Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:28 PM EDT

PDB ID	:	6WOX
Title	:	Thermus thermophilus RNA polymerase initially transcribing complex with 2'dCTP
Authors	:	Shin, Y.; Murakami, K.S.
Deposited on	:	2020-04-26
Resolution	:	3.14 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

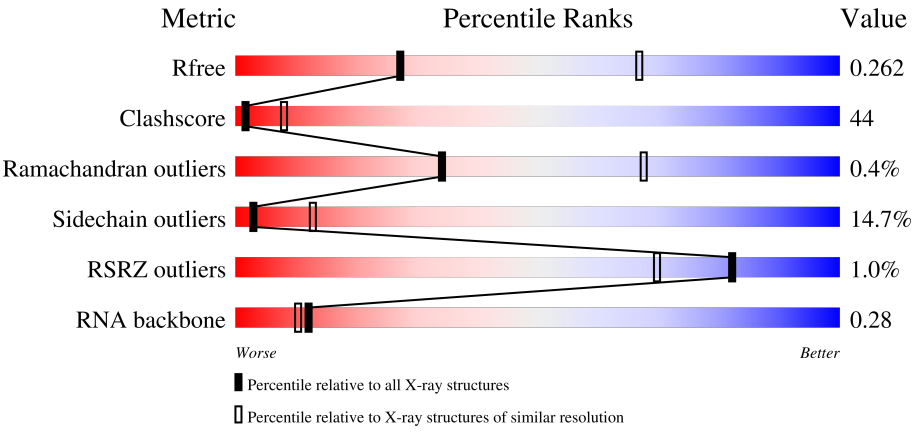
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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.



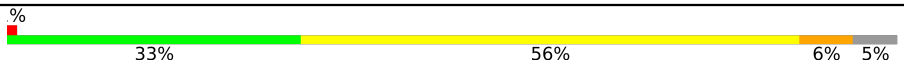
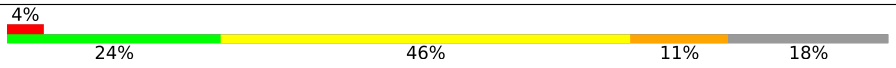
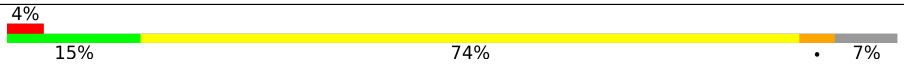
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	315	18% 45% 9% 28%
1	B	315	23% 42% 7% 29%
2	C	1119	% 37% 54% 9%
3	D	1505	% 38% 52% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	
5	F	423	
6	G	22	
7	H	27	
8	I	3	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28581 atoms, of which 12 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11721	7431	2063	2192	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	86	LYS	ARG	conflict	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP *AP*GP*TP*GP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			351	166	65	103	17			

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

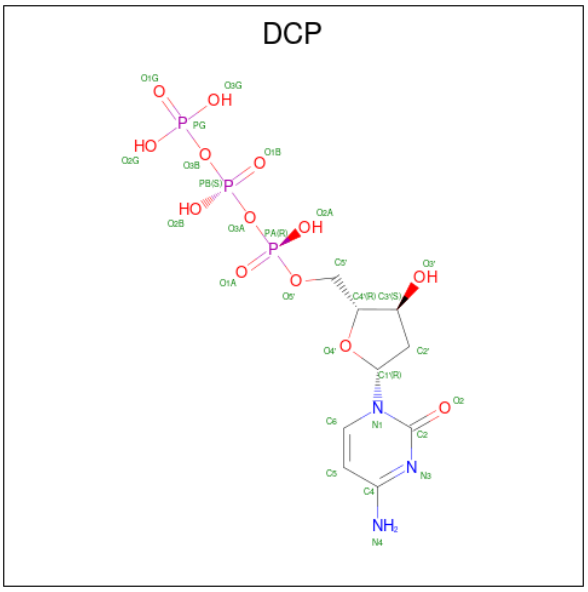
- Molecule 8 is a RNA chain called RNA (5'-R(*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			62	29	13	18	2			

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	D	1	Total	C	H	N	O	P	0	0
			40	9	12	3	13	3		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Mg	0	0
			1	1		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

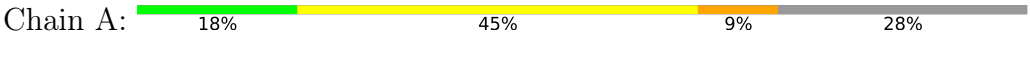
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	2	Total	Zn	0	0
			2	2		

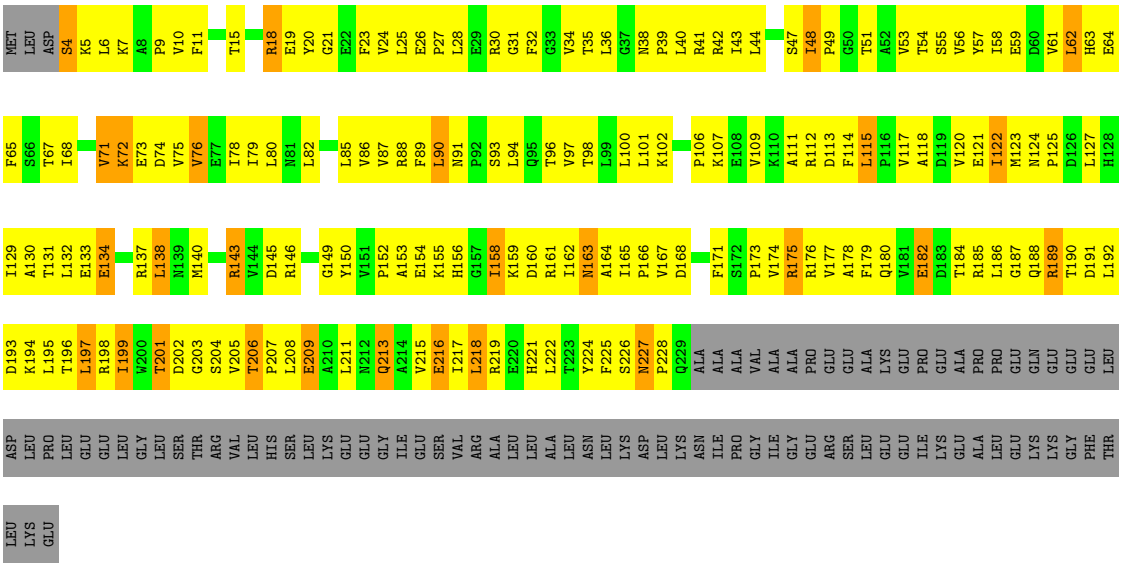
3 Residue-property plots (i)

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

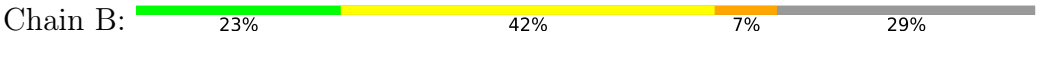
Chain A:

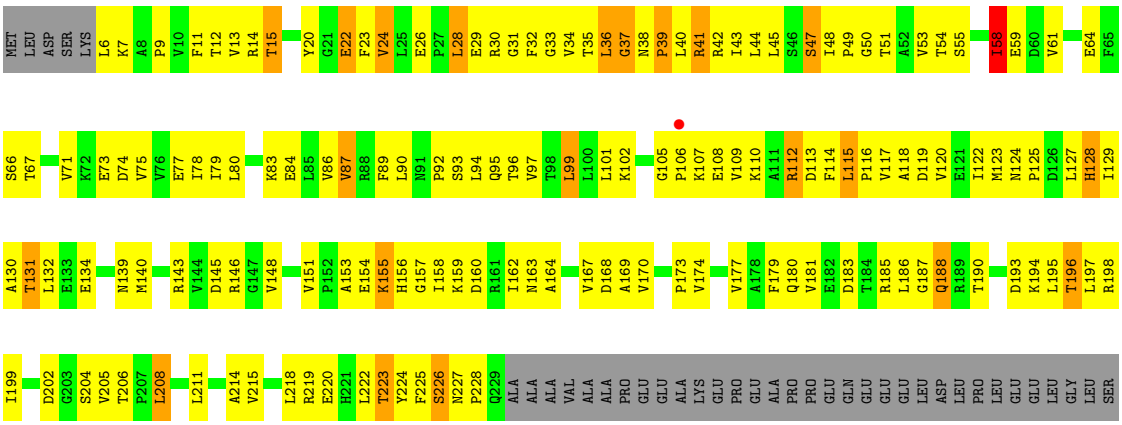




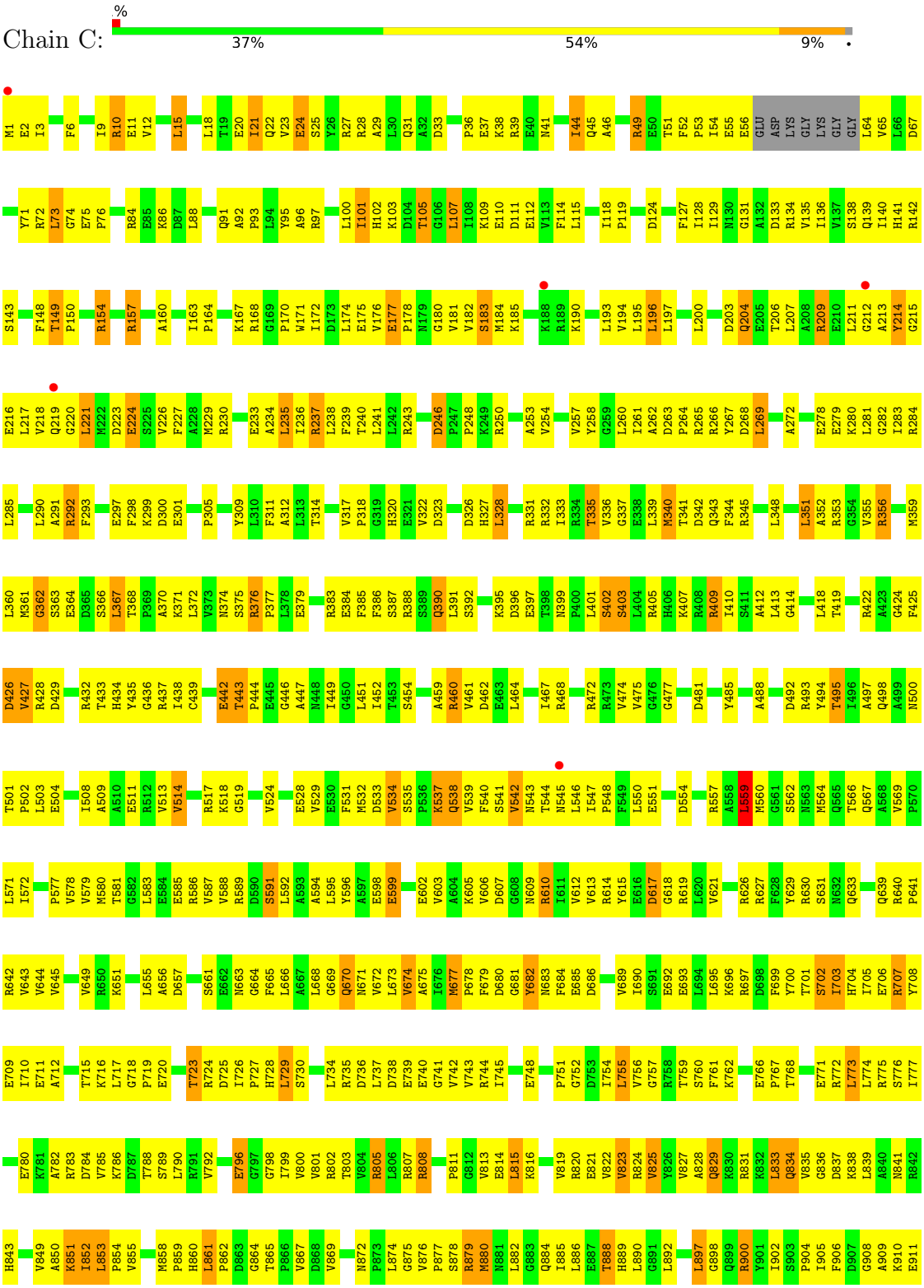
• Molecule 1: DNA-directed RNA polymerase subunit alpha

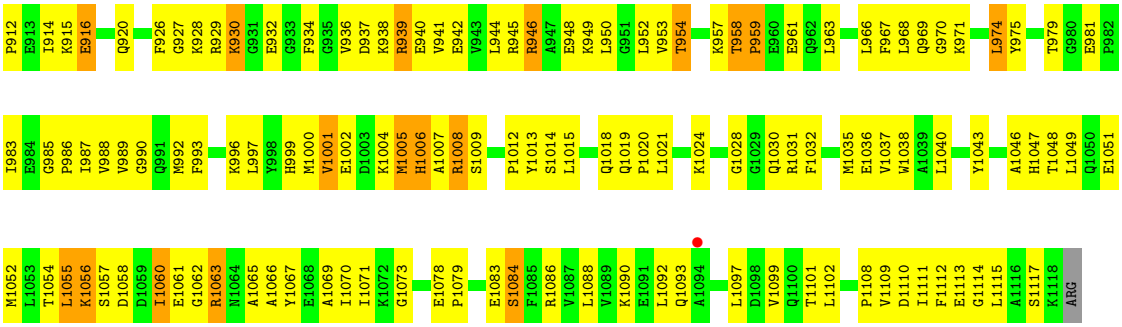
Chain B:



