2	2.12	0.49
3:D:394:ILE:HG12	5:F:536:THR:HG22	1.95	0.49
5:F:600:HIS:HB3	5:F:601:PRO:CD	2.43	0.49
1:A:251:PRO:HD2	5:F:605:GLU:HG3	1.95	0.49
1:G:231:PHE:HB3	1:H:218:ARG:HB3	1.94	0.49
1:H:76:GLU:N	1:H:76:GLU:OE1	2.46	0.49
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.28	0.49
5:L:463:LEU:HA	5:L:466:ILE:HD12	1.95	0.49
1:A:257:VAL:HG13	1:A:276:HIS:O	2.13	0.49
1:A:249:PHE:CD1	1:A:321:TRP:HZ3	2.31	0.49
2:C:61:SER:O	2:C:63:SER:N	2.45	0.49
2:C:796:LEU:H	2:C:796:LEU:HD12	1.78	0.49
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.95	0.49
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.95	0.49
9:E:101:G4P:O1C	9:E:101:G4P:O2'	2.27	0.49
2:I:32:LEU:HD23	2:I:130:MET:SD	2.53	0.49
3:J:288:PRO:O	3:J:292:VAL:HG13	2.13	0.49
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.48	0.49
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.76	0.49
6:M:108:ASP:O	6:M:108:ASP:OD2	2.31	0.49
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.94	0.48
2:C:169:LYS:O	2:C:170:VAL:HG22	2.13	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.76	0.48
5:F:511:ILE:HG21	5:F:522:PHE:CE2	2.48	0.48
5:F:551:LEU:HD11	5:F:598:LEU:HD11	1.94	0.48
1:A:104:LYS:HB3	1:A:110:VAL:HG13	1.95	0.48
2:C:145:ILE:HA	2:C:511:LEU:O	2.13	0.48
2:C:228:VAL:HG22	2:C:245:ARG:HE	1.78	0.48
3:D:53:ARG:HA	3:D:54:ASP:HA	1.56	0.48
4:E:4:VAL:HG13	4:E:5:THR:N	2.28	0.48
5:F:127:ILE:O	5:F:130:VAL:HG22	2.13	0.48
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.28	0.48
5:L:478:PRO:HG2	5:L:483:LEU:HD11	1.95	0.48
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.48	0.48
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.79	0.48
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.48	0.48
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.94	0.48
5:L:469:GLN:O	5:L:473:GLU:HB2	2.12	0.48
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.94	0.48
2:C:1293:VAL:HG11	2:C:1304:MET:HG2	1.95	0.48
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.44	0.48
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.95	0.48
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.94	0.48
2:I:314:ASN:O	2:I:352:ARG:NH1	2.46	0.48
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.43	0.48
3:D:1227:HIS:HB2	3:J:1293:GLU:OE1	2.14	0.48
3:J:88:CYS:O	3:J:90:VAL:N	2.47	0.48
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.70	0.48
1:B:195:ARG:HG3	1:B:198:LEU:HD11	1.96	0.48
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.48	0.48
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.96	0.48
1:H:59:VAL:O	1:H:171:LEU:HB2	2.13	0.48
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.13	0.48
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.44	0.48
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.95	0.48
2:I:903:ARG:HD2	2:I:908:GLU:O	2.13	0.48
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.25	0.48
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.28	0.48
1:A:224:LEU:O	1:A:228:LEU:HD12	2.14	0.48
1:A:23:HIS:HE1	1:A:204:GLU:CG	2.25	0.48
5:F:555:GLU:O	5:F:559:LEU:HB2	2.14	0.48
2:I:518:ASN:O	2:I:691:PRO:HD3	2.13	0.48
1:A:135:ASP:O	1:A:138:ALA:N	2.33	0.48
1:A:220:ALA:O	1:A:223:ILE:HG13	2.14	0.48
2:C:202:ARG:HB2	2:C:369:MET:HG2	1.94	0.48
2:C:47:TYR:OH	2:C:398:SER:HB2	2.12	0.48
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.29	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.78	0.48
3:J:131:PRO:O	3:J:135:ILE:HG13	2.13	0.48
5:L:287:ILE:HD13	5:L:315:TRP:CH2	2.48	0.48
1:B:44:ARG:HE	3:D:538:ARG:HB3	1.79	0.48
1:B:65:LEU:O	1:B:66:HIS:ND1	2.46	0.48
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.45	0.48
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.49	0.48
1:G:13:LEU:H	1:G:13:LEU:HD23	1.78	0.48
2:I:156:PHE:CD2	2:I:175:ARG:HB3	2.48	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.96	0.48
3:J:679:TYR:O	3:J:683:ILE:HG13	2.13	0.48
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1063:GLY:HA3	2:C:1239:VAL:HB	1.95	0.48
2:C:802:VAL:HG11	2:C:1230:MET:HB3	1.96	0.48
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.95	0.48
1:G:140:ILE:O	1:G:140:ILE:HG13	2.14	0.48
3:J:156:ARG:NH2	3:J:191:SER:OG	2.45	0.48
6:M:55:VAL:O	6:M:59:VAL:HG23	2.13	0.48
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.95	0.48
3:D:227:PHE:O	3:D:230:SER:HB3	2.13	0.48
5:F:470:MET:O	5:F:478:PRO:HD3	2.14	0.48
2:I:1086:PRO:HB3	2:I:1212:LEU:HD23	1.95	0.48
2:I:1281:TYR:OH	3:J:434:ILE:O	2.32	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.14	0.48
3:D:746:LEU:O	6:M:84:LEU:HD13	2.14	0.48
2:C:1124:ILE:HG21	2:C:1180:MET:HE2	1.94	0.47
2:C:131:THR:OG1	2:C:135:THR:O	2.32	0.47
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.29	0.47
2:C:27:LEU:O	2:C:528:ARG:NH1	2.46	0.47
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.96	0.47
5:F:253:SER:O	5:F:257:LYS:HG3	2.14	0.47
5:L:308:GLY:HA2	5:L:356:GLU:OE1	2.14	0.47
3:D:11:GLN:HG2	3:D:15:GLU:CD	2.34	0.47
3:D:365:GLN:O	3:D:437:PHE:HD1	1.97	0.47
1:G:76:GLU:OE2	1:G:76:GLU:N	2.47	0.47
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.96	0.47
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.96	0.47
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.80	0.47
3:J:848:VAL:HG12	3:J:857:LEU:CD1	2.44	0.47
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.95	0.47
1:A:295:LEU:HD22	1:A:300:LEU:HD23	1.97	0.47
2:C:201:ARG:NH2	2:C:370:MET:O	2.47	0.47
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.39	0.47
5:F:608:ARG:HH11	5:F:608:ARG:HB2	1.79	0.47
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.94	0.47
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.44	0.47
2:I:239:MET:N	2:I:285:ILE:O	2.45	0.47
2:I:1286:THR:N	3:J:479:GLU:OE2	2.42	0.47
3:J:656:GLU:OE1	3:J:692:ARG:NH2	2.41	0.47
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.96	0.47
3:D:478:LEU:HG	4:E:47:THR:HG23	1.97	0.47
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.97	0.47
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1221:LEU:HB2	3:J:1229:VAL:HG11	1.95	0.47
6:M:144:ILE:HG23	6:M:147:LYS:HE2	1.96	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.49	0.47
3:D:27:PRO:O	3:D:31:ARG:HG3	2.13	0.47
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.47	0.47
3:D:614:LEU:HD22	4:E:7:GLN:HB2	1.97	0.47
1:H:18:GLN:HA	1:H:24:ALA:HA	1.95	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.46	0.47
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.96	0.47
1:B:104:LYS:HG3	1:B:105:SER:N	2.29	0.47
1:B:270:LEU:HD22	1:B:275:ILE:HG21	1.96	0.47
1:B:29:GLU:OE1	1:B:30:PRO:CD	2.62	0.47
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.97	0.47
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.45	0.47
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.44	0.47
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.94	0.47
3:D:638:SER:OG	3:D:639:VAL:N	2.47	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.97	0.47
5:F:130:VAL:HB	5:F:365:MET:HG3	1.97	0.47
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.96	0.47
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.79	0.47
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.30	0.47
2:I:518:ASN:N	2:I:518:ASN:OD1	2.47	0.47
2:I:601:ASP:OD1	2:I:601:ASP:N	2.46	0.47
3:J:337:ARG:NH2	3:J:1323:ALA:HB3	2.29	0.47
3:J:53:ARG:HA	3:J:54:ASP:HA	1.52	0.47
5:L:353:LEU:HD13	5:L:361:ILE:HD12	1.96	0.47
3:D:674:THR:CG2	6:M:139:LYS:HG2	2.43	0.47
1:B:112:ALA:O	1:B:115:ILE:HG13	2.15	0.47
1:B:82:LEU:HD22	1:B:173:VAL:HG12	1.97	0.47
1:B:215:GLU:HA	1:B:218:ARG:HD2	1.95	0.47
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.14	0.47
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.97	0.47
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.96	0.47
3:D:405:GLU:O	3:D:408:VAL:HG22	2.15	0.47
3:D:689:ALA:O	3:D:693:VAL:HG23	2.15	0.47
4:E:2:ALA:HB2	4:E:55:GLU:OE1	2.15	0.47
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.97	0.47
1:G:231:PHE:HA	1:H:218:ARG:HG2	1.97	0.47
2:I:119:GLU:HG3	2:I:489:PRO:CD	2.40	0.47
3:J:214:ARG:HA	3:J:217:LEU:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:275:ARG:HG2	3:J:278:ARG:HH12	1.80	0.47
3:J:355:ILE:HG21	3:J:466:MET:CG	2.45	0.47
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.44	0.47
5:L:114:GLU:O	5:L:117:ILE:N	2.43	0.47
5:L:395:THR:OG1	5:L:396:ASN:N	2.47	0.47
1:B:61:ILE:HG23	1:B:142:MET:HE2	1.97	0.47
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.95	0.47
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.50	0.47
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.29	0.47
1:H:100:LEU:HB3	1:H:115:ILE:CG2	2.45	0.47
3:J:337:ARG:HD2	3:J:1324:SER:HA	1.97	0.47
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.96	0.47
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.97	0.47
5:L:483:LEU:HD12	5:L:483:LEU:H	1.79	0.47
5:L:561:MET:HA	5:L:567:MET:CE	2.45	0.47
1:A:95:LYS:O	1:A:148:ARG:NH2	2.47	0.47
1:B:224:LEU:O	1:B:228:LEU:HD12	2.15	0.47
2:C:155:VAL:HA	2:C:175:ARG:O	2.15	0.47
2:C:325:LEU:O	2:C:330:HIS:HB2	2.15	0.47
3:D:99:ARG:HG3	3:D:249:LEU:HD21	1.97	0.47
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.96	0.47
2:I:1296:ASP:CG	2:I:1322:SER:HB3	2.35	0.47
2:I:384:LEU:O	2:I:388:LEU:HG	2.14	0.47
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.14	0.47
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.97	0.47
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.44	0.47
5:L:489:MET:O	5:L:491:GLU:N	2.47	0.47
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.50	0.47
2:C:620:ASN:ND2	2:C:620:ASN:O	2.47	0.47
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.96	0.47
3:D:43:THR:OG1	5:F:449:THR:O	2.20	0.47
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.96	0.47
1:H:91:ARG:HD2	1:H:210:THR:HB	1.97	0.47
2:I:963:GLU:O	2:I:967:LEU:HB2	2.14	0.47
2:I:1251:TYR:OH	3:J:348:ASP:OD2	2.20	0.47
3:J:678:ARG:O	3:J:682:VAL:HG23	2.15	0.47
3:J:705:THR:OG1	3:J:718:SER:HA	2.14	0.47
5:L:515:GLU:HG2	5:L:516:ASP:H	1.79	0.47
6:M:44:LEU:CD2	6:M:99:ILE:HG23	2.43	0.47
3:D:1239:ASP:O	3:D:1243:LEU:HB2	2.14	0.47
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:598:LYS:O	3:D:601:ILE:HG22	2.14	0.47
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.55	0.47
3:J:268:LEU:CB	3:J:306:LEU:HD23	2.44	0.47
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.80	0.47
1:A:18:GLN:HE22	1:A:213:PRO:HD2	1.79	0.46
2:C:119:GLU:HG3	2:C:489:PRO:HD2	1.96	0.46
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.80	0.46
2:C:338:THR:HG22	2:C:345:PRO:HB3	1.97	0.46
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.97	0.46
3:D:491:LEU:HD22	3:D:496:GLY:O	2.15	0.46
2:I:690:VAL:HB	2:I:1236:ASN:HB3	1.97	0.46
2:I:1313:HIS:HB2	3:J:474:LEU:HD13	1.97	0.46
3:J:694:SER:O	3:J:698:MET:HB2	2.15	0.46
5:L:343:LYS:O	5:L:347:ILE:HG13	2.15	0.46
2:C:106:GLU:HB2	2:C:109:ALA:HB2	1.82	0.46
2:C:739:ASP:OD1	2:C:739:ASP:N	2.48	0.46
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.97	0.46
3:D:556:GLU:O	3:D:564:VAL:HB	2.15	0.46
3:D:850:LYS:HG2	3:D:857:LEU:HD11	1.95	0.46
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.97	0.46
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.73	0.46
3:J:809:VAL:HA	3:J:894:VAL:O	2.14	0.46
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.30	0.46
5:L:584:ARG:HA	5:L:584:ARG:HD2	1.71	0.46
1:B:250:ASP:OD1	1:B:252:ILE:HB	2.16	0.46
1:B:281:LEU:HD11	1:B:303:ILE:HG21	1.97	0.46
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.67	0.46
2:C:518:ASN:OD1	2:C:518:ASN:N	2.48	0.46
3:D:680:ASN:HB2	9:M:202:G4P:C2	2.45	0.46
3:D:786:THR:CG2	6:M:75:ARG:HG2	2.45	0.46
5:F:138:PRO:HD2	5:F:353:LEU:HD11	1.97	0.46
5:F:600:HIS:CB	5:F:601:PRO:CD	2.93	0.46
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.97	0.46
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.80	0.46
2:I:979:LEU:HA	2:I:1002:LEU:HD13	1.97	0.46
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.97	0.46
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.50	0.46
3:J:826:ILE:HD12	3:J:826:ILE:O	2.15	0.46
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.19	0.46
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.97	0.46
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:26:ARG:NH2	4:E:38:LEU:HD13	2.30	0.46
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.62	0.46
2:C:902:LEU:HD12	5:F:607:LEU:HD23	1.98	0.46
3:D:677:GLU:CG	6:M:129:ARG:NH1	2.79	0.46
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.16	0.46
2:C:468:LEU:O	2:C:471:VAL:HG12	2.16	0.46
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.45	0.46
3:D:356:THR:OG1	3:D:357:VAL:N	2.48	0.46
3:D:500:ILE:O	3:D:500:ILE:HG22	2.15	0.46
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.98	0.46
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.97	0.46
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.46	0.46
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.96	0.46
3:J:495:ASN:C	3:J:497:GLU:H	2.19	0.46
3:J:657:ALA:O	3:J:661:VAL:HG13	2.15	0.46
2:C:147:SER:OG	2:C:455:SER:HB3	2.16	0.46
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.60	0.46
3:D:797:THR:O	3:D:801:VAL:HG12	2.15	0.46
3:D:826:ILE:HD12	3:D:826:ILE:O	2.15	0.46
4:E:2:ALA:HB2	4:E:55:GLU:CD	2.36	0.46
3:J:1167:LYS:HG2	3:J:1168:GLU:H	1.80	0.46
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.46
3:J:748:ALA:O	3:J:777:HIS:HD2	1.97	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.31	0.46
1:A:135:ASP:HB2	2:C:726:TYR:HE1	1.80	0.46
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.50	0.46
1:B:185:TYR:HA	1:B:202:VAL:O	2.15	0.46
2:C:928:VAL:HG22	2:C:1054:LEU:HD11	1.98	0.46
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.23	0.46
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.27	0.46
1:G:104:LYS:HG2	1:G:110:VAL:HG13	1.98	0.46
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.44	0.46
2:I:109:ALA:HB1	2:I:110:PRO:HD2	1.97	0.46
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.98	0.46
5:L:147:GLN:O	5:L:151:VAL:HG23	2.16	0.46
1:B:115:ILE:HG22	1:B:116:THR:N	2.29	0.46
1:B:94:GLY:HA2	1:B:277:TYR:HE2	1.81	0.46
3:D:899:TYR:CD1	3:D:915:ILE:HD12	2.51	0.46
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.97	0.46
3:J:255:LEU:HD13	3:J:255:LEU:HA	1.84	0.46
3:J:398:LYS:HE2	5:L:532:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:15:ASN:C	4:K:17:PHE:H	2.20	0.46
3:J:478:LEU:HG	4:K:47:THR:HG23	1.97	0.46
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.46	0.46
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.46	0.46
3:J:57:PHE:CE2	3:J:252:LEU:HD12	2.51	0.46
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.31	0.46
3:J:700:ASN:O	3:J:704:GLU:HB2	2.16	0.46
3:J:901:ARG:HD2	3:J:906:GLY:O	2.15	0.46
6:M:18:ALA:C	6:M:20:VAL:H	2.19	0.46
1:A:223:ILE:HD13	1:B:8:PHE:HE2	1.81	0.46
1:B:187:VAL:HG13	1:B:200:LYS:O	2.16	0.46
2:C:882:ILE:H	2:C:882:ILE:HD12	1.82	0.46
5:F:525:ASP:CG	5:F:528:LEU:HG	2.36	0.46
2:I:673:HIS:O	2:I:1109:ILE:HG22	2.16	0.46
2:I:151:ARG:NH1	2:I:542:ARG:HH12	2.13	0.46
2:I:818:VAL:HB	2:I:1076:ILE:HD11	1.98	0.46
3:J:227:PHE:O	3:J:230:SER:HB3	2.16	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.16	0.46
3:J:479:GLU:CG	4:K:20:VAL:HG11	2.46	0.46
1:A:72:GLU:OE2	2:C:958:LYS:NZ	2.40	0.45
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.81	0.45
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.81	0.45
3:J:803:VAL:HG22	3:J:1259:GLN:HB3	1.98	0.45
1:B:182:ARG:HG2	1:B:183:ILE:N	2.31	0.45
2:C:979:LEU:HD21	2:C:1000:LEU:HD13	1.98	0.45
2:C:820:GLU:N	2:C:1080:ASN:O	2.48	0.45
5:F:226:ALA:O	5:F:229:VAL:HG22	2.16	0.45
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.98	0.45
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.97	0.45
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.28	0.45
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.81	0.45
2:I:478:ARG:NH2	2:I:487:LEU:HD13	2.31	0.45
2:I:617:ALA:HA	2:I:636:CYS:SG	2.56	0.45
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.98	0.45
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.32	0.45
2:I:807:TRP:HE1	2:I:1086:PRO:HD3	1.81	0.45
6:M:91:ARG:NH1	9:M:202:G4P:O2'	2.48	0.45
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.81	0.45
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.98	0.45
3:D:81:ARG:C	3:D:83:VAL:H	2.20	0.45
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:VAL:O	5:F:167:ASP:HB2	2.16	0.45
2:I:802:VAL:HG11	2:I:1230:MET:HB3	1.98	0.45
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.16	0.45
3:J:1293:GLU:HB3	3:J:1294:ALA:H	1.56	0.45
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.30	0.45
3:J:366:CYS:HB3	3:J:437:PHE:CD1	2.51	0.45
3:J:678:ARG:HG3	3:J:679:TYR:N	2.31	0.45
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.99	0.45
1:B:321:TRP:CG	1:B:321:TRP:O	2.70	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.98	0.45
2:C:691:PRO:HA	2:C:788:SER:OG	2.15	0.45
1:H:67:GLU:O	1:H:78:ILE:HB	2.16	0.45
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.99	0.45
2:I:156:PHE:HD2	2:I:175:ARG:HB3	1.79	0.45
3:J:905:ARG:HH12	4:K:10:VAL:HG11	1.81	0.45
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.51	0.45