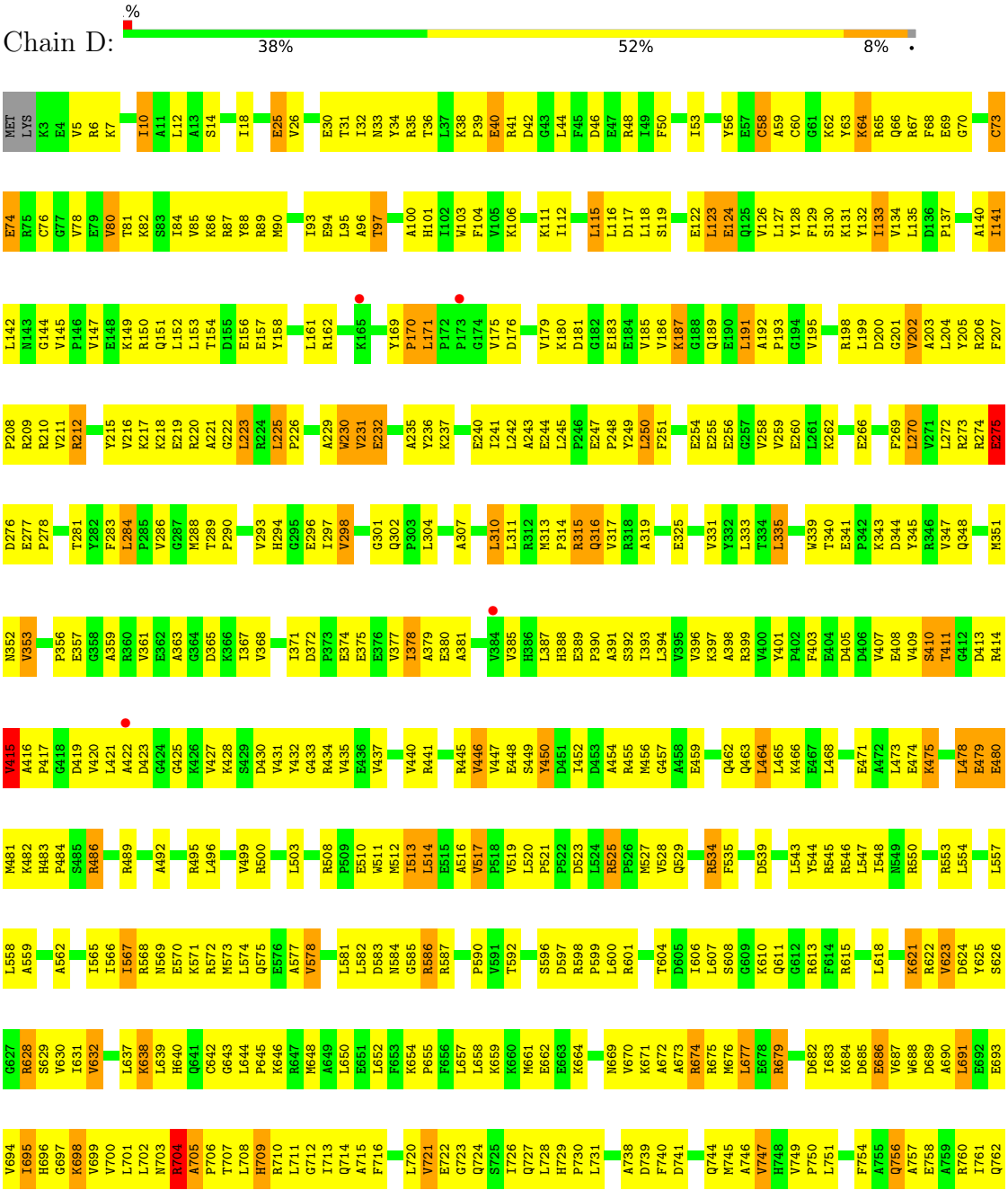


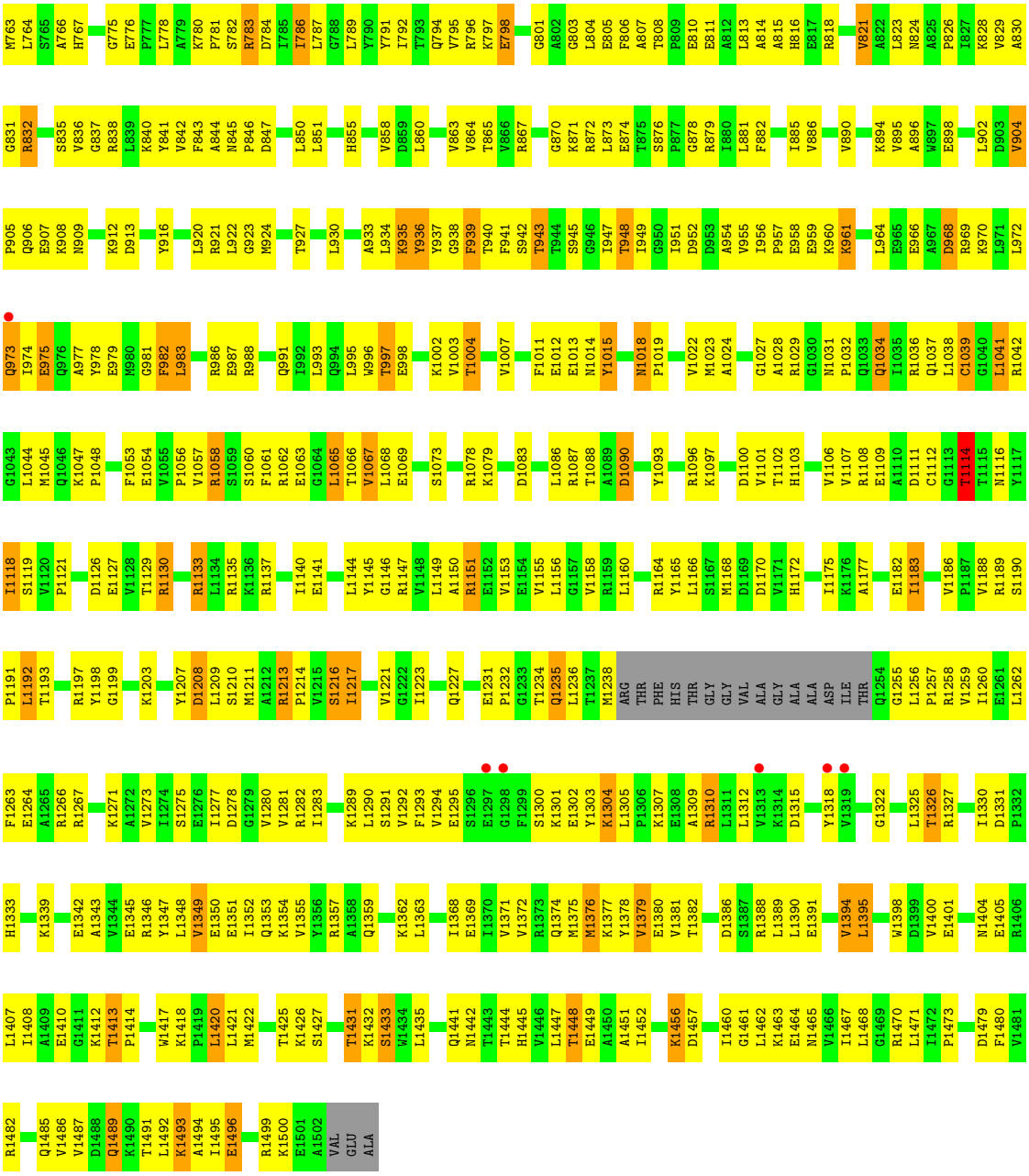
• Molecule 2: DNA-directed RNA polymerase subunit beta





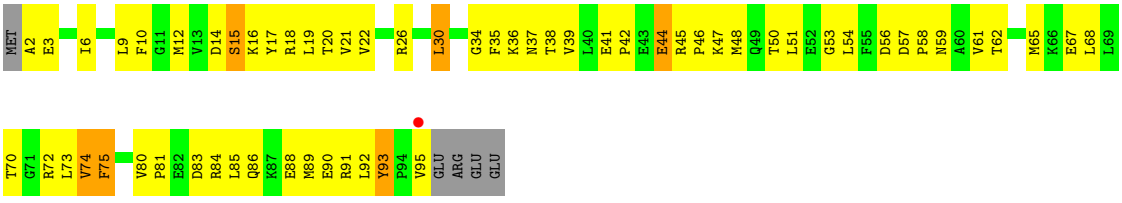
• Molecule 3: DNA-directed RNA polymerase subunit beta'





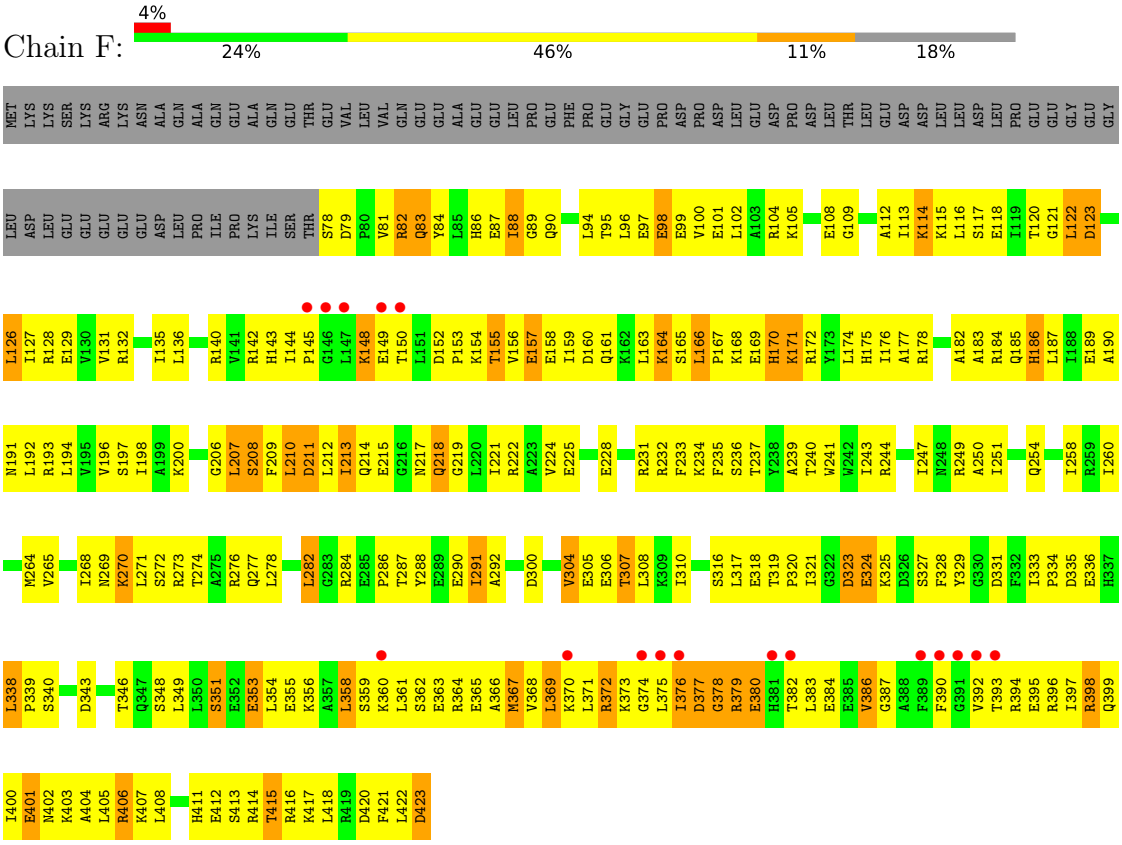
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



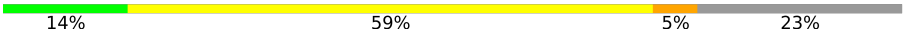
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



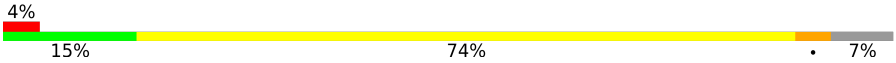
• Molecule 6: DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*G)-3')

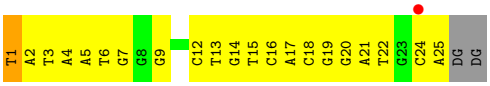
Chain G:



• Molecule 7: DNA (25-MER)

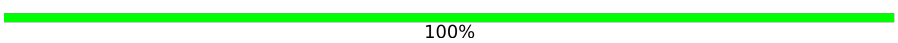
Chain H:





• Molecule 8: RNA (5'-R(*GP*CP*A)-3')

Chain I:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.44Å 102.65Å 295.38Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	29.93 – 3.14 29.93 – 3.14	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.93-3.14) 93.7 (29.93-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.196 , 0.261 0.197 , 0.262	Depositor DCC
R_{free} test set	2001 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å^2)	87.4	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28581	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, MG, ZN, DCP