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.67	0.45
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.31	0.45
3:J:649:LYS:O	3:J:653:ILE:HG13	2.15	0.45
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	2.16	0.45
5:L:247:GLU:O	5:L:251:LYS:HG3	2.16	0.45
5:L:253:SER:O	5:L:257:LYS:HG3	2.16	0.45
2:I:900:LYS:HB3	5:L:563:PHE:HD1	1.82	0.45
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.49	0.45
2:C:106:GLU:HB3	2:C:109:ALA:CA	2.43	0.45
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.81	0.45
3:D:342:LEU:HA	3:D:343:LEU:HA	1.72	0.45
5:F:608:ARG:HH11	5:F:608:ARG:CG	2.30	0.45
2:I:50:GLU:OE1	2:I:54:ARG:NE	2.44	0.45
2:I:836:LEU:HB3	2:I:918:LEU:HD11	1.98	0.45
3:J:801:VAL:O	3:J:805:GLN:HB2	2.17	0.45
4:K:49:ILE:O	4:K:53:GLU:HG3	2.17	0.45
5:L:166:VAL:O	5:L:167:ASP:HB2	2.15	0.45
1:A:195:ARG:HD2	1:A:196:THR:H	1.81	0.45
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.71	0.45
1:B:151:GLY:HA2	1:B:178:SER:HB3	1.98	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
2:C:236:LYS:HA	2:C:236:LYS:HD3	1.76	0.45
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.45
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.99	0.45
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.98	0.45
3:D:905:ARG:CZ	3:D:910:ASN:HD21	2.29	0.45
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.99	0.45
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.81	0.45
3:J:115:TRP:HE1	3:J:308:ASP:HB2	1.82	0.45
3:J:598:LYS:O	3:J:601:ILE:HG22	2.17	0.45
5:L:511:ILE:HG21	5:L:522:PHE:CE2	2.52	0.45
1:B:321:TRP:N	1:B:322:PRO:CD	2.80	0.45
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.52	0.45
2:C:744:GLY:C	2:C:746:ALA:H	2.20	0.45
3:D:682:VAL:O	3:D:685:ILE:HG12	2.17	0.45
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.98	0.45
2:I:1270:PHE:CZ	2:I:1290:MET:HG2	2.52	0.45
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.46	0.45
1:B:35:PHE:HA	1:B:38:THR:HB	1.99	0.45
2:C:587:LEU:HA	2:C:587:LEU:HD23	1.73	0.45
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.81	0.45
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.99	0.45
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.99	0.45
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.99	0.45
2:I:39:ILE:HA	2:I:49:LEU:HD12	1.99	0.45
3:J:331:ILE:O	3:J:337:ARG:HA	2.17	0.45
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.81	0.45
6:M:25:GLU:OE2	6:M:123:ILE:HB	2.17	0.45
1:A:282:VAL:O	1:A:315:GLY:N	2.50	0.45
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.99	0.45
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.51	0.45
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.31	0.45
2:C:73:TYR:HA	2:C:98:VAL:HA	1.98	0.45
3:D:1283:SER:O	3:D:1286:LYS:N	2.49	0.45
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.52	0.45
5:F:324:LYS:HB3	5:F:325:PRO:HD2	1.99	0.45
5:F:452:ILE:HG13	5:F:457:ILE:HG13	1.99	0.45
1:H:219:ARG:HA	1:H:222:THR:HB	1.98	0.45
2:I:961:SER:O	2:I:965:GLN:N	2.40	0.45
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.99	0.45
3:J:449:LEU:HD21	3:J:457:TYR:CD2	2.52	0.45
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.97	0.45
1:B:228:LEU:HA	1:B:231:PHE:HD2	1.82	0.44
1:B:253:LEU:HB2	1:B:321:TRP:HE1	1.81	0.44
1:B:65:LEU:HA	1:B:65:LEU:HD23	1.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1285:TYR:CE1	3:D:475:GLU:HG2	2.52	0.44
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.99	0.44
2:C:565:GLU:HG2	2:C:565:GLU:O	2.16	0.44
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.99	0.44
3:D:122:SER:O	3:D:126:LEU:HG	2.18	0.44
1:H:107:ILE:HG12	1:H:136:GLU:O	2.16	0.44
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.98	0.44
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.72	0.44
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.98	0.44
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.76	0.44
3:J:761:ALA:H	3:J:771:GLN:NE2	2.15	0.44
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.69	0.44
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.99	0.44
2:C:514:PHE:HB3	2:C:760:ASN:HD22	1.82	0.44
3:D:159:ILE:HG13	3:D:159:ILE:O	2.16	0.44
2:I:960:LEU:HB3	2:I:1025:PHE:CE2	2.52	0.44
2:I:1082:ILE:H	2:I:1082:ILE:CD1	2.27	0.44
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.48	0.44
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.48	0.44
1:A:76:GLU:N	1:A:76:GLU:OE2	2.51	0.44
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.17	0.44
2:C:122:VAL:HG23	5:F:472:GLN:HG3	2.00	0.44
2:C:290:GLU:HG2	2:C:319:LEU:CD1	2.47	0.44
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.44
2:C:5:TYR:O	2:C:8:LYS:HG2	2.17	0.44
2:C:73:TYR:CB	2:C:98:VAL:HG22	2.47	0.44
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.87	0.44
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.17	0.44
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.99	0.44
3:D:707:ILE:HD12	3:D:707:ILE:H	1.83	0.44
2:I:198:ILE:HD13	2:I:388:LEU:HD13	1.99	0.44
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.52	0.44
2:I:710:VAL:HG13	2:I:717:VAL:HG21	2.00	0.44
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.98	0.44
5:L:148:TYR:OH	5:L:218:ARG:HA	2.18	0.44
5:L:314:THR:O	5:L:318:ALA:HB3	2.18	0.44
1:B:212:ASP:O	1:B:215:GLU:N	2.50	0.44
2:C:541:GLU:N	2:C:541:GLU:OE1	2.49	0.44
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.83	0.44
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.51	0.44
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:588:GLU:HB3	2:I:607:SER:HA	1.99	0.44
2:I:61:SER:O	2:I:63:SER:N	2.50	0.44
3:J:1349:GLU:N	3:J:1349:GLU:OE2	2.35	0.44
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.74	0.44
1:B:290:LEU:HB3	1:B:291:LYS:HE2	1.98	0.44
2:C:1083:GLU:HG3	2:C:1083:GLU:H	1.60	0.44
2:C:657:THR:HG21	2:C:1188:ASP:HB2	2.00	0.44
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.16	0.44
3:D:334:LYS:HA	3:D:335:GLN:HA	1.80	0.44
3:D:494:ALA:CB	3:D:922:SER:HB3	2.48	0.44
1:H:100:LEU:HB3	1:H:115:ILE:HG22	1.99	0.44
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.50	0.44
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.83	0.44
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.52	0.44
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.99	0.44
3:J:905:ARG:NH1	4:K:10:VAL:HG11	2.31	0.44
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.18	0.44
5:L:143:TYR:CZ	5:L:268:TYR:CE2	3.04	0.44
1:A:228:LEU:CD1	1:B:224:LEU:HD23	2.40	0.44
2:C:161:LYS:HA	2:C:170:VAL:HA	1.99	0.44
2:C:725:GLN:HE22	2:C:966:ILE:HG23	1.82	0.44
3:D:418:GLU:OE1	4:E:3:ARG:NH2	2.48	0.44
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.32	0.44
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.38	0.44
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.98	0.44
2:I:800:MET:HE2	2:I:1095:ASP:HB3	2.00	0.44
2:I:55:SER:OG	2:I:56:VAL:N	2.50	0.44
2:I:93:SER:HA	2:I:128:PRO:HA	2.00	0.44
2:I:1332:SER:HA	3:J:243:PRO:HB2	1.99	0.44
5:L:476:ARG:HH11	5:L:477:GLU:H	1.66	0.44
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	2.00	0.44
2:C:238:GLN:HG2	2:C:286:GLU:HA	2.00	0.44
2:C:533:LEU:HD11	2:C:568:ASN:HD22	1.83	0.44
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.83	0.44
2:C:963:GLU:O	2:C:967:LEU:HB2	2.18	0.44
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.99	0.44
2:I:678:ARG:CG	2:I:1108:ASN:HD22	2.28	0.44
2:I:250:THR:HA	2:I:268:ARG:HA	2.00	0.44
3:J:659:ALA:O	3:J:663:GLU:HG3	2.18	0.44
3:J:825:VAL:C	3:J:826:ILE:HG13	2.38	0.44
5:L:476:ARG:HH11	5:L:476:ARG:HB3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.98	0.44
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.53	0.44
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.00	0.44
1:H:147:GLN:HG3	1:H:148:ARG:H	1.83	0.44
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.33	0.44
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.82	0.44
5:L:470:MET:HB2	5:L:478:PRO:HG3	2.00	0.44
1:A:168:ILE:H	1:A:168:ILE:HG12	1.68	0.44
1:A:315:GLY:C	1:A:316:MET:HG3	2.38	0.44
2:C:169:LYS:HE2	2:C:190:PRO:HA	2.00	0.44
2:C:87:ILE:H	2:C:87:ILE:HG13	1.61	0.44
1:G:100:LEU:HD23	1:G:115:ILE:HG21	2.00	0.44
1:G:166:ARG:O	1:G:167:PRO:C	2.56	0.44
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.82	0.44
2:I:201:ARG:NH2	2:I:370:MET:O	2.37	0.44
2:I:541:GLU:N	2:I:541:GLU:OE1	2.48	0.44
2:I:543:ALA:HA	2:I:544:GLY:HA3	1.71	0.44
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.99	0.44
6:M:70:PRO:HG2	6:M:78:GLN:OE1	2.18	0.44
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.47	0.43
2:C:1240:ASP:OD1	2:C:1240:ASP:N	2.45	0.43
2:C:462:ASN:O	2:C:466:VAL:HG23	2.18	0.43
2:C:716:ALA:HB3	2:C:784:ALA:HB3	2.00	0.43
3:D:1273:ASP:O	3:D:1275:LEU:N	2.47	0.43
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.18	0.43
3:D:850:LYS:HB2	3:D:852:GLY:O	2.18	0.43
5:F:320:ILE:HG21	5:F:331:HIS:CD2	2.53	0.43
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.47	0.43
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.33	0.43
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.00	0.43
2:I:565:GLU:HG2	2:I:565:GLU:O	2.17	0.43
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.17	0.43
3:J:587:LEU:HD23	3:J:591:ILE:HG21	2.00	0.43
5:L:320:ILE:HG23	5:L:327:SER:O	2.16	0.43
1:A:266:SER:HB3	1:A:303:ILE:HD11	2.00	0.43
1:B:262:LEU:H	1:B:262:LEU:HD12	1.82	0.43
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.18	0.43
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.99	0.43
1:G:67:GLU:OE1	2:I:1057:LYS:NZ	2.52	0.43
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.18	0.43
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.83	0.43
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.48	0.43
1:B:286:GLU:OE2	1:B:304:LYS:NZ	2.46	0.43
2:C:1282:GLY:H	3:D:483:LEU:HD13	1.83	0.43
5:F:101:TYR:CE2	5:F:388:ILE:HD11	2.43	0.43
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.86	0.43
2:I:1308:ILE:CG2	3:J:379:PRO:HB2	2.47	0.43
2:I:850:ILE:O	2:I:850:ILE:HG22	2.18	0.43
3:J:358:GLY:N	3:J:359:PRO:HD3	2.32	0.43
5:L:573:LEU:H	5:L:573:LEU:CD2	2.25	0.43
6:M:65:GLU:HB3	6:M:82:PHE:HZ	1.82	0.43
1:A:158:ARG:HH22	1:A:172:LEU:HD23	1.82	0.43
1:B:16:ILE:HG12	1:B:26:VAL:HG13	2.00	0.43
2:C:867:GLU:H	2:C:867:GLU:HG3	1.39	0.43
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.99	0.43
3:D:347:VAL:HG12	3:D:348:ASP:O	2.18	0.43
3:D:680:ASN:O	3:D:683:ILE:HG22	2.19	0.43
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.43
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.43
3:J:128:LEU:HB3	3:J:157:GLN:HE22	1.83	0.43
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.91	0.43
3:J:311:ARG:O	3:J:312:ARG:HD3	2.18	0.43
3:J:342:LEU:HA	3:J:343:LEU:HA	1.71	0.43
3:J:385:LEU:CD2	3:J:411:ILE:HG13	2.48	0.43
3:J:804:ALA:O	3:J:806:ASP:N	2.51	0.43
3:D:674:THR:HG22	6:M:136:ILE:HD12	2.01	0.43
6:M:78:GLN:HG2	6:M:82:PHE:CE2	2.54	0.43
2:C:338:THR:CG2	2:C:345:PRO:HB3	2.49	0.43
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.53	0.43
3:D:215:LYS:HE2	3:D:215:LYS:HB3	1.86	0.43
3:D:201:LEU:CD1	3:D:220:ARG:HG2	2.49	0.43
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.78	0.43
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.83	0.43
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	2.01	0.43
3:J:159:ILE:O	3:J:159:ILE:HG13	2.17	0.43
3:J:513:MET:O	3:J:575:GLY:HA3	2.18	0.43
3:J:850:LYS:HB2	3:J:852:GLY:O	2.18	0.43
2:C:13:LYS:HD3	2:C:1149:TYR:HA	2.00	0.43
2:C:323:ALA:O	2:C:327:GLN:HG3	2.18	0.43
2:C:980:VAL:HA	2:C:984:VAL:HA	2.01	0.43
3:D:505:ASP:HB3	3:D:629:PHE:CE1	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.00	0.43
4:E:19:LEU:HD13	4:E:54:ILE:HG21	1.99	0.43
5:F:320:ILE:O	5:F:327:SER:HB3	2.18	0.43
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.81	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.01	0.43
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.00	0.43
2:I:29:SER:O	2:I:33:ASP:HB2	2.19	0.43
2:I:9:LYS:O	2:I:1175:ASN:ND2	2.49	0.43
3:J:689:ALA:O	3:J:693:VAL:HG23	2.19	0.43
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.68	0.43
1:A:49:SER:O	1:A:51:MET:N	2.47	0.43
1:B:151:GLY:O	1:B:177:TYR:N	2.51	0.43
1:B:155:ALA:H	1:B:174:ASP:HA	1.84	0.43
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.39	0.43
3:D:1165:PHE:CE1	3:D:1200:GLU:HB2	2.52	0.43
2:C:1243:MET:HA	3:D:353:SER:HB3	2.01	0.43
3:D:56:LEU:H	3:D:56:LEU:HD12	1.83	0.43
3:D:258:GLY:HA3	5:F:499:LYS:HE2	2.00	0.43
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.99	0.43
2:I:1066:MET:CE	2:I:1076:ILE:HB	2.49	0.43
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.49	0.43
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.43	0.43
3:J:263:SER:HA	5:L:507:MET:HB2	2.01	0.43
3:J:364:HIS:CE1	4:K:3:ARG:NH2	2.84	0.43
3:J:609:TYR:HA	3:J:617:THR:OG1	2.18	0.43
3:D:681:LYS:NZ	6:M:14:ILE:HD12	2.33	0.43
1:A:195:ARG:HD2	1:A:196:THR:N	2.34	0.43
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	2.00	0.43
5:F:141:ILE:HG21	5:F:228:TYR:CD1	2.53	0.43
5:F:354:THR:O	5:F:358:VAL:HG23	2.19	0.43
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	2.01	0.43
2:I:1340:GLU:CG	3:J:21:LYS:HB2	2.49	0.43
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.99	0.43
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.52	0.43
6:M:93:ARG:O	6:M:97:LYS:HG2	2.19	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.83	0.43
1:A:232:VAL:O	1:B:218:ARG:HG2	2.18	0.43
1:A:44:ARG:HE	1:A:183:ILE:HG22	1.83	0.43
2:C:1002:LEU:HD22	2:C:1007:LYS:CB	2.43	0.43
2:C:88:ARG:NH1	2:C:88:ARG:HB2	2.34	0.43
3:D:823:THR:HA	3:D:835:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:281:ARG:HD3	5:F:285:ARG:NH1	2.33	0.43
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.49	0.43
1:G:197:ASP:O	1:G:198:LEU:HD23	2.19	0.43
1:H:56:VAL:HG11	1:H:144:ILE:HD11	2.01	0.43
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.19	0.43
2:I:553:THR:H	2:I:553:THR:HG1	1.46	0.43
3:J:414:GLU:O	4:K:45:LYS:NZ	2.37	0.43
1:B:192:VAL:O	1:B:193:GLU:C	2.58	0.43
1:B:275:ILE:CD1	1:B:284:ARG:HD3	2.49	0.43
2:C:263:VAL:HG13	2:C:267:ARG:HB3	2.01	0.43
2:C:88:ARG:HA	2:C:934:PHE:CZ	2.54	0.43
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.19	0.43
5:F:394:TYR:O	5:F:404:LEU:HD11	2.19	0.43
2:I:699:LEU:HA	2:I:699:LEU:HD23	1.88	0.43
1:A:178:SER:HA	1:A:179:PRO:HD3	1.84	0.42
1:A:310:ARG:O	5:F:608:ARG:NE	2.52	0.42
1:B:285:THR:OG1	1:B:286:GLU:N	2.52	0.42
2:C:237:LEU:HG	2:C:289:VAL:HA	2.01	0.42
3:D:529:GLY:HA2	3:D:551:ARG:O	2.19	0.42
3:D:903:LEU:HD23	3:D:905:ARG:HD3	2.00	0.42
1:G:219:ARG:HB2	1:G:219:ARG:HE	1.54	0.42
2:I:1319:MET:HA	2:I:1320:PRO:HD3	1.92	0.42
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.54	0.42
2:I:778:GLU:O	2:I:781:ASP:HB2	2.19	0.42
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.19	0.42
3:J:179:LYS:HB2	3:J:184:ALA:HB2	2.02	0.42
1:B:14:VAL:HG23	1:B:27:THR:O	2.19	0.42
2:C:1151:LEU:HD21	2:C:1198:LEU:HB2	2.01	0.42
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.78	0.42
2:C:710:VAL:HG13	2:C:717:VAL:HG21	2.01	0.42
2:C:725:GLN:NE2	2:C:966:ILE:HG23	2.34	0.42
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	2.01	0.42
3:D:416:ILE:HA	3:D:416:ILE:HD13	1.75	0.42
3:D:733:SER:O	3:D:737:ILE:HG12	2.19	0.42
3:D:860:ARG:HA	3:D:860:ARG:HD2	1.82	0.42
2:I:692:THR:OG1	2:I:827:ARG:O	2.37	0.42
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.89	0.42
3:J:594:GLN:HB2	3:J:595:ALA:H	1.60	0.42
5:L:287:ILE:HD13	5:L:315:TRP:HH2	1.84	0.42
1:B:53:GLY:C	1:B:177:TYR:HB3	2.39	0.42
2:C:1111:GLN:HB2	2:C:1230:MET:HE1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.34	0.42
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.50	0.42
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.42
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.19	0.42
3:J:24:LEU:HB2	3:J:232:ASN:OD1	2.19	0.42
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.42
3:J:596:LEU:HD11	3:J:604:MET:CE	2.49	0.42
3:J:650:LYS:O	3:J:654:ILE:HG13	2.19	0.42
5:L:316:PHE:CZ	5:L:334:SER:HA	2.53	0.42
1:A:166:ARG:N	1:A:167:PRO:HD2	2.35	0.42
1:B:183:ILE:HD12	1:B:183:ILE:H	1.83	0.42
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.18	0.42
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.19	0.42
3:D:118:LYS:HE2	3:D:118:LYS:HB3	1.89	0.42
3:D:1192:LYS:HE3	3:D:1192:LYS:HB2	1.90	0.42
3:D:262:THR:HG1	3:D:266:ASN:ND2	2.15	0.42
3:D:518:VAL:HG22	3:D:709:ARG:HB2	2.01	0.42
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.42
5:F:584:ARG:O	5:F:588:ARG:HG3	2.20	0.42
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.50	0.42
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.67	0.42
2:I:402:ARG:HG2	2:I:416:GLY:H	1.83	0.42
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	2.01	0.42
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.53	0.42
1:A:18:GLN:HE22	1:A:213:PRO:CD	2.33	0.42
1:B:317:ARG:O	1:B:318:LEU:HD13	2.19	0.42
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.20	0.42
2:C:696:ASP:HB3	2:C:697:LYS:H	1.61	0.42
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.53	0.42
1:G:89:ALA:HB1	1:G:210:THR:CG2	2.50	0.42
1:G:17:GLU:N	1:G:25:LYS:O	2.43	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.73	0.42