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	0.53	0/1814	0.67	0/2466
1	B	0.51	0/1799	0.70	1/2447 (0.0%)
2	C	0.51	0/8937	0.69	5/12087 (0.0%)
3	D	0.54	2/11927 (0.0%)	0.70	4/16127 (0.0%)
4	E	0.49	0/775	0.64	0/1045
5	F	0.49	0/2852	0.63	0/3837
6	G	1.24	1/393 (0.3%)	1.17	3/605 (0.5%)
7	H	1.15	1/580 (0.2%)	1.11	0/895
8	I	0.89	0/69	1.57	0/106
All	All	0.56	4/29146 (0.0%)	0.71	13/39615 (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
2	C	0	1
3	D	0	5
5	F	0	1
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	GLY	C-N	7.80	1.51	1.34
3	D	1114	THR	CB-CG2	5.39	1.70	1.52
6	G	13	DA	C3'-O3'	-5.39	1.36	1.44
7	H	1	DT	C1'-N1	5.34	1.56	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	13	DA	O4'-C4'-C3'	-7.78	101.33	106.00
3	D	170	PRO	C-N-CA	-6.65	105.08	121.70
3	D	225	LEU	CA-CB-CG	6.03	129.18	115.30
2	C	107	LEU	CA-CB-CG	5.92	128.92	115.30
6	G	14	DG	O5'-P-OP1	-5.87	100.42	105.70
2	C	682	TYR	O-C-N	-5.69	113.59	122.70
2	C	559	LEU	CB-CG-CD1	-5.52	101.61	111.00
3	D	310	LEU	CA-CB-CG	5.49	127.93	115.30
3	D	415	VAL	C-N-CA	5.42	135.26	121.70
2	C	686	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	B	28	LEU	CA-CB-CG	5.34	127.58	115.30
6	G	16	DG	O4'-C4'-C3'	-5.12	102.45	104.50
2	C	142	ARG	C-N-CA	-5.07	109.04	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	ILE	Peptide
2	C	362	GLY	Peptide
3	D	275	GLU	Peptide
3	D	64	LYS	Peptide
3	D	704	ARG	Peptide
3	D	782	SER	Peptide
3	D	983	LEU	Peptide
5	F	323	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	219	0
1	B	1767	0	1816	214	0
2	C	8770	0	8874	815	0
3	D	11721	0	11941	1119	0
4	E	761	0	778	81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	2807	0	2882	288	0
6	G	351	0	192	17	0
7	H	516	0	283	41	0
8	I	62	0	34	0	0
9	C	1	0	0	0	0
10	D	28	12	12	3	0
11	D	1	0	0	0	0
12	D	2	0	0	0	0
All	All	28569	12	28646	2541	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (2541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:ALA:HB1	3:D:393:ILE:HD11	1.17	1.15
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.21	1.14
3:D:1234:THR:HB	3:D:1235:GLN:HB2	1.31	1.13
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.21	1.12
1:A:88:ARG:HB3	1:A:123:MET:HE3	1.29	1.11
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.21	1.11
2:C:805:ARG:HG3	2:C:823:VAL:HG23	1.31	1.10
3:D:367:ILE:HD11	3:D:379:ALA:HB2	1.35	1.09
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.17	1.08
2:C:766:GLU:HG2	2:C:767:PRO:HD2	1.34	1.08
5:F:362:SER:HB3	5:F:365:GLU:HG2	1.30	1.07
2:C:690:ILE:HG13	2:C:852:ILE:HG23	1.37	1.06
3:D:65:ARG:HB3	5:F:377:ASP:HA	1.37	1.06
3:D:1060:SER:HB3	3:D:1063:GLU:HG3	1.32	1.06
1:B:53:VAL:HG12	1:B:167:VAL:HG11	1.33	1.05
2:C:690:ILE:HD11	2:C:852:ILE:HD13	1.38	1.05
2:C:474:VAL:HG11	2:C:529:VAL:HG12	1.38	1.05
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.39	1.05
3:D:70:GLY:H	3:D:80:VAL:HG23	1.19	1.04
5:F:412:GLU:HG3	5:F:418:LEU:HD13	1.40	1.03
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.41	1.02
3:D:791:TYR:CE1	3:D:945:SER:HB2	1.95	1.02
2:C:878:SER:HA	3:D:1034:GLN:HE22	1.22	1.01
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.42	1.01
1:A:25:LEU:HB3	1:A:28:LEU:HD11	1.39	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.42	1.00
2:C:734:LEU:HD23	2:C:737:LEU:HD12	1.44	1.00
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.43	1.00
1:A:155:LYS:O	1:A:155:LYS:NZ	1.95	0.99
2:C:944:LEU:HD11	2:C:963:LEU:HD21	1.46	0.98
3:D:582:LEU:O	3:D:604:THR:HG23	1.65	0.97
1:A:88:ARG:CB	1:A:123:MET:HE3	1.94	0.97
2:C:1012:PRO:HB2	2:C:1021:LEU:HD13	1.46	0.97
2:C:890:LEU:HB2	2:C:914:ILE:HD12	1.46	0.96
3:D:689:ASP:HB3	4:E:51:LEU:HD13	1.44	0.96
5:F:361:LEU:HD11	5:F:411:HIS:HB2	1.48	0.96
2:C:495:THR:HG23	2:C:517:ARG:HG3	1.45	0.95
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.31	0.95
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.48	0.95
3:D:1273:VAL:H	3:D:1326:THR:HG23	1.30	0.95
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.48	0.94
3:D:259:VAL:HG13	3:D:270:LEU:HD21	1.49	0.94
3:D:1234:THR:CB	3:D:1235:GLN:HB2	1.98	0.93
5:F:95:THR:H	5:F:98:GLU:HG3	1.31	0.93
5:F:386:VAL:HA	5:F:390:PHE:CE1	2.02	0.93
2:C:775:ARG:HH11	5:F:422:LEU:HD23	1.30	0.93
3:D:709:HIS:HA	3:D:1227:GLN:HG2	1.48	0.92
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.02	0.92
3:D:65:ARG:CB	5:F:377:ASP:HA	2.00	0.92
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.51	0.92
2:C:182:VAL:HG22	2:C:221:LEU:HD23	1.50	0.91
2:C:674:VAL:HG23	2:C:869:VAL:HB	1.48	0.91
3:D:1042:ARG:HB3	3:D:1057:VAL:HG13	1.52	0.91
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.02	0.91
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.52	0.91
3:D:767:HIS:HA	3:D:924:MET:HE3	1.51	0.91
2:C:958:THR:HG23	2:C:961:GLU:HG3	1.53	0.91
3:D:520:LEU:O	3:D:525:ARG:NH1	2.03	0.91
2:C:878:SER:HA	3:D:1034:GLN:NE2	1.85	0.91
2:C:180:GLY:O	2:C:217:LEU:HD22	1.70	0.90
3:D:67:ARG:NH2	5:F:377:ASP:OD2	2.04	0.90
2:C:751:PRO:HA	2:C:792:VAL:HG22	1.52	0.89
2:C:627:ARG:HH21	2:C:641:PRO:HD3	1.35	0.89
2:C:715:THR:HG22	2:C:717:LEU:H	1.37	0.89
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.53	0.89
3:D:1342:GLU:N	3:D:1342:GLU:OE1	2.03	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:HB3	1:A:123:MET:HE2	1.55	0.89
2:C:690:ILE:CG1	2:C:852:ILE:HG23	2.03	0.89
2:C:815:LEU:HD12	2:C:819:VAL:HG23	1.53	0.89
1:A:62:LEU:HA	1:A:163:ASN:HB3	1.55	0.88
2:C:569:VAL:HG21	2:C:1000:MET:CE	2.03	0.88
3:D:1479:ASP:OD1	3:D:1482:ARG:NH1	2.05	0.88
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.38	0.88
4:E:50:THR:HG22	4:E:53:GLY:O	1.71	0.88
5:F:166:LEU:HB2	5:F:171:LYS:HB2	1.56	0.88
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.06	0.88
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.09	0.88
3:D:181:ASP:HB2	3:D:205:TYR:HD1	1.40	0.87
3:D:1263:PHE:O	3:D:1375:MET:HE2	1.74	0.87
3:D:216:VAL:HA	3:D:340:THR:HG22	1.54	0.87
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.04	0.87
3:D:1410:GLU:HB3	3:D:1412:LYS:HE3	1.57	0.87
5:F:109:GLY:O	5:F:113:ILE:HG13	1.75	0.87
7:H:21:DA:H1'	7:H:22:DT:H5'	1.58	0.86
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.10	0.86
5:F:361:LEU:CD1	5:F:411:HIS:HB2	2.06	0.86
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.07	0.86
2:C:1012:PRO:CB	2:C:1021:LEU:HD13	2.05	0.86
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.55	0.86
3:D:1232:PRO:O	3:D:1235:GLN:HB3	1.75	0.86
5:F:338:LEU:HD23	5:F:339:PRO:CD	2.05	0.86
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.41	0.86
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.57	0.86
1:A:198:ARG:O	1:A:199:ILE:HG12	1.75	0.86
2:C:816:LYS:O	2:C:819:VAL:HG22	1.76	0.86
3:D:1213:ARG:HG3	3:D:1214:PRO:HD2	1.58	0.86
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.09	0.85
3:D:335:LEU:H	3:D:335:LEU:HD12	1.40	0.85
3:D:828:LYS:HE2	3:D:831:GLY:H	1.38	0.85
1:B:36:LEU:O	1:B:38:ASN:N	2.08	0.85
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.58	0.85
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.58	0.85
5:F:95:THR:HG22	5:F:98:GLU:CG	2.06	0.85
3:D:371:ILE:HD13	5:F:232:ARG:HD3	1.58	0.84
3:D:798:GLU:CG	3:D:824:ASN:HB2	2.07	0.84
2:C:853:LEU:HB2	2:C:858:MET:CE	2.07	0.84
2:C:204:GLN:HG2	2:C:227:PHE:CZ	2.12	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.56	0.84
1:A:18:ARG:HH21	1:A:88:ARG:CZ	1.89	0.84
5:F:369:LEU:HD23	5:F:372:ARG:HB2	1.60	0.84
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.59	0.84
5:F:95:THR:HG22	5:F:98:GLU:HG2	1.57	0.84
3:D:474:GLU:OE2	3:D:1388:ARG:NH2	2.11	0.84
3:D:65:ARG:HD3	5:F:377:ASP:HA	1.57	0.83
2:C:888:THR:HG22	2:C:990:GLY:HA3	1.60	0.83
2:C:1008:ARG:HD2	2:C:1028:GLY:O	1.78	0.83
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.13	0.83
3:D:41:ARG:HE	3:D:48:ARG:HD3	1.42	0.83
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.08	0.83
3:D:795:VAL:O	3:D:797:LYS:NZ	2.12	0.83
1:B:86:VAL:HG12	1:B:124:ASN:OD1	1.79	0.83
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.60	0.82
2:C:938:LYS:O	2:C:941:VAL:HG22	1.78	0.82
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.61	0.82
3:D:810:GLU:N	3:D:810:GLU:OE2	2.12	0.82
5:F:390:PHE:CD2	5:F:397:ILE:HG12	2.15	0.82
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.59	0.81
5:F:362:SER:HB3	5:F:365:GLU:CG	2.10	0.81
5:F:112:ALA:O	5:F:116:LEU:HB2	1.80	0.81
3:D:1236:LEU:HD22	3:D:1359:GLN:HG3	1.61	0.81
5:F:364:ARG:HA	5:F:367:MET:HG2	1.61	0.81
1:B:117:VAL:HG12	1:B:118:ALA:H	1.43	0.81
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.61	0.81
2:C:1055:LEU:CD2	2:C:1079:PRO:HB3	2.10	0.81
2:C:808:ARG:NH2	2:C:808:ARG:HB3	1.96	0.81
2:C:715:THR:HG22	2:C:717:LEU:N	1.96	0.80
3:D:838:ARG:HD3	3:D:874:GLU:HG2	1.63	0.80
3:D:1192:LEU:HD23	3:D:1369:GLU:HB3	1.62	0.80
1:B:107:LYS:NZ	1:B:113:ASP:OD2	2.13	0.80
1:A:55:SER:CB	1:A:158:ILE:HG22	2.09	0.80
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.63	0.80
1:A:115:LEU:O	1:A:115:LEU:HD23	1.81	0.80
3:D:137:PRO:HB3	3:D:147:VAL:HG23	1.64	0.80
1:A:222:LEU:CD2	1:B:218:LEU:HD23	2.07	0.80
7:H:20:DG:H2"	7:H:21:DA:H5'	1.63	0.80
2:C:102:HIS:HB2	2:C:107:LEU:HB2	1.63	0.79
3:D:1376:MET:HE1	3:D:1421:LEU:HD13	1.63	0.79
2:C:109:LYS:HD2	2:C:110:GLU:H	1.47	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:495:THR:HG23	2:C:517:ARG:CG	2.11	0.79
3:D:401:TYR:OH	3:D:430:ASP:HB2	1.82	0.79