2:I:1156:ARG:HB2	2:I:1156:ARG:HH11	1.84	0.42
2:I:148:GLN:HG3	2:I:511:LEU:HD11	2.01	0.42
2:I:79:VAL:HG23	2:I:80:PHE:H	1.85	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.54	0.42
5:L:343:LYS:HD2	5:L:343:LYS:H	1.84	0.42
9:M:202:G4P:HO2'	9:M:202:G4P:PC	2.41	0.42
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.84	0.42
2:C:528:ARG:NH2	2:C:576:SER:O	2.52	0.42
2:C:920:VAL:HA	2:C:921:PRO:HD3	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.49	0.42
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.52	0.42
3:D:126:LEU:H	3:D:126:LEU:HG	1.65	0.42
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.81	0.42
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.48	0.42
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.35	0.42
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.89	0.42
1:H:158:ARG:HB3	1:H:172:LEU:HD23	2.00	0.42
3:J:649:LYS:HA	3:J:649:LYS:HD3	1.77	0.42
5:L:476:ARG:HD2	5:L:477:GLU:HG2	2.01	0.42
1:A:195:ARG:HE	1:A:198:LEU:HD21	1.85	0.42
1:A:321:TRP:HA	1:A:322:PRO:HA	1.78	0.42
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.83	0.42
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.85	0.42
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.50	0.42
4:E:58:LEU:H	4:E:58:LEU:HD12	1.84	0.42
5:F:125:ASP:O	5:F:129:GLN:HG3	2.19	0.42
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.20	0.42
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.42
1:A:104:LYS:HG3	1:A:105:SER:N	2.35	0.42
1:B:185:TYR:HB2	1:B:201:LEU:HD11	2.02	0.42
1:B:265:ARG:O	1:B:269:CYS:HB2	2.20	0.42
1:B:48:LEU:HA	1:B:180:VAL:HG21	2.01	0.42
2:C:253:PHE:O	2:C:255:ILE:HG13	2.20	0.42
3:D:271:ARG:HD3	3:D:275:ARG:NH2	2.35	0.42
3:D:349:TYR:CD1	3:D:472:LEU:HD21	2.55	0.42
3:D:494:ALA:HB2	3:D:922:SER:HB3	2.02	0.42
5:F:379:MET:O	5:F:383:ASN:ND2	2.52	0.42
3:J:126:LEU:H	3:J:126:LEU:HG	1.67	0.42
3:J:405:GLU:O	3:J:408:VAL:HG22	2.20	0.42
3:J:902:ASP:OD1	3:J:903:LEU:N	2.53	0.42
5:L:161:LEU:C	5:L:262:VAL:HG23	2.39	0.42
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.55	0.42
1:A:286:GLU:HA	1:A:289:LEU:HD12	2.01	0.42
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.78	0.42
2:C:109:ALA:HA	2:C:110:PRO:HD3	1.91	0.42
2:C:297:VAL:HG23	2:C:333:ILE:HG23	2.02	0.42
2:C:198:ILE:HD13	2:C:388:LEU:HD13	2.02	0.42
2:C:466:VAL:O	2:C:470:ARG:HG2	2.19	0.42
2:C:602:GLU:O	2:C:602:GLU:HG3	2.20	0.42
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:355:ILE:HG22	3:D:447:ILE:HB	2.01	0.42
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.54	0.42
3:D:572:THR:OG1	3:D:576:ARG:HB2	2.20	0.42
3:D:683:ILE:HD11	3:D:754:ILE:HG23	2.01	0.42
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.34	0.42
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.83	0.42
3:J:308:ASP:CG	3:J:311:ARG:HE	2.22	0.42
2:I:1274:GLU:HA	3:J:428:THR:HG21	2.02	0.42
3:J:515:ARG:NH2	3:J:717:VAL:O	2.52	0.42
3:J:596:LEU:HD11	3:J:604:MET:HE3	2.02	0.42
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.59	0.42
5:L:513:ASP:C	5:L:515:GLU:H	2.22	0.42
6:M:47:TRP:O	6:M:51:LEU:HG	2.20	0.42
2:C:1131:MET:HE1	2:C:1141:LEU:HD12	2.01	0.42
2:C:117:ILE:H	2:C:117:ILE:HG12	1.62	0.42
2:C:1066:MET:HG2	2:C:1234:LYS:HA	2.01	0.42
3:D:266:ASN:O	3:D:270:ARG:HB2	2.20	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
3:D:487:THR:HB	3:D:618:VAL:HG21	2.01	0.42
3:D:827:GLU:O	3:D:829:GLY:N	2.50	0.42
1:G:75:GLN:HA	2:I:729:ALA:H	1.83	0.42
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.42
3:J:647:PRO:HG3	3:J:697:MET:CA	2.50	0.42
5:L:233:ASP:O	5:L:236:LYS:HE2	2.20	0.42
1:A:192:VAL:HG12	1:A:195:ARG:HB2	2.02	0.41
1:A:315:GLY:O	1:A:316:MET:HG3	2.20	0.41
2:C:593:LYS:HG3	2:C:595:THR:HG23	2.00	0.41
3:D:1299:GLY:HA2	3:D:1300:ALA:HA	1.86	0.41
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.85	0.41
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.55	0.41
2:I:896:THR:HB	2:I:897:PRO:HD2	2.02	0.41
2:I:975:ILE:O	2:I:979:LEU:HB2	2.20	0.41
3:J:362:ARG:HH21	9:J:2004:G4P:C1'	2.33	0.41
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.55	0.41
2:C:162:GLY:O	2:C:164:THR:N	2.52	0.41
2:C:421:SER:H	2:C:424:ASP:HB2	1.85	0.41
2:C:487:LEU:HD23	2:C:487:LEU:H	1.85	0.41
2:C:117:ILE:HD12	2:C:488:MET:HG2	2.02	0.41
2:C:463:GLN:NE2	2:C:501:ALA:O	2.53	0.41
2:C:830:THR:HG23	2:C:832:HIS:NE2	2.35	0.41
3:D:130:MET:HB2	3:D:157:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:ASN:O	3:D:46:TYR:HD2	2.02	0.41
3:D:835:LEU:O	3:D:839:VAL:HG23	2.20	0.41
5:F:471:LEU:HD23	5:F:476:ARG:O	2.21	0.41
1:G:192:VAL:O	1:G:194:GLN:N	2.54	0.41
1:H:67:GLU:HA	1:H:78:ILE:HG21	2.02	0.41
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.54	0.41
5:L:470:MET:O	5:L:478:PRO:HD3	2.21	0.41
3:D:786:THR:HG21	6:M:75:ARG:HG2	2.00	0.41
1:A:237:VAL:O	1:B:13:LEU:HA	2.20	0.41
2:C:42:ASP:C	2:C:44:GLU:H	2.24	0.41
3:D:661:VAL:HG12	3:D:682:VAL:HG13	2.02	0.41
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.41
5:F:515:GLU:HG2	5:F:516:ASP:N	2.35	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.01	0.41
3:J:154:LEU:HD22	3:J:160:LEU:HD11	2.02	0.41
3:J:460:ASP:OD1	3:J:462:ASP:OD1	2.39	0.41
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.50	0.41
5:L:152:GLU:OE2	5:L:218:ARG:HG3	2.19	0.41
5:L:603:ARG:HD3	5:L:603:ARG:HA	1.84	0.41
6:M:57:ARG:O	6:M:60:THR:N	2.47	0.41
6:M:59:VAL:HA	6:M:62:MET:HB2	2.03	0.41
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	2.01	0.41
3:D:24:LEU:HD13	3:D:24:LEU:HA	1.90	0.41
3:D:425:ARG:HD2	3:D:459:ALA:HB2	2.02	0.41
5:F:483:LEU:H	5:F:483:LEU:HD12	1.85	0.41
5:F:530:LEU:HD12	5:F:533:ASP:H	1.84	0.41
1:G:51:MET:HA	1:G:52:PRO:HD3	1.93	0.41
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.51	0.41
1:H:217:ILE:HA	1:H:220:ALA:HB3	2.02	0.41
2:I:194:LEU:HA	2:I:194:LEU:HD12	1.88	0.41
2:I:871:VAL:HG12	2:I:883:LEU:O	2.20	0.41
3:J:430:HIS:NE2	3:J:456:ALA:O	2.49	0.41
3:J:460:ASP:CG	3:J:462:ASP:OD1	2.59	0.41
1:B:134:THR:OG1	1:B:135:ASP:N	2.52	0.41
1:B:269:CYS:SG	1:B:295:LEU:HG	2.60	0.41
2:C:1230:MET:HG2	2:C:1232:MET:HG3	2.03	0.41
2:C:800:MET:HB3	2:C:800:MET:HE3	1.81	0.41
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.35	0.41
3:D:279:LEU:HD12	3:D:295:GLU:HG3	2.01	0.41
3:D:317:THR:HB	3:D:324:LEU:HB3	2.01	0.41
3:D:615:LYS:HA	4:E:5:THR:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:744:ARG:HG3	3:D:744:ARG:O	2.21	0.41
1:G:22:THR:OG1	1:G:23:HIS:N	2.54	0.41
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.51	0.41
2:I:686:GLN:HG2	2:I:796:LEU:HD22	2.03	0.41
2:I:829:THR:HA	2:I:1059:ARG:HA	2.03	0.41
3:J:147:ILE:HG13	3:J:147:ILE:O	2.20	0.41
3:J:332:LYS:HA	3:J:337:ARG:H	1.85	0.41
3:J:638:SER:OG	3:J:639:VAL:N	2.53	0.41
6:M:17:ILE:CG2	6:M:50:GLN:HG3	2.49	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.81	0.41
2:C:1124:ILE:HG13	2:C:1180:MET:HE3	2.03	0.41
2:C:943:LYS:O	2:C:947:GLU:HG3	2.20	0.41
3:D:1167:LYS:HB3	3:D:1167:LYS:HE3	1.85	0.41
3:D:248:ASP:O	3:D:251:PRO:HG3	2.21	0.41
3:D:355:ILE:HG21	3:D:466:MET:HG3	2.02	0.41
5:F:139:GLU:HG3	5:F:351:THR:HG22	2.01	0.41
1:G:35:PHE:HA	1:G:35:PHE:HD1	1.78	0.41
1:H:7:GLU:HG2	1:H:8:PHE:H	1.85	0.41
2:I:1083:GLU:HG3	2:I:1083:GLU:H	1.64	0.41
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	2.01	0.41
2:I:127:ILE:HG22	2:I:502:VAL:HG11	2.02	0.41
2:I:80:PHE:HB3	2:I:84:GLU:HB2	2.03	0.41
3:J:239:LEU:HD23	3:J:239:LEU:HA	1.88	0.41
3:J:686:TRP:CD1	3:J:758:PRO:HD3	2.56	0.41
5:L:316:PHE:CE1	5:L:337:VAL:HB	2.56	0.41
1:B:189:ALA:HB1	1:B:191:ARG:HH12	1.86	0.41
2:C:1054:LEU:HD12	2:C:1054:LEU:HA	1.86	0.41
2:C:1252:SER:HB3	2:C:1255:THR:O	2.21	0.41
2:C:81:ASP:HA	2:C:92:TYR:HE1	1.86	0.41
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.84	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.91	0.41
3:D:735:ALA:O	3:D:738:ARG:HB3	2.21	0.41
3:D:905:ARG:NH2	3:D:907:HIS:HB2	2.22	0.41
1:G:57:THR:HG22	1:G:58:GLU:HG3	2.02	0.41
2:I:896:THR:O	2:I:897:PRO:C	2.58	0.41
3:J:761:ALA:H	3:J:771:GLN:HE22	1.67	0.41
6:M:111:PHE:CE2	6:M:126:LEU:HD13	2.56	0.41
1:A:124:VAL:HG11	1:A:210:THR:HG23	2.02	0.41
1:B:153:VAL:N	1:B:175:ALA:O	2.54	0.41
1:B:29:GLU:O	1:B:31:LEU:HD23	2.11	0.41
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:591:ILE:HA	3:D:591:ILE:HD12	1.89	0.41
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	2.21	0.41
4:E:15:ASN:O	4:E:16:ARG:HB3	2.21	0.41
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.86	0.41
2:I:1111:GLN:HB2	2:I:1230:MET:HE2	2.03	0.41
2:I:1276:TRP:HD1	2:I:1279:GLU:OE1	2.02	0.41
2:I:157:PHE:O	2:I:443:ASP:N	2.52	0.41
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.03	0.41
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.36	0.41
3:J:1179:PRO:HD2	3:J:1184:ASP:HB3	2.01	0.41
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	2.02	0.41
3:J:514:THR:HB	3:J:576:ARG:HG2	2.02	0.41
3:J:849:LEU:HD22	3:J:849:LEU:H	1.85	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.86	0.41
1:A:97:GLU:HA	1:A:146:VAL:O	2.21	0.41
1:A:187:VAL:HG23	1:A:187:VAL:O	2.21	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.89	0.41
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.75	0.41
3:D:1183:SER:CB	3:J:206:ASN:HD21	2.33	0.41
3:D:460:ASP:OD2	6:M:71:ASP:OD2	2.39	0.41
1:G:192:VAL:O	1:G:192:VAL:HG12	2.20	0.41
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.03	0.41
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.43	0.41
2:I:1281:TYR:OH	3:J:431:ARG:O	2.38	0.41
3:J:657:ALA:CB	3:J:689:ALA:HB2	2.50	0.41
3:J:647:PRO:HG3	3:J:697:MET:N	2.35	0.41
5:L:285:ARG:HA	5:L:288:MET:HB3	2.02	0.41
5:L:377:LYS:O	5:L:381:GLU:HG3	2.21	0.41
5:L:493:LYS:HA	5:L:496:LYS:HG3	2.02	0.41
6:M:140:THR:O	6:M:144:ILE:HG12	2.21	0.41
1:B:120:ASP:OD1	1:B:276:HIS:CD2	2.74	0.41
1:B:16:ILE:HG12	1:B:26:VAL:HG22	2.03	0.41
1:B:62:ASP:HB2	1:B:141:SER:O	2.21	0.41
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.42	0.41
2:C:206:ALA:O	2:C:209:ILE:HG22	2.21	0.41
2:C:42:ASP:O	2:C:44:GLU:N	2.52	0.41
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.35	0.41
3:D:1156:LEU:HD23	3:D:1219:ASP:HB3	2.02	0.41
3:D:1282:TYR:HD2	3:D:1286:LYS:HZ2	1.68	0.41
3:D:147:ILE:HG13	3:D:147:ILE:O	2.21	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:VAL:HG12	1:H:66:HIS:H	1.85	0.41
2:I:297:VAL:HB	2:I:317:LEU:HD21	2.02	0.41
2:I:734:ILE:O	2:I:748:ILE:HB	2.21	0.41
3:J:1167:LYS:HE3	3:J:1167:LYS:HB3	1.92	0.41
2:I:1294:LYS:HD2	3:J:348:ASP:O	2.21	0.41
3:J:504:GLN:OE1	3:J:731:ARG:HD2	2.21	0.41
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.20	0.41
2:C:169:LYS:HE2	2:C:190:PRO:O	2.20	0.41
3:D:17:PHE:HZ	3:D:1353:VAL:HG21	1.85	0.41
3:D:45:ASN:O	3:D:46:TYR:CD2	2.74	0.41
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.55	0.41
1:H:183:ILE:HG23	1:H:205:MET:HG3	2.03	0.41
1:H:211:ILE:HD12	1:H:211:ILE:HA	1.97	0.41
2:I:1086:PRO:CB	2:I:1212:LEU:HD23	2.51	0.41
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.95	0.41
2:I:1225:VAL:HA	3:J:638:SER:CB	2.51	0.41
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.95	0.41
5:L:226:ALA:O	5:L:229:VAL:HG22	2.21	0.41
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.22	0.40
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.86	0.40
3:D:460:ASP:OD1	3:D:464:ASP:OD2	2.39	0.40
5:F:143:TYR:CD2	5:F:269:LEU:HD21	2.56	0.40
2:I:149:LEU:HD13	2:I:453:ILE:HG13	2.02	0.40
2:I:452:ARG:HH12	2:I:585:GLY:HA3	1.86	0.40
2:I:5:TYR:O	2:I:8:LYS:HG2	2.22	0.40
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.03	0.40
2:I:828:PHE:HD1	2:I:828:PHE:HA	1.71	0.40
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.86	0.40
3:J:1239:ASP:O	3:J:1243:LEU:HB2	2.21	0.40
3:J:361:LEU:HD13	3:J:366:CYS:HA	2.03	0.40
3:J:668:PHE:CE1	3:J:678:ARG:HG2	2.56	0.40
3:J:860:ARG:HB3	3:J:861:ASN:H	1.55	0.40
5:L:322:MET:HB3	5:L:324:LYS:HZ3	1.86	0.40
1:B:106:GLY:O	1:B:108:GLY:N	2.54	0.40
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.86	0.40
2:C:12:ARG:HG3	2:C:1181:PRO:HB2	2.04	0.40
2:C:145:ILE:HG22	2:C:456:VAL:HG22	2.03	0.40
2:C:221:LEU:HD12	2:C:298:ALA:O	2.21	0.40
2:C:202:ARG:HD3	2:C:369:MET:HG2	2.02	0.40
2:C:79:VAL:HG23	2:C:80:PHE:H	1.85	0.40
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:742:GLY:O	3:D:762:ASN:HB3	2.21	0.40
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.35	0.40
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.27	0.40
2:I:540:ARG:HD2	2:I:540:ARG:H	1.86	0.40
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.03	0.40
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.21	0.40
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.57	0.40
3:J:709:ARG:HD2	3:J:710:ASP:H	1.86	0.40
3:J:839:VAL:HG12	3:J:864:LEU:HD12	2.03	0.40
6:M:112:GLY:HA2	6:M:126:LEU:HD11	2.03	0.40
6:M:136:ILE:HA	6:M:136:ILE:HD12	1.89	0.40
6:M:36:GLN:O	6:M:39:HIS:HB3	2.21	0.40
1:A:110:VAL:HG21	1:A:140:ILE:HD11	2.03	0.40
2:C:1248:THR:HG22	2:C:1251:TYR:OH	2.21	0.40
2:C:1319:MET:HA	2:C:1320:PRO:HD3	1.90	0.40
3:D:1168:GLU:O	3:D:1170:LYS:N	2.54	0.40
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.54	0.40
3:D:490:ILE:N	3:D:490:ILE:HD13	2.29	0.40
5:F:281:ARG:O	5:F:285:ARG:HG3	2.20	0.40
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.21	0.40
1:H:178:SER:HA	1:H:179:PRO:HD3	1.86	0.40
1:H:74:VAL:HG11	1:H:81:ILE:HD11	2.02	0.40
2:I:521:LEU:O	2:I:525:THR:HB	2.22	0.40
3:J:416:ILE:HA	3:J:416:ILE:HD12	1.83	0.40
3:J:709:ARG:HD2	3:J:710:ASP:N	2.36	0.40
3:J:923:ILE:O	3:J:926:PRO:HD2	2.21	0.40
1:A:89:ALA:O	1:A:124:VAL:HG12	2.22	0.40
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.86	0.40
1:A:323:PRO:HB2	1:A:324:ALA:HB2	2.04	0.40
1:B:104:LYS:HD3	1:B:114:ASP:OD2	2.20	0.40
1:B:49:SER:O	1:B:51:MET:N	2.54	0.40
2:C:601:ASP:N	2:C:601:ASP:OD1	2.46	0.40
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.36	0.40
3:D:681:LYS:NZ	6:M:12:LEU:HD13	2.37	0.40
3:D:707:ILE:HD11	3:D:716:GLN:HG2	2.03	0.40
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.87	0.40
3:D:860:ARG:HB3	3:D:861:ASN:H	1.81	0.40
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.49	0.40
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.37	0.40
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.91	0.40
2:I:402:ARG:HG2	2:I:416:GLY:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:195:GLU:H	3:J:195:GLU:HG3	1.61	0.40
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.37	0.40
3:J:514:THR:CB	3:J:576:ARG:HG2	2.51	0.40
3:J:664:ILE:HG21	3:J:681:LYS:HG2	2.04	0.40
6:M:90:ASP:O	6:M:94:LYS:HG3	2.22	0.40
1:A:262:LEU:HD12	1:A:262:LEU:H	1.86	0.40
2:C:149:LEU:HD12	2:C:452:ARG:O	2.21	0.40
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.03	0.40
3:D:789:LYS:HZ3	3:D:932:MET:CB	2.35	0.40
5:F:511:ILE:HG22	5:F:517:SER:O	2.22	0.40
1:G:31:LEU:HD23	1:G:31:LEU:HA	1.88	0.40
2:I:388:LEU:HD23	2:I:388:LEU:HA	1.86	0.40
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.24	0.40
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.51	0.40
3:J:161:THR:H	3:J:164:GLN:HB2	1.86	0.40
3:J:322:ARG:HG3	3:J:323:PRO:HD2	2.04	0.40
4:K:56:GLU:HB2	4:K:58:LEU:HD11	2.04	0.40
5:L:363:ARG:O	5:L:367:ILE:HG13	2.20	0.40
5:L:544:THR:HG22	5:L:607:LEU:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASP:OD2	3:J:675:ALA:N[2_555]	2.03	0.17

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	317/329 (96%)	249 (78%)	53 (17%)	15 (5%)	3 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	291/329 (88%)	225 (77%)	45 (16%)	21 (7%)	1	20
1	G	225/329 (68%)	200 (89%)	21 (9%)	4 (2%)	10	50
1	H	212/329 (64%)	197 (93%)	11 (5%)	4 (2%)	9	49
2	C	1338/1342 (100%)	1201 (90%)	114 (8%)	23 (2%)	11	52
2	I	1338/1342 (100%)	1196 (89%)	119 (9%)	23 (2%)	11	52
3	D	1169/1407 (83%)	1042 (89%)	99 (8%)	28 (2%)	7	44
3	J	1151/1407 (82%)	1024 (89%)	100 (9%)	27 (2%)	7	45
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	7	45
4	K	77/91 (85%)	68 (88%)	5 (6%)	4 (5%)	2	27
5	F	462/613 (75%)	425 (92%)	28 (6%)	9 (2%)	9	49
5	L	463/613 (76%)	424 (92%)	32 (7%)	7 (2%)	12	54
6	M	138/151 (91%)	128 (93%)	7 (5%)	3 (2%)	8	46
All	All	7268/8373 (87%)	6460 (89%)	638 (9%)	170 (2%)	7	45

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	167	PRO
1	A	242	VAL
1	A	320	ASN
1	B	20	SER
1	B	29	GLU
1	B	30	PRO
1	B	32	GLU
1	B	107	ILE
1	B	320	ASN
1	B	323	PRO
1	B	324	ALA
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1153	ALA
2	C	1159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	566	ASP
5	F	569	THR
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	710	ASP
3	J	712	GLN
3	J	850	LYS
3	J	854	ALA
3	J	1294	ALA
4	K	4	VAL
4	K	15	ASN
4	K	33	GLY
5	L	584	ARG
6	M	31	TYR
1	A	50	SER
1	A	119	GLY
1	A	232	VAL
1	A	315	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	50	SER
1	B	62	ASP
1	B	119	GLY
1	B	135	ASP
1	B	315	GLY
2	C	121	GLU
2	C	237	LEU
2	C	1154	ASP
3	D	89	GLY
3	D	805	GLN
3	D	933	ARG
3	D	934	THR
5	F	584	ARG
1	G	162	GLU
1	G	167	PRO
1	H	138	ALA
2	I	237	LEU
2	I	1059	ARG
2	I	1165	SER
3	J	89	GLY
3	J	314	ARG
3	J	339	ARG
3	J	496	GLY
3	J	745	GLY
3	J	805	GLN
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
1	A	62	ASP
1	B	319	GLU
1	B	321	TRP
2	C	163	LYS
2	C	236	LYS
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY
3	D	314	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	417	ARG
3	D	1274	PHE