1:A:89:PHE:HB2	1:A:146:ARG:HH22	1.45	0.79
1:A:218:LEU:O	1:A:222:LEU:HD12	1.82	0.79
2:C:460:ARG:HD2	2:C:485:TYR:CE1	2.17	0.79
2:C:833:LEU:HD12	2:C:834:GLN:N	1.97	0.79
3:D:683:ILE:CG2	3:D:687:VAL:HG11	2.12	0.79
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.64	0.79
5:F:123:ASP:OD1	5:F:126:LEU:N	2.14	0.79
2:C:25:SER:OG	2:C:335:THR:OG1	2.01	0.79
2:C:627:ARG:NH2	2:C:640:ARG:HA	1.97	0.79
2:C:1055:LEU:HD21	2:C:1079:PRO:HB3	1.63	0.79
5:F:120:THR:HG23	5:F:122:LEU:H	1.46	0.79
2:C:109:LYS:CG	2:C:368:THR:HG22	2.08	0.79
3:D:175:VAL:CG1	3:D:193:PRO:HG2	2.13	0.79
2:C:569:VAL:HG21	2:C:1000:MET:HE1	1.65	0.79
3:D:1493:LYS:NZ	3:D:1496:GLU:OE2	2.16	0.79
2:C:140:ILE:HD13	2:C:331:ARG:HH11	1.48	0.78
3:D:421:LEU:HD13	3:D:428:LYS:HA	1.64	0.78
3:D:885:ILE:HD13	3:D:937:TYR:CD1	2.19	0.78
2:C:710:ILE:HG22	2:C:823:VAL:HG12	1.63	0.78
3:D:65:ARG:HD3	5:F:377:ASP:CA	2.13	0.78
1:A:164:ALA:O	1:A:166:PRO:HD3	1.84	0.78
2:C:149:THR:HA	2:C:322:VAL:HG13	1.66	0.78
3:D:776:GLU:OE2	3:D:1362:LYS:HD3	1.82	0.78
3:D:410:SER:O	3:D:435:VAL:HG11	1.84	0.78
1:A:40:LEU:HD23	1:A:218:LEU:HD12	1.66	0.78
2:C:260:LEU:C	2:C:261:ILE:HD12	2.04	0.78
3:D:671:LYS:HZ2	5:F:423:ASP:HA	1.47	0.78
1:A:20:TYR:O	1:A:207:PRO:HG2	1.84	0.78
1:B:185:ARG:NH1	1:B:187:GLY:O	2.16	0.78
2:C:859:PRO:O	2:C:867:VAL:HG22	1.84	0.78
2:C:967:PHE:O	2:C:970:GLY:N	2.15	0.78
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.19	0.78
2:C:260:LEU:HB3	2:C:261:ILE:CD1	2.13	0.77
2:C:366:SER:O	2:C:371:LYS:NZ	2.17	0.77
2:C:424:GLY:O	2:C:428:ARG:HD2	1.83	0.77
3:D:657:LEU:O	3:D:661:MET:HE2	1.84	0.77
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.12	0.77
2:C:474:VAL:HG11	2:C:529:VAL:CG1	2.13	0.77
1:B:115:LEU:HD22	1:B:116:PRO:HD2	1.64	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:HIS:HE1	1:B:131:THR:HG22	1.50	0.77
2:C:65:VAL:HG22	2:C:101:ILE:HG23	1.67	0.77
2:C:1115:LEU:HD23	3:D:85:VAL:CG1	2.15	0.77
3:D:721:VAL:HG23	3:D:722:GLU:O	1.83	0.77
3:D:254:GLU:O	3:D:255:GLU:HG2	1.85	0.77
3:D:315:ARG:H	3:D:315:ARG:HD2	1.48	0.77
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.18	0.76
1:B:115:LEU:HD22	1:B:116:PRO:CD	2.15	0.76
5:F:392:VAL:HG21	5:F:396:ARG:HG2	1.65	0.76
2:C:808:ARG:HB3	2:C:808:ARG:HH21	1.47	0.76
2:C:196:LEU:O	2:C:196:LEU:HD22	1.86	0.76
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.68	0.76
3:D:241:ILE:HD12	3:D:310:LEU:HD23	1.65	0.76
3:D:650:LEU:HD12	3:D:657:LEU:HD22	1.67	0.76
6:G:3:DT:H2"	6:G:4:DG:C8	2.21	0.76
1:A:101:LEU:HD23	1:A:102:LYS:N	2.00	0.76
5:F:287:THR:HG23	5:F:290:GLU:OE2	1.86	0.76
3:D:275:GLU:O	3:D:277:GLU:N	2.18	0.76
3:D:558:LEU:HD23	3:D:567:ILE:CD1	2.16	0.76
3:D:1489:GLN:HE22	3:D:1492:LEU:HD12	1.48	0.76
5:F:274:THR:O	5:F:278:LEU:HG	1.86	0.76
1:A:18:ARG:HH11	1:A:18:ARG:HG3	1.49	0.76
1:A:79:ILE:HD12	1:A:167:VAL:CG2	2.16	0.76
3:D:1496:GLU:O	3:D:1500:LYS:HG2	1.86	0.76
5:F:96:LEU:O	5:F:100:VAL:HG23	1.86	0.76
3:D:284:LEU:HD23	3:D:290:PRO:HG3	1.68	0.75
3:D:407:VAL:HA	3:D:422:ALA:HB1	1.68	0.75
5:F:131:VAL:HG11	5:F:177:ALA:HB1	1.68	0.75
5:F:354:LEU:HD12	5:F:355:GLU:N	2.01	0.75
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.68	0.75
3:D:473:LEU:HD21	3:D:495:ARG:NH2	2.01	0.75
2:C:317:VAL:HB	2:C:320:HIS:CD2	2.21	0.75
5:F:361:LEU:HG	5:F:411:HIS:HD2	1.50	0.75
2:C:124:ASP:HA	2:C:592:LEU:HD13	1.67	0.75
2:C:513:VAL:HG22	2:C:524:VAL:O	1.84	0.75
2:C:905:ILE:HG23	2:C:906:PHE:HD1	1.52	0.75
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.22	0.75
1:A:18:ARG:HH11	1:A:18:ARG:CG	2.00	0.75
1:A:150:TYR:CE1	2:C:696:LYS:HG2	2.22	0.75
2:C:211:LEU:HD23	2:C:218:VAL:HG22	1.68	0.75
3:D:259:VAL:HG13	3:D:270:LEU:CD2	2.17	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:767:HIS:HA	3:D:924:MET:CE	2.16	0.75
2:C:886:LEU:HD11	3:D:951:ILE:HD13	1.69	0.74
3:D:1236:LEU:CD2	3:D:1359:GLN:HG3	2.16	0.74
2:C:56:GLU:OE2	2:C:103:LYS:HE2	1.86	0.74
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	1.88	0.74
3:D:169:TYR:O	3:D:392:SER:OG	2.06	0.74
3:D:671:LYS:NZ	5:F:423:ASP:HA	2.03	0.74
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.69	0.74
3:D:1042:ARG:HB3	3:D:1057:VAL:CG1	2.17	0.74
1:A:35:THR:OG1	1:B:42:ARG:HD3	1.88	0.74
2:C:880:MET:HE2	3:D:1061:PHE:HE2	1.51	0.74
2:C:988:VAL:HG23	3:D:948:THR:CG2	2.18	0.74
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.51	0.74
3:D:864:VAL:HG12	3:D:865:THR:N	2.03	0.74
3:D:1028:ALA:O	3:D:1029:ARG:HG2	1.86	0.74
2:C:805:ARG:HG3	2:C:823:VAL:CG2	2.15	0.73
3:D:864:VAL:HG12	3:D:865:THR:H	1.51	0.73
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.70	0.73
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.53	0.73
3:D:62:LYS:HD2	3:D:63:TYR:CE2	2.23	0.73
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.68	0.73
1:A:206:THR:HG22	1:A:209:GLU:CG	2.18	0.73
2:C:143:SER:HB2	2:C:332:ARG:HD2	1.68	0.73
2:C:690:ILE:CD1	2:C:852:ILE:HG23	2.18	0.73
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.19	0.73
3:D:1494:ALA:CB	4:E:92:LEU:HD11	2.17	0.73
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.02	0.73
2:C:49:ARG:NH1	2:C:52:PHE:O	2.21	0.73
2:C:718:GLY:HA3	2:C:761:PHE:CE1	2.24	0.73
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.69	0.73
5:F:362:SER:CB	5:F:365:GLU:HG2	2.14	0.73
2:C:564:MET:HG2	2:C:997:LEU:HD11	1.70	0.73
3:D:236:TYR:H	3:D:319:ALA:HB3	1.53	0.73
3:D:930:LEU:HD11	3:D:934:LEU:HD11	1.69	0.73
1:A:11:PHE:CD2	1:B:225:PHE:HA	2.24	0.73
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.19	0.73
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.70	0.73
2:C:958:THR:HG23	2:C:961:GLU:CG	2.18	0.73
3:D:82:LYS:HB2	3:D:84:ILE:HG22	1.69	0.73
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.70	0.73
2:C:418:LEU:HD21	2:C:427:VAL:HG11	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:298:VAL:HG12	3:D:302:GLN:CD	2.09	0.73
1:B:86:VAL:CG1	1:B:123:MET:HB2	2.19	0.73
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.71	0.73
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.20	0.73
3:D:348:GLN:HB2	3:D:351:MET:HG3	1.69	0.72
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.71	0.72
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.54	0.72
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.54	0.72
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.71	0.72
2:C:1005:MET:SD	3:D:648:MET:HG3	2.29	0.72
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.24	0.72
3:D:973:GLN:HG3	3:D:973:GLN:O	1.89	0.72
1:A:20:TYR:OH	1:A:198:ARG:NE	2.22	0.72
7:H:24:DC:H2"	7:H:25:DA:OP2	1.90	0.72
1:A:226:SER:O	1:A:228:PRO:HD3	1.90	0.72
1:B:84:GLU:OE2	3:D:867:ARG:NH1	2.22	0.72
1:B:220:GLU:O	1:B:223:THR:OG1	2.06	0.72
2:C:937:ASP:OD1	2:C:939:ARG:HG2	1.90	0.72
3:D:122:GLU:HG2	3:D:152:LEU:HD11	1.71	0.72
3:D:185:VAL:HG13	3:D:189:GLN:OE1	1.90	0.72
2:C:906:PHE:CE2	3:D:1067:VAL:HA	2.25	0.72
1:B:106:PRO:HD3	1:B:134:GLU:HG2	1.71	0.72
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.19	0.72
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.25	0.72
4:E:30:LEU:HD22	4:E:35:PHE:HD1	1.55	0.72
3:D:475:LYS:HA	3:D:478:LEU:HD11	1.72	0.71
3:D:486:ARG:HG3	3:D:489:ARG:NH2	2.04	0.71
2:C:767:PRO:HG3	2:C:782:ALA:HB1	1.72	0.71
2:C:879:ARG:NH2	10:D:1601:DCP:O1G	2.22	0.71
3:D:475:LYS:O	3:D:478:LEU:HD12	1.91	0.71
1:B:73:GLU:OE1	1:B:73:GLU:N	2.22	0.71
2:C:835:VAL:HA	2:C:849:VAL:HG12	1.72	0.71
2:C:503:LEU:HD22	2:C:508:ILE:HA	1.71	0.71
1:B:127:LEU:HD23	1:B:128:HIS:N	2.05	0.71
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.26	0.71
3:D:684:LYS:O	3:D:687:VAL:HG12	1.90	0.71
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	1.90	0.71
6:G:6:DA:H2"	6:G:7:DT:O5'	1.91	0.71
3:D:1431:THR:HG23	3:D:1433:SER:N	2.06	0.71
2:C:176:VAL:HG11	2:C:217:LEU:HD13	1.71	0.71
2:C:317:VAL:HG13	2:C:318:PRO:HD2	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1213:ARG:HG3	3:D:1214:PRO:CD	2.21	0.71
3:D:1499:ARG:NH1	4:E:84:ARG:HG2	2.06	0.71
1:A:101:LEU:O	1:A:102:LYS:HG2	1.90	0.71
3:D:30:GLU:OE1	3:D:40:GLU:HG2	1.90	0.71
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	2.05	0.71
3:D:1078:ARG:HG2	3:D:1078:ARG:HH11	1.54	0.71
1:A:73:GLU:OE2	1:A:130:ALA:HA	1.90	0.70
1:B:96:THR:HG22	1:B:97:VAL:H	1.56	0.70
2:C:1066:ALA:O	2:C:1069:ALA:N	2.24	0.70
3:D:975:GLU:O	3:D:979:GLU:HB2	1.90	0.70
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.73	0.70
1:A:55:SER:HB3	1:A:158:ILE:HG22	1.72	0.70
1:B:124:ASN:ND2	1:B:127:LEU:HD12	2.06	0.70
2:C:143:SER:HB2	2:C:332:ARG:CD	2.20	0.70
2:C:775:ARG:NH1	5:F:422:LEU:HD23	2.05	0.70
2:C:833:LEU:HD12	2:C:834:GLN:H	1.56	0.70
3:D:1389:LEU:O	3:D:1390:LEU:HD23	1.90	0.70
5:F:364:ARG:HA	5:F:367:MET:CG	2.22	0.70
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.74	0.70
3:D:982:PHE:O	3:D:983:LEU:HG	1.91	0.70
3:D:1156:LEU:HD23	3:D:1182:GLU:OE1	1.91	0.70
5:F:353:GLU:OE2	5:F:417:LYS:HG3	1.90	0.70
1:A:30:ARG:HB2	1:A:191:ASP:O	1.91	0.70
2:C:102:HIS:HB2	2:C:107:LEU:CB	2.22	0.70
2:C:878:SER:CA	3:D:1034:GLN:HE22	2.00	0.70
2:C:988:VAL:HG21	3:D:949:ILE:O	1.91	0.70
2:C:223:ASP:O	2:C:226:VAL:HG23	1.92	0.70
2:C:811:PRO:O	2:C:813:VAL:HG12	1.91	0.70
3:D:697:GLY:O	3:D:760:ARG:NH1	2.23	0.70
5:F:234:LYS:HD3	7:H:5:DA:OP2	1.92	0.70
5:F:328:PHE:HB2	5:F:331:ASP:OD2	1.92	0.70
1:A:39:PRO:HG3	1:B:39:PRO:HG2	1.72	0.70
1:B:197:LEU:HD12	1:B:198:ARG:N	2.07	0.70
2:C:352:ALA:O	2:C:356:ARG:HD2	1.92	0.69