3	D	1344	LEU
5	F	600	HIS
1	G	229	GLU
1	H	193	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	332	LYS
3	J	417	ARG
6	M	58	THR
1	A	319	GLU
1	A	324	ALA
1	B	13	LEU
1	B	322	PRO
2	C	813	GLU
2	C	1059	ARG
3	D	1297	LYS
1	H	20	SER
2	I	696	ASP
2	I	813	GLU
2	I	892	GLU
3	J	344	GLY
3	J	1344	LEU
4	K	14	GLY
1	A	318	LEU
1	B	318	LEU
2	C	62	TYR
2	C	983	GLY
2	C	1158	LYS
3	D	46	TYR
3	D	345	LYS
5	F	602	SER
2	I	201	ARG
2	I	236	LYS
3	J	338	PHE
3	J	357	VAL
2	C	1256	GLN
3	D	357	VAL
3	D	828	GLY
3	D	1375	ALA
2	I	160	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	756	TYR
3	J	333	GLY
5	L	585	GLU
6	M	27	PRO
1	A	19	VAL
1	B	19	VAL
3	D	826	ILE
5	F	96	ASP
3	J	173	GLY
3	J	336	GLY
3	D	120	LEU
3	D	831	VAL
5	F	361	ILE
5	F	601	PRO
3	J	639	VAL
1	B	217	ILE
4	E	86	ILE
2	I	1202	GLY
5	L	475	GLY
1	B	293	PRO
2	C	110	PRO
3	D	850	LYS
1	H	30	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	278/286 (97%)	230 (83%)	48 (17%)	2	16
1	B	256/286 (90%)	224 (88%)	32 (12%)	5	29
1	G	193/286 (68%)	169 (88%)	24 (12%)	5	29
1	H	183/286 (64%)	171 (93%)	12 (7%)	19	54
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	12	43
2	I	1154/1157 (100%)	1059 (92%)	95 (8%)	13	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	962/1168 (82%)	879 (91%)	83 (9%)	12	45
3	J	960/1168 (82%)	875 (91%)	85 (9%)	11	42
4	E	72/75 (96%)	64 (89%)	8 (11%)	7	33
4	K	67/75 (89%)	60 (90%)	7 (10%)	8	35
5	F	417/540 (77%)	387 (93%)	30 (7%)	17	51
5	L	418/540 (77%)	380 (91%)	38 (9%)	11	41
6	M	121/131 (92%)	111 (92%)	10 (8%)	13	46
All	All	6236/7155 (87%)	5662 (91%)	574 (9%)	11	41

All (574) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	18	GLN
1	A	26	VAL
1	A	29	GLU
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	66	HIS
1	A	70	THR
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL
1	A	99	ILE
1	A	105	SER
1	A	116	THR
1	A	125	LYS
1	A	133	LEU
1	A	139	SER
1	A	159	ILE
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	ARG
1	A	207	THR
1	A	211	ILE
1	A	223	ILE
1	A	231	PHE
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	258	ASP
1	A	262	LEU
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU
1	A	302	GLU
1	A	306	VAL
1	A	316	MET
1	A	318	LEU
1	A	320	ASN
1	B	8	PHE
1	B	9	LEU
1	B	18	GLN
1	B	29	GLU
1	B	45	ARG
1	B	50	SER
1	B	54	CYS
1	B	70	THR
1	B	71	LYS
1	B	75	GLN
1	B	77	ASP
1	B	83	LEU
1	B	98	VAL
1	B	133	LEU
1	B	139	SER
1	B	159	ILE
1	B	183	ILE
1	B	186	ASN
1	B	195	ARG
1	B	223	ILE
1	B	258	ASP
1	B	262	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	ASP
1	B	282	VAL
1	B	284	ARG
1	B	285	THR
1	B	300	LEU
1	B	302	GLU
1	B	306	VAL
1	B	316	MET
1	B	318	LEU
1	B	320	ASN
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	23	ASP
2	C	46	GLN
2	C	81	ASP
2	C	103	VAL
2	C	107	ARG
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR
2	C	135	THR
2	C	150	HIS
2	C	164	THR
2	C	201	ARG
2	C	208	ILE
2	C	236	LYS
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	377	THR
2	C	384	LEU
2	C	423	ASP
2	C	455	SER
2	C	471	VAL
2	C	481	LEU
2	C	484	LEU
2	C	485	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	490	GLN
2	C	492	MET
2	C	518	ASN
2	C	525	THR
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	553	THR
2	C	561	ILE
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	663	VAL
2	C	672	GLU
2	C	694	ARG
2	C	697	LYS
2	C	714	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	778	GLU
2	C	781	ASP
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1054	LEU
2	C	1059	ARG
2	C	1076	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1082	ILE
2	C	1134	GLN
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1233	LEU
2	C	1237	HIS
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1296	ASP
2	C	1310	ASP
2	C	1313	HIS
2	C	1327	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	11	GLN
3	D	46	TYR
3	D	47	ARG
3	D	54	ASP
3	D	79	LYS
3	D	93	THR
3	D	95	THR
3	D	97	VAL
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	248	ASP
3	D	252	LEU
3	D	259	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	292	VAL
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	413	ASP
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	490	ILE
3	D	505	ASP
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	560	ASN
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	639	VAL
3	D	641	ILE
3	D	678	ARG
3	D	680	ASN
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	753	SER
3	D	754	ILE
3	D	764	ARG
3	D	772	TYR
3	D	797	THR
3	D	801	VAL
3	D	810	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	890	THR
3	D	897	HIS
3	D	901	ARG
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	918	ILE
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1199	PHE
3	D	1221	LEU
3	D	1251	LYS
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1366	HIS
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU
4	E	62	GLN
5	F	98	VAL
5	F	114	GLU
5	F	154	GLU
5	F	163	THR
5	F	261	LEU
5	F	277	MET
5	F	305	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	306	PHE
5	F	338	HIS
5	F	401	PHE
5	F	449	THR
5	F	471	LEU
5	F	472	GLN
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	516	ASP
5	F	526	THR
5	F	527	THR
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	569	THR
5	F	572	THR
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	33	ARG
1	G	50	SER
1	G	70	THR
1	G	79	LEU
1	G	90	VAL
1	G	101	THR
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	145	LYS
1	G	156	SER
1	G	171	LEU
1	G	178	SER
1	G	187	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	219	ARG
1	G	231	PHE
1	H	18	GLN
1	H	27	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	95	LYS
1	H	102	LEU
1	H	124	VAL
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	46	GLN
2	I	86	GLN
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	131	THR
2	I	132	ASP
2	I	138	ILE
2	I	156	PHE
2	I	164	THR
2	I	197	ARG
2	I	201	ARG
2	I	208	ILE
2	I	236	LYS
2	I	285	ILE
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	423	ASP
2	I	453	ILE
2	I	455	SER
2	I	471	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	481	LEU
2	I	484	LEU
2	I	485	ASP
2	I	490	GLN
2	I	492	MET
2	I	518	ASN
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	540	ARG
2	I	542	ARG
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	596	ASP
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	633	LEU
2	I	635	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	694	ARG
2	I	705	GLU
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	764	CYS
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	828	PHE
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	919	ARG
2	I	922	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	951	MET
2	I	992	LEU
2	I	1037	THR
2	I	1054	LEU
2	I	1082	ILE
2	I	1083	GLU
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1198	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER
2	I	1254	VAL
2	I	1265	PHE
2	I	1287	LEU
2	I	1296	ASP
2	I	1313	HIS
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	47	ARG
3	J	54	ASP
3	J	79	LYS
3	J	92	VAL
3	J	93	THR
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	206	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	259	ARG
3	J	292	VAL
3	J	324	LEU
3	J	343	LEU
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE
3	J	413	ASP
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	505	ASP
3	J	510	LEU
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	560	ASN
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	641	ILE
3	J	678	ARG
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	772	TYR
3	J	797	THR
3	J	801	VAL
3	J	810	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	827	GLU
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	897	HIS
3	J	898	CYS
3	J	901	ARG
3	J	908	ILE
3	J	910	ASN
3	J	918	ILE
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1186	TYR
3	J	1194	ARG
3	J	1199	PHE
3	J	1221	LEU
3	J	1251	LYS
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1282	TYR
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	3	ARG
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	102	MET
5	L	114	GLU
5	L	154	GLU
5	L	261	LEU
5	L	266	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	277	MET
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	401	PHE
5	L	405	ILE
5	L	429	THR
5	L	445	ASP
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP
5	L	526	THR
5	L	527	THR
5	L	552	THR
5	L	558	VAL
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
6	M	42	ARG
6	M	50	GLN
6	M	52	ARG
6	M	53	ASP
6	M	69	PHE
6	M	72	PRO
6	M	88	ASN
6	M	129	ARG
6	M	136	ILE
6	M	146	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	B	186	ASN