2:C:910:LYS:O	2:C:914:ILE:HG22	1.92	0.69
1:A:211:LEU:O	1:A:215:VAL:HG23	1.92	0.69
3:D:65:ARG:HD3	5:F:377:ASP:H	1.58	0.69
3:D:615:ARG:HD2	3:D:1096:ARG:NH2	2.07	0.69
3:D:885:ILE:HG23	3:D:937:TYR:CE1	2.27	0.69
1:A:72:LYS:NZ	2:C:643:VAL:O	2.23	0.69
1:B:106:PRO:CD	1:B:134:GLU:HG2	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.74	0.69
2:C:756:VAL:HG21	2:C:823:VAL:CG1	2.22	0.69
3:D:116:LEU:HB2	3:D:118:LEU:HD12	1.74	0.69
3:D:371:ILE:HG13	3:D:372:ASP:N	2.07	0.69
3:D:816:HIS:HB2	3:D:836:VAL:HG11	1.75	0.69
3:D:1137:ARG:O	3:D:1141:GLU:HG3	1.92	0.69
3:D:1271:LYS:HD2	3:D:1331:ASP:HB2	1.73	0.69
5:F:369:LEU:O	5:F:369:LEU:HD22	1.93	0.69
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.74	0.69
1:B:226:SER:O	1:B:228:PRO:HD3	1.93	0.69
2:C:585:GLU:O	2:C:588:VAL:HG12	1.90	0.69
2:C:263:ASP:O	2:C:265:ARG:N	2.24	0.69
3:D:645:PRO:HG2	3:D:724:GLN:O	1.91	0.69
1:B:38:ASN:HB3	1:B:39:PRO:CD	2.22	0.69
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.56	0.69
3:D:573:MET:SD	5:F:210:LEU:HB3	2.33	0.69
2:C:874:LEU:HD12	3:D:784:ASP:OD1	1.93	0.69
3:D:7:LYS:HD3	3:D:1456:LYS:NZ	2.06	0.69
3:D:116:LEU:HB2	3:D:118:LEU:CD1	2.23	0.69
2:C:195:LEU:CD1	2:C:234:ALA:HB1	2.23	0.69
2:C:587:VAL:O	2:C:591:SER:HB3	1.93	0.69
5:F:286:PRO:HB2	5:F:291:ILE:HD12	1.73	0.69
6:G:6:DA:H5"	6:G:6:DA:C8	2.28	0.69
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.23	0.69
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.74	0.69
4:E:50:THR:CG2	4:E:53:GLY:H	2.05	0.69
5:F:157:GLU:O	5:F:161:GLN:HG2	1.93	0.69
3:D:65:ARG:HB3	5:F:377:ASP:CA	2.20	0.68
3:D:431:VAL:HG21	3:D:448:GLU:OE1	1.93	0.68
3:D:62:LYS:HB3	3:D:63:TYR:CD2	2.28	0.68
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.27	0.68
2:C:644:VAL:HG22	2:C:645:VAL:H	1.59	0.68
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.75	0.68
3:D:739:ASP:OD1	3:D:741:ASP:OD1	2.11	0.68
3:D:1024:ALA:HA	3:D:1029:ARG:O	1.94	0.68
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.74	0.68
2:C:234:ALA:HA	2:C:237:ARG:HB2	1.75	0.68
2:C:260:LEU:CB	2:C:261:ILE:HD12	2.22	0.68
3:D:226:PRO:HD3	3:D:249:TYR:CD2	2.28	0.68
3:D:262:LYS:HE2	3:D:341:GLU:OE2	1.94	0.68
1:B:102:LYS:HG3	1:B:139:ASN:OD1	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1009:SER:O	3:D:624:ASP:HB3	1.94	0.68
3:D:93:ILE:HD13	3:D:548:ILE:HG12	1.75	0.68
3:D:1234:THR:CA	3:D:1235:GLN:HB2	2.24	0.68
3:D:1496:GLU:O	3:D:1496:GLU:HG3	1.93	0.68
4:E:39:VAL:HG21	4:E:72:ARG:HB3	1.75	0.68
5:F:361:LEU:HD11	5:F:411:HIS:CB	2.21	0.68
1:A:206:THR:HB	1:A:209:GLU:OE1	1.93	0.68
2:C:861:LEU:HD12	2:C:865:THR:HB	1.75	0.68
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.42	0.68
3:D:41:ARG:NE	3:D:48:ARG:HD3	2.09	0.68
3:D:1057:VAL:HG23	3:D:1069:GLU:CD	2.13	0.68
2:C:681:GLY:HA2	3:D:939:PHE:CE1	2.28	0.68
2:C:719:PRO:HD2	2:C:761:PHE:CE1	2.28	0.68
3:D:103:TRP:HE1	3:D:604:THR:HG21	1.57	0.68
3:D:208:PRO:CG	3:D:353:VAL:HG11	2.24	0.68
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.28	0.68
3:D:1003:VAL:O	3:D:1007:VAL:HG23	1.94	0.68
2:C:54:ILE:HG21	2:C:355:VAL:CG2	2.24	0.68
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.27	0.68
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.29	0.68
1:A:106:PRO:HD3	1:A:134:GLU:OE1	1.94	0.68
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.74	0.68
2:C:1001:VAL:CG1	3:D:724:GLN:HB2	2.24	0.67
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.27	0.67
3:D:156:GLU:N	3:D:156:GLU:OE2	2.24	0.67
4:E:80:VAL:HG12	4:E:81:PRO:O	1.93	0.67
2:C:513:VAL:HG21	2:C:529:VAL:HG21	1.76	0.67
3:D:650:LEU:HD12	3:D:657:LEU:CD2	2.25	0.67
3:D:814:ALA:O	3:D:818:ARG:HG3	1.94	0.67
1:A:55:SER:HB2	1:A:158:ILE:HG22	1.76	0.67
1:B:185:ARG:HB2	1:B:190:THR:OG1	1.95	0.67
2:C:176:VAL:HG22	2:C:182:VAL:HG12	1.76	0.67
2:C:715:THR:HB	2:C:718:GLY:O	1.94	0.67
3:D:1486:VAL:HA	4:E:74:VAL:O	1.93	0.67
5:F:104:ARG:HG2	5:F:108:GLU:OE2	1.95	0.67
1:A:107:LYS:NZ	1:A:113:ASP:OD2	2.20	0.67
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.30	0.67
2:C:1056:LYS:HD3	3:D:751:LEU:HD11	1.76	0.67
5:F:371:LEU:CD1	5:F:379:ARG:HG3	2.24	0.67
1:B:24:VAL:HG13	1:B:196:THR:OG1	1.93	0.67
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:560:MET:O	2:C:564:MET:HB2	1.94	0.67
2:C:588:VAL:HG11	2:C:664:GLY:O	1.93	0.67
3:D:93:ILE:CD1	3:D:548:ILE:HG12	2.25	0.67
2:C:547:ILE:O	2:C:905:ILE:HD11	1.95	0.67
3:D:250:LEU:N	3:D:250:LEU:HD23	2.09	0.67
3:D:411:THR:HG22	5:F:178:ARG:HB3	1.77	0.67
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	1.77	0.67
5:F:375:LEU:HD23	5:F:375:LEU:O	1.95	0.67
6:G:6:DA:H5"	6:G:6:DA:H8	1.59	0.67
2:C:337:GLY:O	2:C:341:THR:HG23	1.95	0.67
2:C:751:PRO:HA	2:C:792:VAL:CG2	2.24	0.67
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.29	0.67
2:C:182:VAL:HG22	2:C:221:LEU:CD2	2.22	0.67
2:C:359:MET:O	2:C:360:LEU:HD13	1.95	0.67
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.76	0.67
3:D:916:TYR:CE2	3:D:920:LEU:HD11	2.30	0.67
3:D:1310:ARG:HB2	3:D:1327:ARG:HD2	1.76	0.67
1:B:109:VAL:C	1:B:110:LYS:HD2	2.16	0.67
2:C:221:LEU:O	2:C:221:LEU:HD22	1.95	0.67
2:C:928:LYS:O	2:C:932:GLU:HG3	1.95	0.67
3:D:226:PRO:HD3	3:D:249:TYR:CE2	2.30	0.67
5:F:222:ARG:NE	5:F:222:ARG:HA	2.10	0.67
1:A:86:VAL:HG21	1:A:202:ASP:HB2	1.76	0.66
1:A:213:GLN:O	1:A:217:ILE:HG13	1.94	0.66
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.30	0.66
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.78	0.66
2:C:888:THR:HG22	2:C:990:GLY:CA	2.24	0.66
3:D:154:THR:OG1	3:D:157:GLU:HG3	1.95	0.66
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.76	0.66
5:F:129:GLU:HG2	5:F:144:ILE:HG13	1.77	0.66
5:F:370:LYS:O	5:F:371:LEU:HD22	1.95	0.66
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.77	0.66
3:D:791:TYR:CD1	3:D:945:SER:HB2	2.31	0.66
3:D:948:THR:HG23	3:D:949:ILE:N	2.10	0.66
3:D:65:ARG:CD	5:F:377:ASP:HA	2.26	0.66
3:D:66:GLN:OE1	5:F:376:ILE:HG12	1.95	0.66
3:D:1290:LEU:HB2	3:D:1307:LYS:HG2	1.77	0.66
3:D:1413:THR:HG22	3:D:1414:PRO:HD2	1.77	0.66
5:F:355:GLU:OE2	5:F:370:LYS:NZ	2.22	0.66
7:H:21:DA:H1'	7:H:22:DT:C5'	2.26	0.66
1:A:67:THR:HG21	2:C:609:ASN:OD1	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLN:NE2	1:A:213:GLN:HA	2.09	0.66
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.76	0.66
1:B:94:LEU:HD23	1:B:95:GLN:N	2.10	0.66
2:C:54:ILE:HG21	2:C:355:VAL:HG23	1.78	0.66
2:C:503:LEU:CD2	2:C:508:ILE:HA	2.25	0.66
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.77	0.66
3:D:479:GLU:OE2	3:D:482:LYS:NZ	2.25	0.66
3:D:645:PRO:HB3	3:D:723:GLY:O	1.96	0.66
3:D:940:THR:O	3:D:943:THR:HG23	1.95	0.66
5:F:365:GLU:OE2	5:F:407:LYS:HD2	1.96	0.66
1:A:9:PRO:HB3	1:A:27:PRO:O	1.96	0.66
3:D:175:VAL:HG11	3:D:193:PRO:HG2	1.76	0.66
3:D:241:ILE:CD1	3:D:310:LEU:HD23	2.24	0.66
3:D:367:ILE:HB	3:D:377:VAL:CG2	2.26	0.66
3:D:658:LEU:HD23	3:D:661:MET:CE	2.21	0.66
3:D:882:PHE:CE2	3:D:906:GLN:HG3	2.31	0.66
3:D:519:VAL:HG22	3:D:544:TYR:CE1	2.31	0.66
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.77	0.66
1:A:19:GLU:O	1:A:207:PRO:HG3	1.94	0.66
2:C:206:THR:HA	2:C:209:ARG:HB3	1.77	0.66
2:C:946:ARG:HH21	2:C:946:ARG:HG3	1.60	0.66
5:F:386:VAL:HA	5:F:390:PHE:HE1	1.56	0.66
2:C:317:VAL:CG1	2:C:318:PRO:HD2	2.25	0.66
2:C:1060:ILE:HD11	2:C:1083:GLU:HB2	1.76	0.66
3:D:258:VAL:HG12	3:D:273:ARG:O	1.95	0.66
5:F:260:ILE:HG13	5:F:265:VAL:HG23	1.78	0.66
5:F:392:VAL:HG22	5:F:393:THR:H	1.60	0.66
2:C:564:MET:HG2	2:C:997:LEU:CD1	2.25	0.66
3:D:664:LYS:HE3	3:D:693:GLU:OE2	1.95	0.65
7:H:13:DT:H3'	7:H:14:DG:H5'	1.78	0.65
3:D:1126:ASP:O	3:D:1130:ARG:HA	1.96	0.65
2:C:177:GLU:CG	2:C:178:PRO:HD2	2.23	0.65
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.79	0.65
3:D:529:GLN:HG3	3:D:535:PHE:CE2	2.30	0.65
5:F:291:ILE:HG21	5:F:304:VAL:HG21	1.78	0.65
1:A:10:VAL:N	1:A:26:GLU:O	2.24	0.65
2:C:926:PHE:O	2:C:929:ARG:HB3	1.96	0.65
2:C:266:ARG:O	2:C:266:ARG:HG3	1.95	0.65
2:C:540:PHE:HB3	2:C:544:THR:CG2	2.26	0.65
2:C:1054:THR:OG1	2:C:1055:LEU:HD23	1.96	0.65
3:D:116:LEU:HD21	3:D:465:LEU:HD12	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:HD11	1:B:109:VAL:CG1	2.27	0.65
3:D:478:LEU:O	3:D:481:MET:N	2.30	0.65
3:D:1065:LEU:HD23	3:D:1069:GLU:CB	2.14	0.65
4:E:50:THR:HG23	4:E:53:GLY:H	1.60	0.65
1:B:112:ARG:HG3	1:B:113:ASP:OD1	1.96	0.65
2:C:312:ALA:HB1	2:C:317:VAL:HG21	1.78	0.65
3:D:256:GLU:HG2	3:D:274:ARG:NH1	2.12	0.65
3:D:823:LEU:HD11	3:D:837:GLY:HA2	1.78	0.65
2:C:890:LEU:HB2	2:C:914:ILE:CD1	2.24	0.65
3:D:103:TRP:HE1	3:D:604:THR:CG2	2.10	0.65
3:D:111:LYS:HD2	3:D:1452:ILE:CD1	2.27	0.65
3:D:284:LEU:HD12	3:D:288:MET:HE1	1.78	0.65
5:F:101:GLU:O	5:F:105:LYS:HG3	1.97	0.65
1:B:96:THR:HG22	1:B:97:VAL:N	2.12	0.65
2:C:250:ARG:HD2	2:C:250:ARG:O	1.97	0.65
2:C:446:GLY:O	2:C:449:ILE:HG22	1.96	0.65
2:C:605:LYS:O	2:C:606:VAL:HG23	1.97	0.65
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.79	0.65
3:D:65:ARG:HD3	5:F:377:ASP:N	2.11	0.65
3:D:1380:GLU:N	3:D:1420:LEU:HD22	2.11	0.65
7:H:13:DT:H3'	7:H:14:DG:C5'	2.26	0.65
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.11	0.65
2:C:64:LEU:HD23	2:C:102:HIS:HA	1.78	0.65
3:D:904:VAL:HG22	3:D:905:PRO:CD	2.27	0.65
2:C:356:ARG:HA	2:C:359:MET:HB2	1.79	0.64
2:C:474:VAL:CG1	2:C:529:VAL:HG12	2.23	0.64
2:C:889:HIS:CD2	3:D:951:ILE:HG22	2.31	0.64
3:D:764:LEU:HB3	3:D:767:HIS:HD2	1.62	0.64
3:D:801:GLY:HA3	3:D:821:VAL:HG22	1.78	0.64