1	B	268	ASN
1	B	276	HIS
1	B	320	ASN
2	C	46	GLN
2	C	69	GLN
2	C	133	ASN
2	C	139	ASN
2	C	343	HIS
2	C	513	GLN
2	C	620	ASN
2	C	760	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1237	HIS
2	C	1288	GLN
3	D	157	GLN
3	D	200	GLN
3	D	320	ASN
3	D	424	ASN
3	D	680	ASN
3	D	690	ASN
3	D	777	HIS
3	D	817	HIS
3	D	910	ASN
5	F	406	GLN
5	F	446	GLN
5	F	579	GLN
5	F	600	HIS
1	G	66	HIS
2	I	46	GLN
2	I	139	ASN
2	I	357	ASN
2	I	620	ASN
2	I	808	ASN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1220	GLN
2	I	1237	HIS
2	I	1244	HIS
2	I	1288	GLN
2	I	1314	GLN
3	J	200	GLN
3	J	206	ASN
3	J	364	HIS
3	J	419	HIS
3	J	424	ASN
3	J	465	GLN
3	J	716	GLN
3	J	861	ASN
5	L	301	ASN
5	L	345	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	579	GLN
6	M	36	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	G4P	E	101	-	32,38,38	1.72	7 (21%)	35,61,61	1.65	6 (17%)
9	G4P	J	2004	-	32,38,38	1.87	8 (25%)	35,61,61	1.55	6 (17%)
9	G4P	M	202	-	32,38,38	1.88	9 (28%)	35,61,61	1.68	6 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	G4P	E	101	-	-	0/23/43/43	0/3/3/3
9	G4P	J	2004	-	-	0/23/43/43	0/3/3/3
9	G4P	M	202	-	-	0/23/43/43	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	2004	G4P	C2'-C1'	-5.19	1.45	1.53
9	M	202	G4P	C2'-C1'	-4.62	1.46	1.53
9	E	101	G4P	C2'-C1'	-4.53	1.46	1.53
9	M	202	G4P	C5-C4	-3.82	1.31	1.40
9	J	2004	G4P	C5-C4	-3.75	1.32	1.40
9	M	202	G4P	C2'-C3'	-3.48	1.45	1.53
9	E	101	G4P	C5-C4	-3.47	1.32	1.40
9	J	2004	G4P	C2'-C3'	-3.20	1.45	1.53
9	E	101	G4P	C2'-C3'	-2.92	1.46	1.53
9	M	202	G4P	C3'-C4'	-2.72	1.45	1.52
9	J	2004	G4P	C3'-C4'	-2.44	1.46	1.52
9	E	101	G4P	C3'-C4'	-2.35	1.46	1.52
9	M	202	G4P	C6-C5	-2.07	1.37	1.41
9	M	202	G4P	O4'-C1'	2.05	1.44	1.41
9	J	2004	G4P	O4'-C1'	2.11	1.44	1.41
9	M	202	G4P	C8-N7	2.19	1.38	1.34
9	J	2004	G4P	C4-N3	2.30	1.39	1.35
9	E	101	G4P	C4-N3	2.43	1.39	1.35
9	J	2004	G4P	C8-N7	2.48	1.39	1.34
9	M	202	G4P	C4-N3	2.49	1.39	1.35
9	E	101	G4P	C8-N7	2.57	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	101	G4P	C2-N2	4.05	1.42	1.34
9	J	2004	G4P	C2-N2	4.22	1.42	1.34
9	M	202	G4P	C2-N2	4.33	1.42	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	202	G4P	N3-C2-N1	-4.02	121.59	127.46
9	J	2004	G4P	C4'-O4'-C1'	-3.73	105.80	109.77
9	J	2004	G4P	N3-C2-N1	-3.51	122.33	127.46
9	E	101	G4P	N3-C2-N1	-3.16	122.84	127.46
9	J	2004	G4P	C5-C6-N1	-2.84	119.45	123.48
9	E	101	G4P	C5-C6-N1	-2.61	119.76	123.48
9	M	202	G4P	C4'-O4'-C1'	-2.52	107.09	109.77
9	M	202	G4P	C5-C6-N1	-2.29	120.22	123.48
9	J	2004	G4P	C4-C5-N7	2.68	112.00	109.41
9	E	101	G4P	C4-C5-N7	2.79	112.11	109.41
9	E	101	G4P	C3'-C2'-C1'	2.83	106.30	99.95
9	M	202	G4P	C4-C5-N7	2.89	112.20	109.41
9	E	101	G4P	C6-N1-C2	3.04	120.43	116.06
9	M	202	G4P	C6-N1-C2	3.14	120.57	116.06
9	J	2004	G4P	C6-N1-C2	3.31	120.82	116.06
9	J	2004	G4P	O3C-PC-O3'	4.86	110.74	102.05
9	M	202	G4P	O3C-PC-O3'	6.10	112.95	102.05
9	E	101	G4P	O3C-PC-O3'	6.59	113.83	102.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	101	G4P	3	0
9	J	2004	G4P	4	0
9	M	202	G4P	7	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	0.42	43 (13%) 3 5	211, 260, 453, 474	0
1	B	297/329 (90%)	0.07	14 (4%) 32 26	204, 303, 444, 497	0
1	G	227/329 (68%)	-0.11	5 (2%) 62 55	257, 320, 369, 399	0
1	H	216/329 (65%)	0.21	18 (8%) 12 11	288, 336, 378, 393	0
2	C	1340/1342 (99%)	-0.21	25 (1%) 67 60	154, 240, 335, 399	0
2	I	1340/1342 (99%)	-0.03	41 (3%) 49 40	200, 281, 382, 521	0
3	D	1173/1407 (83%)	-0.21	10 (0%) 84 78	152, 223, 328, 395	0
3	J	1155/1407 (82%)	-0.14	17 (1%) 74 66	197, 262, 344, 388	0
4	E	89/91 (97%)	-0.20	1 (1%) 80 73	202, 266, 330, 365	0
4	K	79/91 (86%)	0.89	11 (13%) 3 5	336, 411, 518, 552	0
5	F	468/613 (76%)	-0.08	18 (3%) 41 33	188, 293, 445, 515	0
5	L	469/613 (76%)	-0.17	12 (2%) 56 47	223, 313, 427, 446	0
6	M	140/151 (92%)	0.18	10 (7%) 17 14	317, 361, 378, 386	0
All	All	7312/8373 (87%)	-0.08	225 (3%) 49 40	152, 271, 395, 552	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	ASN	11.3
1	A	244	GLU	10.9
1	B	314	LEU	9.8
2	C	252	SER	9.1
1	A	323	PRO	8.6
1	A	245	GLU	6.9
1	A	321	TRP	6.8
1	B	315	GLY	6.3
1	B	284	ARG	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	K	36	ASP	5.9
1	H	158	ARG	5.8
1	A	243	LYS	5.7
1	G	205	MET	5.6
1	G	204	GLU	5.4
1	A	322	PRO	5.3
1	A	246	LYS	5.1
2	I	976	ARG	5.0
5	F	301	ASN	5.0
3	J	747	MET	5.0
5	F	300	LYS	4.9
2	C	332	ARG	4.8
1	A	293	PRO	4.7
4	K	35	LYS	4.7
1	B	298	LYS	4.7
1	H	57	THR	4.7
2	C	317	LEU	4.6
5	F	287	ILE	4.6
1	B	316	MET	4.5
1	A	281	LEU	4.3
2	C	540	ARG	4.3
3	J	1296	GLY	4.2
1	H	172	LEU	4.2
5	F	304	THR	4.1
1	A	284	ARG	4.1
5	F	259	PHE	4.1
1	H	56	VAL	4.0
5	L	167	ASP	3.9
3	J	748	ALA	3.9
6	M	123	ILE	3.9
5	F	165	PHE	3.9
2	I	334	GLU	3.9
1	B	297	LYS	3.9
3	D	878	ASP	3.9
6	M	44	LEU	3.8
1	H	12	ARG	3.8
4	K	33	GLY	3.8
3	J	1215	GLU	3.8
2	C	253	PHE	3.8
2	I	975	ILE	3.8
1	B	303	ILE	3.8
2	C	265	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	J	1198	VAL	3.7
1	A	270	LEU	3.7
1	A	269	CYS	3.7
2	C	266	GLY	3.6
3	J	746	LEU	3.6
5	L	314	THR	3.6
1	A	279	GLY	3.5
2	I	981	ALA	3.4
6	M	151	GLY	3.4
1	A	253	LEU	3.3
1	B	282	VAL	3.3
1	A	249	PHE	3.3
2	C	292	ILE	3.3
2	I	973	SER	3.3
1	A	277	TYR	3.3
1	A	280	ASP	3.3
1	H	147	GLN	3.2
1	A	278	ILE	3.2
2	I	1005	GLU	3.2
5	L	259	PHE	3.2
5	F	299	LYS	3.2
2	I	230	PHE	3.1
2	C	188	PHE	3.1
1	G	203	ILE	3.1
4	K	58	LEU	3.1
2	I	734	ILE	3.1
2	C	254	ASP	3.0
4	K	37	PRO	3.0
2	I	1000	LEU	3.0
2	C	207	THR	3.0
3	J	730	ALA	3.0
6	M	124	ARG	3.0
5	L	165	PHE	3.0
2	C	282	VAL	3.0
1	A	268	ASN	3.0
5	F	283	GLN	3.0
1	A	294	ASN	3.0
5	F	167	ASP	2.9
5	F	286	LEU	2.9
2	C	187	GLU	2.9
3	J	1203	ARG	2.9
2	I	1180	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	242	VAL	2.9
1	A	248	GLU	2.9
1	H	146	VAL	2.9
4	K	12	LYS	2.9
1	B	59	VAL	2.9
4	K	47	THR	2.9
5	F	261	LEU	2.8
2	I	190	PRO	2.8
5	L	317	ASN	2.8
3	J	731	ARG	2.8
1	A	271	LYS	2.8
2	I	974	ARG	2.8
2	I	998	LEU	2.8
3	D	905	ARG	2.8
2	I	420	LEU	2.8
2	I	883	LEU	2.8
2	C	241	LEU	2.8
6	M	106	VAL	2.8
3	J	815	GLY	2.8
1	H	67	GLU	2.7
2	C	331	LYS	2.7
1	A	241	GLU	2.7
1	B	296	GLY	2.7
2	I	186	PHE	2.7
2	I	987	GLU	2.7
3	D	214	ARG	2.7
1	H	98	VAL	2.7
3	D	1198	VAL	2.7
5	L	318	ALA	2.7
6	M	66	ALA	2.7
2	I	725	GLN	2.7
3	D	1199	PHE	2.6
1	A	312	LEU	2.6
2	I	1011	LEU	2.6
1	A	254	LEU	2.6
2	I	200	ARG	2.6
2	I	882	ILE	2.6
1	H	90	VAL	2.6
5	F	162	ILE	2.6
2	C	194	LEU	2.6
2	I	194	LEU	2.6
1	H	176	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	260	ARG	2.6
1	A	262	LEU	2.6
1	B	283	GLN	2.5
3	D	1203	ARG	2.5
1	A	283	GLN	2.5
5	L	325	PRO	2.5
2	I	231	GLU	2.5
1	A	275	ILE	2.5
1	G	184	ALA	2.5
1	A	318	LEU	2.5
5	F	161	LEU	2.5
2	C	206	ALA	2.5
1	A	272	ALA	2.5
3	J	732	GLY	2.4
2	I	979	LEU	2.4
2	I	1010	GLN	2.4
1	H	144	ILE	2.4
1	A	247	PRO	2.4
2	I	310	ILE	2.4
5	F	288	MET	2.4
3	D	1302	TYR	2.4
6	M	103	LEU	2.4
2	I	492	MET	2.4
2	I	1008	GLN	2.4
4	K	30	MET	2.4
2	I	980	VAL	2.4
2	I	203	LYS	2.3
2	I	336	LEU	2.3
1	A	282	VAL	2.3
5	F	340	ALA	2.3
2	I	330	HIS	2.3
1	H	112	ALA	2.3
1	B	313	SER	2.3
1	H	129	VAL	2.3
3	D	1204	VAL	2.3
5	L	312	SER	2.3
1	A	273	GLU	2.3
2	C	541	GLU	2.3
4	K	34	GLY	2.3
1	A	304	LYS	2.3
2	C	492	MET	2.3
1	H	123	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	GLU	2.3
1	B	263	THR	2.2
5	L	490	PRO	2.2
1	B	319	GLU	2.2
2	I	982	GLY	2.2
1	A	274	ALA	2.2
5	L	319	ALA	2.2
2	C	231	GLU	2.2
1	G	47	LEU	2.2
2	I	299	LYS	2.2
1	H	58	GLU	2.2
3	J	1152	GLU	2.2
2	C	295	LYS	2.2
2	I	991	LYS	2.2
4	K	3	ARG	2.2
1	A	292	THR	2.2
3	J	756	GLU	2.1
2	C	338	THR	2.1
3	D	879	ALA	2.1
6	M	16	ALA	2.1
3	J	758	PRO	2.1
2	I	1007	LYS	2.1
2	I	224	PHE	2.1
1	A	267	ALA	2.1
1	A	307	LEU	2.1
1	A	291	LYS	2.1
2	I	565	GLU	2.1
4	K	57	GLY	2.1
6	M	17	ILE	2.1
2	I	187	GLU	2.1
2	I	1006	GLU	2.1
2	C	485	ASP	2.1
2	C	350	THR	2.0
5	F	307	THR	2.0
5	F	337	VAL	2.0
6	M	43	ILE	2.0
2	I	724	VAL	2.0
3	J	879	ALA	2.0
5	L	305	LEU	2.0
1	A	285	THR	2.0
3	D	848	VAL	2.0
3	J	1175	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	L	315	TRP	2.0
3	J	850	LYS	2.0
1	H	59	VAL	2.0
1	H	99	ILE	2.0
2	C	264	GLU	2.0
4	E	59	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	G4P	M	202	36/36	0.85	0.32	1.08	267,326,403,408	0
9	G4P	E	101	36/36	0.91	0.28	0.63	199,253,286,301	0
9	G4P	J	2004	36/36	0.76	0.39	0.20	306,370,455,463	0
8	ZN	D	2003	1/1	0.96	0.38	-0.51	295,295,295,295	0
8	ZN	D	2002	1/1	0.98	0.12	-0.88	273,273,273,273	0
8	ZN	J	2002	1/1	0.87	0.12	-1.00	264,264,264,264	0
8	ZN	M	201	1/1	0.94	0.05	-1.01	662,662,662,662	0
8	ZN	J	2003	1/1	0.97	0.28	-1.20	176,176,176,176	0
7	MG	D	2001	1/1	0.97	0.18	-1.45	162,162,162,162	0
7	MG	J	2001	1/1	0.96	0.40	-	184,184,184,184	0

6.5 Other polymers [i](#)

There are no such residues in this entry.