2:C:193:LEU:HG	2:C:197:LEU:CD1	2.28	0.64
2:C:605:LYS:HB2	2:C:612:VAL:HG12	1.80	0.64
5:F:153:PRO:HA	5:F:156:VAL:HG12	1.78	0.64
5:F:412:GLU:CG	5:F:418:LEU:HD13	2.21	0.64
2:C:605:LYS:HB2	2:C:612:VAL:CG1	2.28	0.64
2:C:689:VAL:HG11	2:C:853:LEU:HD11	1.79	0.64
3:D:236:TYR:CE1	3:D:242:LEU:HB2	2.33	0.64
3:D:791:TYR:CZ	3:D:945:SER:HB2	2.32	0.64
5:F:171:LYS:HD3	5:F:175:HIS:CE1	2.32	0.64
1:A:4:SER:O	1:A:189:ARG:NH2	2.29	0.64
2:C:1110:ASP:OD1	2:C:1112:PHE:N	2.28	0.64
3:D:256:GLU:HG2	3:D:274:ARG:HH11	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1405:GLU:HA	3:D:1408:ILE:CG1	2.28	0.64
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.06	0.64
2:C:238:LEU:HD12	2:C:241:LEU:HB2	1.80	0.64
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.79	0.64
3:D:972:LEU:HA	3:D:975:GLU:HB3	1.78	0.64
4:E:75:PHE:H	4:E:75:PHE:HD2	1.44	0.64
5:F:402:ASN:O	5:F:406:ARG:HB2	1.97	0.64
1:A:219:ARG:HG3	1:B:219:ARG:HG3	1.79	0.64
3:D:1405:GLU:HA	3:D:1408:ILE:HG13	1.79	0.64
5:F:393:THR:HG22	5:F:394:ARG:H	1.60	0.64
1:A:9:PRO:HB2	1:A:26:GLU:O	1.98	0.64
5:F:260:ILE:HG13	5:F:265:VAL:CG2	2.28	0.64
1:A:44:LEU:O	1:A:174:VAL:HG21	1.98	0.64
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.80	0.64
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.78	0.64
3:D:1097:LYS:HD3	3:D:1425:THR:OG1	1.98	0.64
4:E:30:LEU:HD22	4:E:35:PHE:CD1	2.32	0.64
5:F:392:VAL:CG2	5:F:396:ARG:HG2	2.26	0.64
2:C:692:GLU:HG2	2:C:696:LYS:HE3	1.80	0.64
4:E:9:LEU:HD23	4:E:12:MET:HE2	1.80	0.64
5:F:271:LEU:HD21	5:F:307:THR:HG21	1.80	0.64
1:B:64:GLU:HG3	1:B:79:ILE:CD1	2.28	0.64
1:B:117:VAL:HG12	1:B:118:ALA:N	2.13	0.64
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.11	0.64
2:C:477:GLY:O	2:C:508:ILE:HG13	1.98	0.64
2:C:884:GLN:HB2	2:C:992:MET:CE	2.28	0.64
3:D:554:LEU:CD1	3:D:570:GLU:HB3	2.28	0.64
2:C:808:ARG:HD3	2:C:814:GLU:HG3	1.79	0.63
3:D:1273:VAL:H	3:D:1326:THR:CG2	2.08	0.63
5:F:373:LYS:HD3	5:F:380:GLU:OE1	1.96	0.63
2:C:23:VAL:HG23	2:C:24:GLU:H	1.63	0.63
3:D:407:VAL:O	5:F:171:LYS:HE2	1.99	0.63
2:C:211:LEU:HB3	2:C:218:VAL:CG2	2.28	0.63
3:D:63:TYR:OH	3:D:74:GLU:OE1	2.14	0.63
3:D:203:ALA:CB	3:D:393:ILE:HD11	2.11	0.63
1:A:222:LEU:HD21	1:B:218:LEU:CD2	2.11	0.63
2:C:339:LEU:HD11	2:C:391:LEU:HD12	1.79	0.63
5:F:368:VAL:CB	5:F:397:ILE:HD11	2.28	0.63
2:C:403:SER:O	2:C:407:LYS:HG3	1.99	0.63
2:C:748:GLU:HG3	2:C:799:ILE:HD11	1.80	0.63
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1130:ARG:HB3	3:D:1130:ARG:NH1	2.13	0.63
5:F:116:LEU:O	5:F:116:LEU:HD23	1.98	0.63
1:B:32:PHE:HA	1:B:35:THR:HB	1.79	0.63
1:B:107:LYS:HG2	1:B:108:GLU:H	1.63	0.63
2:C:683:ASN:CB	2:C:872:ASN:HB2	2.27	0.63
5:F:157:GLU:HA	5:F:157:GLU:OE1	1.98	0.63
2:C:716:LYS:C	2:C:717:LEU:HD12	2.17	0.63
3:D:1065:LEU:CD2	3:D:1069:GLU:HB3	2.12	0.63
5:F:372:ARG:HA	5:F:372:ARG:HE	1.62	0.63
2:C:762:LYS:HG2	2:C:786:LYS:HG3	1.79	0.63
2:C:1060:ILE:CD1	2:C:1083:GLU:HB2	2.29	0.63
3:D:63:TYR:CE2	3:D:73:CYS:HB2	2.33	0.63
3:D:1494:ALA:HB1	4:E:92:LEU:HD11	1.80	0.63
2:C:875:GLY:O	2:C:879:ARG:HB2	1.99	0.63
2:C:963:LEU:N	2:C:963:LEU:HD23	2.12	0.63
3:D:242:LEU:HD21	3:D:311:LEU:CD1	2.29	0.63
5:F:408:LEU:HA	5:F:411:HIS:HB3	1.80	0.63
2:C:237:ARG:O	2:C:240:THR:OG1	2.16	0.62
3:D:38:LYS:HB3	3:D:39:PRO:HD2	1.80	0.62
3:D:408:GLU:OE1	3:D:408:GLU:HA	1.98	0.62
3:D:986:ARG:NH1	3:D:986:ARG:HB2	2.14	0.62
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.34	0.62
2:C:944:LEU:HD11	2:C:963:LEU:CD2	2.27	0.62
5:F:376:ILE:O	5:F:377:ASP:HB3	1.98	0.62
1:A:47:SER:O	1:A:49:PRO:HD3	2.00	0.62
2:C:257:VAL:HG23	2:C:258:TYR:H	1.63	0.62
1:B:53:VAL:HG12	1:B:167:VAL:CG1	2.22	0.62
2:C:409:ARG:NH1	2:C:442:GLU:OE2	2.32	0.62
2:C:726:ILE:HG21	2:C:729:LEU:HD22	1.80	0.62
3:D:204:LEU:O	3:D:393:ILE:HG13	1.98	0.62
3:D:601:ARG:HD2	5:F:318:GLU:HG2	1.82	0.62
3:D:955:VAL:O	3:D:957:PRO:HD3	1.99	0.62
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.80	0.62
3:D:130:SER:O	3:D:131:LYS:HG3	2.00	0.62
3:D:761:ILE:HD13	4:E:19:LEU:CD2	2.29	0.62
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.81	0.62
5:F:358:LEU:HD12	5:F:370:LYS:HD2	1.81	0.62
3:D:82:LYS:O	3:D:85:VAL:HG22	2.00	0.62
3:D:597:ASP:O	3:D:599:PRO:HD3	1.99	0.62
3:D:1353:GLN:O	3:D:1357:ARG:HG3	1.98	0.62
2:C:73:LEU:HD22	2:C:92:ALA:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:30:LEU:HD23	4:E:35:PHE:HA	1.81	0.62
2:C:683:ASN:CB	2:C:872:ASN:HD22	2.13	0.62
2:C:755:LEU:CD1	2:C:792:VAL:HG12	2.30	0.62
2:C:1067:TYR:CE1	2:C:1071:ILE:HD13	2.34	0.62
3:D:368:VAL:HB	3:D:377:VAL:HG13	1.81	0.62
5:F:206:GLY:O	5:F:207:LEU:HD23	1.99	0.62
1:A:122:ILE:O	1:A:122:ILE:HG22	2.00	0.62
1:A:224:TYR:CG	1:B:9:PRO:HG2	2.34	0.62
2:C:339:LEU:CD1	2:C:391:LEU:HD12	2.29	0.62
3:D:236:TYR:N	3:D:319:ALA:HB3	2.14	0.62
3:D:835:SER:H	3:D:838:ARG:HG3	1.63	0.62
1:B:118:ALA:O	1:B:119:ASP:HB2	1.99	0.62
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.80	0.62
3:D:221:ALA:O	3:D:335:LEU:HD12	1.99	0.62
3:D:407:VAL:HA	3:D:422:ALA:CB	2.29	0.62
2:C:193:LEU:HG	2:C:197:LEU:HD11	1.82	0.61
2:C:897:LEU:N	2:C:897:LEU:HD23	2.15	0.61
3:D:407:VAL:HG13	3:D:422:ALA:CB	2.28	0.61
3:D:407:VAL:CG1	3:D:422:ALA:HB2	2.27	0.61
3:D:231:VAL:HG13	3:D:242:LEU:O	2.01	0.61
3:D:558:LEU:HD23	3:D:567:ILE:HD11	1.81	0.61
3:D:689:ASP:HB3	4:E:51:LEU:CD1	2.27	0.61
2:C:755:LEU:HD11	2:C:792:VAL:HG12	1.81	0.61
3:D:208:PRO:HG3	3:D:353:VAL:HG11	1.82	0.61
3:D:572:ARG:NH1	5:F:83:GLN:HG2	2.14	0.61
3:D:703:ASN:HB3	3:D:746:ALA:HB3	1.82	0.61
3:D:1090:ASP:N	3:D:1090:ASP:OD1	2.28	0.61
5:F:364:ARG:O	5:F:367:MET:HG3	1.99	0.61
1:A:79:ILE:HD12	1:A:167:VAL:HG22	1.81	0.61
1:A:133:GLU:OE2	2:C:605:LYS:HD3	2.01	0.61
2:C:53:PRO:HB3	2:C:67:ASP:OD2	2.00	0.61
5:F:367:MET:HA	5:F:370:LYS:HB3	1.83	0.61
7:H:17:DA:H2"	7:H:18:DC:H5'	1.83	0.61
1:B:53:VAL:CG1	1:B:167:VAL:HG11	2.21	0.61
2:C:1092:LEU:CD1	2:C:1099:VAL:HG21	2.30	0.61
3:D:1410:GLU:CB	3:D:1412:LYS:HE3	2.29	0.61
5:F:196:VAL:HG11	7:H:7:DG:H4'	1.83	0.61
1:A:215:VAL:HG13	1:B:222:LEU:CD2	2.25	0.61
3:D:417:PRO:HG3	3:D:430:ASP:O	2.01	0.61
3:D:704:ARG:HG2	3:D:705:ALA:H	1.65	0.61
2:C:23:VAL:HG23	2:C:24:GLU:N	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.36	0.61
5:F:368:VAL:HB	5:F:397:ILE:HD11	1.82	0.61
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.83	0.61
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.82	0.61
2:C:257:VAL:HG23	2:C:258:TYR:N	2.16	0.61
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.36	0.61
1:B:30:ARG:NE	2:C:854:PRO:HG3	2.15	0.61
1:B:94:LEU:HD21	1:B:96:THR:O	2.01	0.61
2:C:598:GLU:O	2:C:651:LYS:HE3	2.00	0.61
3:D:36:THR:O	3:D:38:LYS:HG3	2.01	0.61
3:D:705:ALA:CB	3:D:706:PRO:CD	2.77	0.61
1:A:180:GLN:HG3	2:C:934:PHE:CD1	2.35	0.60
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.01	0.60
3:D:700:VAL:O	3:D:701:LEU:HD23	2.00	0.60
3:D:930:LEU:CD1	3:D:934:LEU:HD11	2.31	0.60
3:D:1045:MET:HA	3:D:1045:MET:CE	2.30	0.60
3:D:298:VAL:HA	3:D:302:GLN:OE1	2.01	0.60
3:D:314:PRO:HD2	3:D:317:VAL:CG1	2.30	0.60
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.02	0.60
3:D:1078:ARG:HG2	3:D:1078:ARG:NH1	2.17	0.60
5:F:95:THR:N	5:F:98:GLU:HG3	2.10	0.60
2:C:944:LEU:CD1	2:C:963:LEU:HD21	2.29	0.60
3:D:7:LYS:HD3	3:D:1456:LYS:HZ3	1.66	0.60
3:D:781:PRO:HB2	3:D:786:ILE:HG22	1.83	0.60
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.82	0.60
1:B:211:LEU:O	1:B:215:VAL:HG23	2.00	0.60
2:C:355:VAL:HG23	2:C:356:ARG:N	2.17	0.60
2:C:462:ASP:HB3	2:C:468:ARG:CD	2.31	0.60
2:C:723:THR:OG1	2:C:725:ASP:N	2.33	0.60
3:D:657:LEU:HG	3:D:661:MET:CE	2.31	0.60
5:F:364:ARG:HD2	5:F:364:ARG:C	2.22	0.60
1:A:39:PRO:O	1:A:43:ILE:HG13	2.00	0.60
1:B:202:ASP:OD1	1:B:204:SER:HB3	2.01	0.60
2:C:627:ARG:NH2	2:C:641:PRO:HD3	2.13	0.60
2:C:1047:HIS:CE1	3:D:1471:LEU:HD21	2.37	0.60
3:D:801:GLY:CA	3:D:821:VAL:HG22	2.31	0.60
1:A:38:ASN:HB3	1:A:39:PRO:CD	2.31	0.60
3:D:180:LYS:O	3:D:183:GLU:HB2	2.01	0.60
3:D:750:PRO:HB2	3:D:756:GLN:HE22	1.65	0.60
3:D:970:LYS:HA	3:D:973:GLN:HB3	1.83	0.60
3:D:1126:ASP:OD2	3:D:1133:ARG:HG3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:153:PRO:O	5:F:156:VAL:HG12	2.02	0.60
1:A:153:ALA:C	1:A:155:LYS:H	2.03	0.60
2:C:492:ASP:HB3	2:C:518:LYS:HG2	1.84	0.60
2:C:167:LYS:HE3	7:H:12:DC:C5	2.37	0.60
2:C:1055:LEU:HD23	2:C:1055:LEU:N	2.17	0.60
3:D:347:VAL:HA	3:D:351:MET:HE3	1.84	0.60
3:D:1442:ASN:HD21	6:G:11:DT:H4'	1.66	0.60
5:F:236:SER:OG	7:H:5:DA:OP2	2.15	0.60
1:A:9:PRO:CD	1:B:224:TYR:CD2	2.85	0.60
1:A:222:LEU:HD23	1:B:215:VAL:HG13	1.84	0.60
3:D:415:VAL:HG22	3:D:419:ASP:OD2	2.01	0.60
3:D:1290:LEU:CB	3:D:1307:LYS:HG2	2.32	0.60
4:E:9:LEU:HD23	4:E:12:MET:CE	2.31	0.60
1:A:55:SER:HB2	1:A:158:ILE:O	2.01	0.60
2:C:65:VAL:CG2	2:C:101:ILE:HG23	2.31	0.60
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.17	0.60
3:D:711:LEU:HD22	3:D:714:GLN:NE2	2.17	0.60
5:F:401:GLU:O	5:F:405:LEU:HD13	2.01	0.60
1:A:182:GLU:HG3	1:A:194:LYS:HE2	1.83	0.59
3:D:411:THR:HG22	5:F:178:ARG:CB	2.32	0.59
3:D:687:VAL:O	3:D:690:ALA:HB3	2.01	0.59
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.28	0.59
3:D:1267:ARG:NH2	3:D:1331:ASP:OD2	2.34	0.59
3:D:1394:VAL:HG22	3:D:1420:LEU:HD23	1.83	0.59
5:F:89:GLY:HA3	7:H:7:DG:C6	2.37	0.59
1:B:97:VAL:HG12	1:B:99:LEU:HD12	1.83	0.59
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.38	0.59
3:D:547:LEU:HD12	3:D:577:ALA:CB	2.32	0.59
3:D:823:LEU:HD11	3:D:837:GLY:CA	2.33	0.59
3:D:1057:VAL:HG21	3:D:1065:LEU:HD21	1.83	0.59
1:A:18:ARG:HH21	1:A:88:ARG:NH1	2.00	0.59
1:B:106:PRO:CG	1:B:134:GLU:HG2	2.32	0.59
2:C:666:LEU:HD11	2:C:668:LEU:HD21	1.84	0.59
3:D:242:LEU:CD2	3:D:311:LEU:HD12	2.31	0.59
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.37	0.59
1:B:26:GLU:CD	1:B:194:LYS:HG3	2.22	0.59
3:D:411:THR:HA	3:D:435:VAL:HG13	1.83	0.59
3:D:547:LEU:HD12	3:D:577:ALA:HB3	1.84	0.59
3:D:760:ARG:HH22	4:E:62:THR:HG22	1.67	0.59
3:D:1160:LEU:HD23	3:D:1164:ARG:NH1	2.17	0.59
7:H:15:DT:H2"	7:H:16:DC:H5'	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:O	1:A:173:PRO:HD3	2.03	0.59
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.84	0.59
3:D:314:PRO:HB2	3:D:317:VAL:CG1	2.32	0.59
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.85	0.59
3:D:1371:VAL:O	3:D:1374:GLN:N	2.33	0.59
2:C:361:MET:HG3	2:C:361:MET:O	2.01	0.59
2:C:1099:VAL:CG2	3:D:10:ILE:HG13	2.33	0.59
3:D:652:LEU:HB3	3:D:749:VAL:CG2	2.32	0.59
3:D:1118:ILE:HD13	3:D:1190:SER:CB	2.32	0.59
2:C:425:PHE:HE2	3:D:1086:LEU:HD12	1.67	0.59
2:C:759:THR:HA	2:C:786:LYS:O	2.02	0.59
3:D:483:HIS:ND1	3:D:484:PRO:O	2.33	0.59
3:D:1422:MET:HE3	3:D:1426:LYS:CG	2.32	0.59
3:D:1422:MET:CE	3:D:1426:LYS:HG2	2.31	0.59
4:E:83:ASP:HA	4:E:86:GLN:HG2	1.83	0.59
5:F:360:LYS:O	5:F:361:LEU:HD23	2.03	0.59
5:F:371:LEU:HD12	5:F:379:ARG:HG3	1.84	0.59
1:A:185:ARG:NH2	1:A:187:GLY:O	2.35	0.59
2:C:367:LEU:HA	2:C:371:LYS:HZ2	1.67	0.59
3:D:807:ALA:O	3:D:830:ALA:HB2	2.03	0.59
3:D:885:ILE:HG23	3:D:937:TYR:CD1	2.38	0.59
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.68	0.59
3:D:1156:LEU:O	3:D:1158:VAL:HG23	2.03	0.59
1:A:150:TYR:HE1	2:C:696:LYS:HA	1.67	0.59
2:C:91:GLN:HA	2:C:119:PRO:HA	1.85	0.59
2:C:644:VAL:HG22	2:C:645:VAL:N	2.17	0.59
2:C:705:ILE:HG23	2:C:827:VAL:O	2.02	0.59
2:C:727:PRO:HB2	2:C:728:HIS:CD2	2.36	0.59
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.84	0.59
3:D:566:ILE:HD11	5:F:192:LEU:CD2	2.33	0.59
3:D:1234:THR:H	3:D:1235:GLN:CB	2.16	0.59
1:A:196:THR:HG21	2:C:934:PHE:CE1	2.38	0.58
1:B:38:ASN:OD1	2:C:979:THR:HG22	2.03	0.58
2:C:139:GLN:HB2	2:C:391:LEU:HD11	1.84	0.58
2:C:217:LEU:O	2:C:220:GLY:N	2.36	0.58
2:C:626:ARG:H	2:C:639:GLN:HE21	1.50	0.58
3:D:1130:ARG:HB3	3:D:1130:ARG:HH11	1.68	0.58
4:E:95:VAL:O	4:E:95:VAL:HG12	2.03	0.58
5:F:208:SER:OG	5:F:211:ASP:HB2	2.03	0.58
1:A:188:GLN:OE1	1:A:188:GLN:HA	2.03	0.58
2:C:838:LYS:HD3	2:C:997:LEU:HD12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:853:LEU:HD12	2:C:858:MET:CE	2.33	0.58
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.68	0.58
2:C:952:LEU:HD12	2:C:969:GLN:OE1	2.03	0.58
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.84	0.58
3:D:284:LEU:HA	3:D:288:MET:HE2	1.85	0.58
3:D:403:PHE:HB2	3:D:423:ASP:OD2	2.03	0.58
3:D:704:ARG:CB	3:D:745:MET:HE2	2.26	0.58
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.85	0.58
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.85	0.58
2:C:841:ASN:HD22	2:C:992:MET:CE	2.17	0.58
2:C:1031:ARG:HB2	3:D:622:ARG:NH1	2.18	0.58
3:D:95:LEU:HD22	3:D:574:LEU:HD21	1.85	0.58
3:D:140:ALA:HA	3:D:450:TYR:CD1	2.39	0.58
3:D:882:PHE:CZ	3:D:906:GLN:HG3	2.38	0.58
3:D:1060:SER:HB3	3:D:1063:GLU:CG	2.22	0.58
2:C:21:ILE:HD11	2:C:461:VAL:HG11	1.85	0.58
2:C:422:ARG:HH22	7:H:13:DT:C3'	2.17	0.58
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.85	0.58
3:D:696:HIS:CE1	4:E:48:MET:HB3	2.38	0.58
3:D:750:PRO:HB2	3:D:756:GLN:NE2	2.18	0.58
1:B:162:ILE:HD12	1:B:163:ASN:H	1.69	0.58
2:C:12:VAL:HG21	2:C:472:ARG:NE	2.19	0.58
2:C:127:PHE:O	2:C:133:ASP:HA	2.03	0.58
2:C:502:PRO:O	2:C:503:LEU:HD23	2.04	0.58
3:D:529:GLN:HA	3:D:534:ARG:O	2.03	0.58
1:A:57:TYR:HE2	1:A:59:GLU:HA	1.69	0.58
1:B:64:GLU:O	1:B:75:VAL:HB	2.04	0.58
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.67	0.58
3:D:103:TRP:CZ2	3:D:1444:THR:HG22	2.39	0.58
3:D:202:VAL:O	3:D:202:VAL:HG22	2.02	0.58
3:D:230:TRP:CZ3	3:D:333:LEU:HD21	2.39	0.58
3:D:646:LYS:CB	3:D:720:LEU:HD23	2.33	0.58
3:D:983:LEU:HB3	3:D:987:GLU:OE2	2.03	0.58
5:F:166:LEU:CB	5:F:171:LYS:HB2	2.32	0.58
3:D:728:LEU:HD12	3:D:729:HIS:H	1.67	0.58
3:D:806:PHE:O	3:D:829:VAL:HA	2.04	0.58
2:C:167:LYS:HE3	7:H:12:DC:H5	1.68	0.58
3:D:185:VAL:CG1	3:D:186:VAL:N	2.67	0.58
3:D:628:ARG:HD3	6:G:17:DC:H4'	1.85	0.58
3:D:851:LEU:HD11	3:D:855:HIS:HE1	1.69	0.58
2:C:501:THR:CG2	2:C:514:VAL:HG23	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:657:ASP:OD2	2:C:663:ASN:N	2.33	0.58
3:D:398:ALA:HB1	3:D:446:VAL:O	2.04	0.58
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.37	0.58
5:F:163:LEU:HB3	5:F:174:LEU:HD13	1.85	0.58
1:A:31:GLY:N	1:A:193:ASP:OD2	2.36	0.57
2:C:974:LEU:HD11	2:C:989:VAL:HG21	1.86	0.57
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.39	0.57
3:D:293:VAL:HG23	3:D:294:HIS:O	2.04	0.57
3:D:1422:MET:HE3	3:D:1426:LYS:HG2	1.85	0.57
7:H:16:DC:H2"	7:H:17:DA:C8	2.39	0.57
3:D:93:ILE:HD11	3:D:548:ILE:HD11	1.85	0.57
3:D:137:PRO:CB	3:D:147:VAL:HG23	2.32	0.57
3:D:221:ALA:CB	3:D:281:THR:HG22	2.34	0.57
3:D:557:LEU:HD13	3:D:566:ILE:CG2	2.35	0.57
3:D:216:VAL:HA	3:D:340:THR:CG2	2.30	0.57
3:D:1004:THR:OG1	3:D:1036:ARG:HD3	2.04	0.57
5:F:404:ALA:O	5:F:408:LEU:HG	2.04	0.57
2:C:767:PRO:CG	2:C:782:ALA:HB1	2.35	0.57
2:C:880:MET:HE2	3:D:1061:PHE:CE2	2.37	0.57
3:D:378:ILE:HD12	3:D:378:ILE:N	2.19	0.57
5:F:219:GLY:O	5:F:222:ARG:N	2.38	0.57
2:C:128:ILE:O	2:C:129:ILE:HD12	2.04	0.57
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.35	0.57
3:D:706:PRO:CB	3:D:708:LEU:HD21	2.35	0.57
3:D:117:ASP:HB2	3:D:495:ARG:NH1	2.19	0.57
3:D:223:LEU:HD11	3:D:288:MET:SD	2.44	0.57
1:B:170:VAL:O	1:B:170:VAL:HG12	2.05	0.57
3:D:1305:LEU:HD13	3:D:1309:ALA:CB	2.35	0.57
5:F:369:LEU:CD2	5:F:372:ARG:HB2	2.35	0.57
1:A:25:LEU:HD23	1:A:28:LEU:HD21	1.86	0.57
1:A:34:VAL:HG21	1:B:42:ARG:CZ	2.33	0.57
1:A:156:HIS:NE2	1:A:167:VAL:O	2.31	0.57
1:B:208:LEU:HD12	1:B:208:LEU:O	2.05	0.57
2:C:388:ARG:HG3	2:C:388:ARG:HH11	1.70	0.57
3:D:371:ILE:HG13	3:D:372:ASP:H	1.68	0.57
3:D:930:LEU:O	3:D:934:LEU:HD12	2.04	0.57
3:D:1101:VAL:HG22	3:D:1101:VAL:O	2.05	0.57
5:F:271:LEU:CD2	5:F:307:THR:HG21	2.35	0.57
5:F:338:LEU:CD2	5:F:339:PRO:HD2	2.14	0.57
1:B:33:GLY:C	1:B:181:VAL:HG21	2.25	0.57
3:D:97:THR:HG22	3:D:554:LEU:HD21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:574:LEU:O	3:D:578:VAL:HG12	2.05	0.57
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.40	0.57
2:C:798:GLY:HA3	2:C:828:ALA:O	2.05	0.57
2:C:1019:GLN:HE21	3:D:621:LYS:HE3	1.70	0.57
3:D:135:LEU:O	3:D:149:LYS:HE3	2.05	0.57
3:D:140:ALA:HA	3:D:450:TYR:CE1	2.39	0.57
3:D:235:ALA:HB1	3:D:319:ALA:O	2.05	0.57
3:D:885:ILE:HD13	3:D:937:TYR:HD1	1.70	0.57
5:F:207:LEU:HB2	5:F:212:LEU:HD21	1.87	0.57
4:E:41:GLU:N	4:E:44:GLU:OE2	2.34	0.56
1:A:26:GLU:OE2	1:A:194:LYS:HD3	2.05	0.56
1:B:66:SER:O	1:B:75:VAL:HG23	2.05	0.56
1:B:107:LYS:HG2	1:B:108:GLU:N	2.20	0.56
2:C:214:TYR:HD2	2:C:218:VAL:CG2	2.17	0.56
2:C:670:GLN:HG2	2:C:699:PHE:CE2	2.40	0.56
1:A:62:LEU:HD12	1:A:62:LEU:N	2.21	0.56
2:C:74:GLY:O	2:C:92:ALA:HB1	2.05	0.56
2:C:405:ARG:NE	2:C:566:THR:HG21	2.21	0.56
2:C:1009:SER:HA	3:D:625:TYR:HD1	1.70	0.56
3:D:141:ILE:HD12	3:D:145:VAL:C	2.26	0.56
3:D:171:LEU:HD21	3:D:390:PRO:HD2	1.88	0.56
3:D:180:LYS:HA	3:D:205:TYR:OH	2.05	0.56
3:D:242:LEU:HD23	3:D:311:LEU:HD12	1.87	0.56
3:D:691:LEU:O	3:D:694:VAL:HB	2.05	0.56
3:D:864:VAL:CG1	3:D:865:THR:H	2.15	0.56
3:D:955:VAL:O	3:D:955:VAL:HG23	2.04	0.56
3:D:1057:VAL:HG23	3:D:1069:GLU:OE2	2.03	0.56
5:F:131:VAL:HG11	5:F:177:ALA:CB	2.33	0.56
5:F:234:LYS:HD3	7:H:5:DA:P	2.46	0.56
2:C:376:ARG:HD3	5:F:276:ARG:HD2	1.87	0.56
2:C:640:ARG:O	2:C:656:ALA:HB1	2.05	0.56
3:D:646:LYS:HB3	3:D:720:LEU:HD23	1.87	0.56
3:D:761:ILE:HD13	4:E:19:LEU:HD21	1.87	0.56
3:D:1217:ILE:HG21	3:D:1480:PHE:CG	2.41	0.56
3:D:1295:GLU:HA	3:D:1300:SER:CB	2.36	0.56
2:C:428:ARG:NH2	2:C:447:ALA:O	2.39	0.56
2:C:569:VAL:HG21	2:C:1000:MET:HE2	1.85	0.56
3:D:171:LEU:HD11	3:D:390:PRO:O	2.05	0.56
3:D:284:LEU:HD12	3:D:288:MET:CE	2.34	0.56
3:D:993:LEU:O	3:D:997:THR:OG1	2.21	0.56
4:E:61:VAL:O	4:E:65:MET:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:ALA:O	2:C:264:PRO:HD3	2.06	0.56
2:C:727:PRO:HB3	2:C:783:ARG:NH1	2.21	0.56
3:D:40:GLU:OE1	3:D:40:GLU:HA	2.04	0.56
3:D:711:LEU:HD22	3:D:714:GLN:HE21	1.71	0.56
3:D:821:VAL:CG1	3:D:836:VAL:HG21	2.36	0.56
3:D:951:ILE:HD11	3:D:1062:ARG:HG3	1.85	0.56
3:D:968:ASP:O	3:D:972:LEU:HG	2.05	0.56
3:D:1258:ARG:NH2	3:D:1262:LEU:HD21	2.20	0.56
1:A:32:PHE:HA	1:A:35:THR:HB	1.88	0.56
1:A:201:THR:HG23	1:A:203:GLY:H	1.69	0.56
2:C:95:TYR:CE2	2:C:114:PHE:HD1	2.24	0.56
2:C:326:ASP:OD2	2:C:426:ASP:HB3	2.06	0.56
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.17	0.56
2:C:614:ARG:NH2	2:C:618:GLY:O	2.39	0.56
2:C:971:LYS:HA	2:C:987:ILE:O	2.06	0.56
3:D:662:GLU:OE2	3:D:669:ASN:HA	2.06	0.56
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.87	0.56
3:D:885:ILE:HG21	3:D:937:TYR:HD1	1.70	0.56
3:D:1031:ASN:HB2	3:D:1032:PRO:CD	2.36	0.56
5:F:171:LYS:HD3	5:F:175:HIS:HE1	1.69	0.56
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.35	0.56
2:C:836:GLY:HA3	2:C:1001:VAL:CG2	2.36	0.56
2:C:1015:LEU:HD11	5:F:333:ILE:HG21	1.86	0.56
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.06	0.56
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.87	0.56
3:D:1190:SER:OG	3:D:1191:PRO:HD2	2.06	0.56
4:E:36:LYS:HB2	4:E:93:TYR:HB3	1.88	0.56
1:A:65:PHE:CE2	2:C:703:ILE:CG2	2.89	0.56
2:C:278:GLU:HG2	2:C:283:ILE:O	2.05	0.56
2:C:878:SER:OG	3:D:1029:ARG:HD2	2.06	0.56
3:D:126:VAL:O	3:D:457:GLY:N	2.38	0.56
3:D:1197:ARG:HD3	3:D:1198:TYR:CE2	2.41	0.56
1:A:64:GLU:HA	1:A:165:ILE:HD13	1.86	0.56
2:C:258:TYR:CD1	2:C:263:ASP:HB2	2.41	0.56
2:C:879:ARG:HH22	10:D:1601:DCP:PG	2.29	0.56
2:C:1019:GLN:NE2	3:D:621:LYS:HE3	2.21	0.56
3:D:18:ILE:HD13	3:D:516:ALA:O	2.06	0.56
3:D:131:LYS:H	3:D:456:MET:HE2	1.71	0.56
3:D:879:ARG:HB3	3:D:902:LEU:CD1	2.35	0.56
5:F:316:SER:O	5:F:319:THR:OG1	2.19	0.56
2:C:586:ARG:O	2:C:589:ARG:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:617:ASP:N	2:C:617:ASP:OD1	2.39	0.55
2:C:742:VAL:CG1	2:C:803:THR:HG21	2.36	0.55
3:D:348:GLN:H	3:D:351:MET:CE	2.19	0.55
2:C:150:PRO:HD3	2:C:322:VAL:HG21	1.88	0.55
2:C:551:GLU:OE2	2:C:551:GLU:N	2.30	0.55
2:C:1018:GLN:NE2	5:F:335:ASP:OD2	2.35	0.55
3:D:41:ARG:HH21	3:D:48:ARG:HH11	1.54	0.55
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.42	0.55
5:F:260:ILE:HD11	5:F:265:VAL:HG22	1.87	0.55
1:B:59:GLU:HB2	1:B:139:ASN:HB3	1.89	0.55
1:B:99:LEU:HD23	1:B:114:PHE:HB3	1.88	0.55
1:B:197:LEU:HD12	1:B:198:ARG:H	1.70	0.55
2:C:139:GLN:HB2	2:C:391:LEU:CD1	2.36	0.55
2:C:726:ILE:CG2	2:C:729:LEU:HD22	2.36	0.55
2:C:948:GLU:HG3	2:C:953:VAL:HG23	1.86	0.55
3:D:658:LEU:CD2	3:D:661:MET:HE3	2.30	0.55
3:D:676:MET:HE3	3:D:684:LYS:H	1.71	0.55
3:D:961:LYS:HA	3:D:964:LEU:HB2	1.88	0.55
5:F:390:PHE:CE2	5:F:397:ILE:HG12	2.42	0.55
2:C:577:PRO:HB3	2:C:993:PHE:CD1	2.41	0.55
2:C:581:THR:HB	2:C:905:ILE:HD13	1.89	0.55
3:D:70:GLY:N	3:D:80:VAL:HG23	2.04	0.55
3:D:554:LEU:HB2	3:D:570:GLU:HG3	1.87	0.55
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.89	0.55
3:D:885:ILE:CG2	3:D:937:TYR:HD1	2.19	0.55
3:D:1155:VAL:HG11	3:D:1183:ILE:HD12	1.88	0.55
3:D:1234:THR:N	3:D:1235:GLN:CB	2.69	0.55
3:D:1264:GLU:OE1	3:D:1264:GLU:HA	2.06	0.55
4:E:45:ARG:O	4:E:47:LYS:HG2	2.06	0.55
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.87	0.55
3:D:528:VAL:O	3:D:535:PHE:HA	2.06	0.55
3:D:1047:LYS:HG3	3:D:1053:PHE:CZ	2.40	0.55
7:H:21:DA:H2"	7:H:22:DT:OP2	2.05	0.55
1:A:68:ILE:HG22	1:A:71:VAL:HG13	1.89	0.55
2:C:598:GLU:O	2:C:599:GLU:HG2	2.05	0.55
3:D:187:LYS:HD2	3:D:200:ASP:OD2	2.07	0.55
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.89	0.55
3:D:709:HIS:O	3:D:711:LEU:N	2.39	0.55
3:D:864:VAL:CG1	3:D:865:THR:N	2.70	0.55
3:D:1047:LYS:HG3	3:D:1053:PHE:CE2	2.41	0.55
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1495:ILE:HG23	4:E:88:GLU:OE2	2.07	0.55
5:F:135:ILE:HD11	5:F:182:ALA:HB2	1.87	0.55
5:F:372:ARG:HA	5:F:372:ARG:NE	2.21	0.55
1:A:206:THR:HG22	1:A:209:GLU:HG2	1.89	0.55
2:C:820:ARG:NH1	2:C:820:ARG:HB3	2.21	0.55
3:D:1198:TYR:CE2	3:D:1460:ILE:HD13	2.42	0.55
5:F:237:THR:HG21	7:H:3:DT:H5"	1.88	0.55
1:A:18:ARG:NH2	1:A:88:ARG:CZ	2.66	0.55
1:A:23:PHE:CD2	1:A:211:LEU:HD23	2.42	0.55
1:B:162:ILE:HD12	1:B:163:ASN:N	2.22	0.55
2:C:181:VAL:HG23	2:C:221:LEU:HA	1.89	0.55
2:C:375:SER:OG	2:C:379:GLU:OE1	2.24	0.55
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.06	0.55
2:C:1019:GLN:HG2	2:C:1057:SER:OG	2.07	0.55
3:D:421:LEU:HD13	3:D:428:LYS:CA	2.35	0.55
3:D:977:ALA:O	3:D:982:PHE:HB3	2.06	0.55
1:A:6:LEU:HD23	1:A:7:LYS:N	2.21	0.55
1:A:65:PHE:CE2	2:C:703:ILE:HG21	2.42	0.55
1:B:12:THR:HB	1:B:24:VAL:HG23	1.89	0.55
1:B:44:LEU:HD21	1:B:211:LEU:HA	1.88	0.55
2:C:36:PRO:HA	2:C:39:ARG:HG3	1.88	0.55
2:C:111:ASP:OD2	2:C:370:ALA:HB2	2.07	0.55
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	1.87	0.55
3:D:183:GLU:HG3	3:D:185:VAL:HG23	1.88	0.55
3:D:371:ILE:HD11	5:F:232:ARG:NH1	2.21	0.55
3:D:650:LEU:CD1	3:D:657:LEU:CD2	2.84	0.55
3:D:767:HIS:CE1	4:E:3:GLU:HB2	2.42	0.55
3:D:885:ILE:CG2	3:D:937:TYR:CD1	2.90	0.55
2:C:150:PRO:CG	2:C:322:VAL:HG21	2.36	0.55
2:C:422:ARG:HH22	7:H:13:DT:H3'	1.72	0.55
5:F:240:THR:O	5:F:240:THR:HG22	2.07	0.55
1:A:153:ALA:O	1:A:155:LYS:N	2.39	0.54
2:C:736:ASP:O	2:C:744:ARG:HG2	2.07	0.54
2:C:915:LYS:HE3	2:C:968:LEU:O	2.07	0.54
3:D:59:ALA:CB	3:D:78:VAL:HG21	2.32	0.54
3:D:409:VAL:HG23	3:D:435:VAL:HG21	1.88	0.54
5:F:129:GLU:CG	5:F:144:ILE:HG13	2.36	0.54
5:F:153:PRO:HA	5:F:156:VAL:CG1	2.37	0.54
1:B:101:LEU:HD12	1:B:113:ASP:O	2.06	0.54
1:B:117:VAL:CG1	1:B:118:ALA:H	2.16	0.54
1:B:224:TYR:N	1:B:224:TYR:CD1	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:PHE:HD1	2:C:298:PHE:CE1	2.25	0.54
2:C:367:LEU:HA	2:C:371:LYS:NZ	2.22	0.54
2:C:1101:THR:HG21	2:C:1111:ILE:HG21	1.89	0.54
3:D:258:VAL:HA	3:D:296:GLU:O	2.07	0.54
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.89	0.54
3:D:315:ARG:H	3:D:315:ARG:CD	2.19	0.54
1:A:34:VAL:CG2	1:B:42:ARG:CZ	2.85	0.54
1:B:173:PRO:CB	1:B:205:VAL:HG12	2.38	0.54
2:C:281:LEU:HD23	2:C:309:TYR:HD1	1.72	0.54
2:C:362:GLY:O	2:C:363:SER:HB3	2.06	0.54
2:C:559:LEU:C	2:C:559:LEU:HD23	2.28	0.54
2:C:708:TYR:OH	2:C:796:GLU:HG2	2.08	0.54
5:F:272:SER:O	5:F:276:ARG:HG3	2.07	0.54
5:F:387:GLY:CA	5:F:394:ARG:HG2	2.38	0.54
1:B:219:ARG:HA	1:B:222:LEU:HD12	1.89	0.54
2:C:540:PHE:HB3	2:C:544:THR:HG21	1.88	0.54
2:C:719:PRO:CD	2:C:761:PHE:HE1	2.21	0.54
2:C:911:GLU:N	2:C:912:PRO:HD2	2.23	0.54
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.90	0.54
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.88	0.54
3:D:1376:MET:HE1	3:D:1421:LEU:CD1	2.36	0.54
5:F:265:VAL:O	5:F:269:ASN:ND2	2.40	0.54
1:B:89:PHE:HB2	1:B:146:ARG:HH21	1.72	0.54
1:B:128:HIS:C	1:B:128:HIS:CD2	2.81	0.54
3:D:361:VAL:HG21	3:D:379:ALA:HB1	1.89	0.54
3:D:697:GLY:HA3	4:E:59:ASN:HD22	1.72	0.54
3:D:1211:MET:HE2	4:E:16:LYS:HD2	1.88	0.54
3:D:1492:LEU:O	3:D:1492:LEU:HD13	2.08	0.54
1:A:175:ARG:HH12	1:A:176:ARG:NH1	2.06	0.54
1:B:64:GLU:OE2	1:B:79:ILE:HD13	2.08	0.54
2:C:136:ILE:HG21	2:C:336:VAL:HG23	1.90	0.54
2:C:742:VAL:HG12	2:C:743:VAL:O	2.08	0.54
2:C:1001:VAL:HG11	3:D:724:GLN:HB2	1.89	0.54
3:D:284:LEU:CB	3:D:288:MET:HE2	2.38	0.54
1:A:9:PRO:HD3	1:B:224:TYR:CD2	2.42	0.54
1:B:26:GLU:CB	1:B:194:LYS:HG3	2.36	0.54
2:C:598:GLU:C	2:C:599:GLU:HG2	2.28	0.54
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.08	0.54
3:D:1492:LEU:O	3:D:1492:LEU:HD22	2.07	0.54
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.22	0.54
2:C:1004:LYS:HD3	3:D:744:GLN:HE22	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:529:GLN:HG3	3:D:535:PHE:CZ	2.43	0.54
7:H:19:DG:H2"	7:H:20:DG:C8	2.42	0.54
1:A:111:ALA:HB2	1:A:127:LEU:HB3	1.89	0.54
1:B:33:GLY:O	1:B:181:VAL:HG21	2.07	0.54
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.38	0.54
2:C:626:ARG:H	2:C:639:GLN:NE2	2.05	0.54
2:C:748:GLU:HA	2:C:799:ILE:HD13	1.89	0.54
3:D:93:ILE:HD11	3:D:548:ILE:CG1	2.38	0.54
3:D:124:GLU:OE2	3:D:587:ARG:NH1	2.40	0.54
3:D:378:ILE:HD12	3:D:378:ILE:H	1.73	0.54
3:D:749:VAL:HG12	3:D:750:PRO:O	2.08	0.54
3:D:1045:MET:HG3	3:D:1073:SER:HA	1.90	0.54
3:D:1192:LEU:CD2	3:D:1369:GLU:HB3	2.36	0.54
5:F:164:LYS:HD2	5:F:164:LYS:O	2.06	0.54
5:F:319:THR:HG22	5:F:320:PRO:HD2	1.90	0.54
1:A:40:LEU:CD2	1:A:218:LEU:HD12	2.37	0.54
1:A:94:LEU:O	1:A:146:ARG:NH1	2.41	0.54
1:B:44:LEU:HB2	1:B:177:VAL:HG21	1.89	0.54
1:B:54:THR:CG2	1:B:143:ARG:HG2	2.38	0.54
1:B:173:PRO:HB2	1:B:205:VAL:HG12	1.90	0.54
2:C:84:ARG:HD3	2:C:629:TYR:OH	2.08	0.54
3:D:141:ILE:HD12	3:D:145:VAL:N	2.23	0.54
3:D:207:PHE:HB2	3:D:391:ALA:HB2	1.90	0.54
3:D:446:VAL:O	3:D:446:VAL:HG12	2.08	0.54
3:D:850:LEU:HD11	3:D:881:LEU:HD13	1.89	0.54
3:D:936:TYR:C	3:D:936:TYR:HD2	2.11	0.54
3:D:996:TRP:HH2	3:D:1058:ARG:HH22	1.56	0.54
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.23	0.54
5:F:153:PRO:C	5:F:156:VAL:HG12	2.28	0.54
2:C:418:LEU:CD2	2:C:427:VAL:HG11	2.38	0.53
2:C:596:TYR:O	2:C:655:LEU:HD13	2.08	0.53
2:C:988:VAL:HG21	3:D:949:ILE:C	2.29	0.53
3:D:180:LYS:O	3:D:183:GLU:CB	2.57	0.53
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.89	0.53
3:D:209:ARG:NH2	3:D:391:ALA:HA	2.23	0.53
3:D:766:ALA:HB3	4:E:2:ALA:HA	1.89	0.53
3:D:966:GLU:HG2	3:D:969:ARG:NH1	2.22	0.53
5:F:397:ILE:O	5:F:401:GLU:HB2	2.07	0.53
1:A:82:LEU:HD23	1:A:129:ILE:HD12	1.89	0.53
2:C:12:VAL:HG21	2:C:472:ARG:CD	2.38	0.53
2:C:211:LEU:HB3	2:C:218:VAL:HG22	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:116:LEU:HD11	3:D:465:LEU:CD1	2.38	0.53
3:D:135:LEU:HD11	3:D:463:GLN:CG	2.38	0.53
3:D:157:GLU:O	3:D:161:LEU:HG	2.08	0.53
1:A:6:LEU:HD23	1:A:7:LYS:H	1.73	0.53
1:A:11:PHE:CE2	1:B:225:PHE:HA	2.43	0.53
1:A:34:VAL:HG23	1:A:35:THR:N	2.24	0.53
2:C:128:ILE:C	2:C:129:ILE:HD12	2.28	0.53
2:C:988:VAL:HG23	3:D:948:THR:HG23	1.90	0.53
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.41	0.53
3:D:758:GLU:HA	3:D:762:GLN:OE1	2.08	0.53
5:F:161:GLN:O	5:F:165:SER:OG	2.20	0.53
5:F:372:ARG:O	5:F:373:LYS:HG2	2.08	0.53
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.43	0.53
2:C:578:VAL:HG13	2:C:671:ASN:CG	2.29	0.53
2:C:670:GLN:HB2	2:C:700:TYR:CE1	2.43	0.53
2:C:729:LEU:HD21	2:C:754:ILE:HD11	1.90	0.53
3:D:26:VAL:HG12	3:D:548:ILE:HD13	1.90	0.53
3:D:767:HIS:CE1	4:E:6:ILE:HD13	2.43	0.53
3:D:1291:SER:OG	3:D:1302:GLU:HG3	2.08	0.53
3:D:1300:SER:OG	3:D:1301:LYS:N	2.40	0.53
5:F:81:VAL:HG12	5:F:82:ARG:N	2.23	0.53
5:F:264:MET:O	5:F:268:ILE:HG13	2.08	0.53
6:G:8:DC:H42	7:H:20:DG:H1	1.55	0.53
1:B:74:ASP:O	1:B:78:ILE:HG13	2.08	0.53
2:C:56:GLU:CD	2:C:103:LYS:HE2	2.28	0.53
2:C:112:GLU:HG3	2:C:112:GLU:O	2.07	0.53
2:C:805:ARG:CG	2:C:823:VAL:HG23	2.22	0.53
2:C:950:LEU:HB2	2:C:952:LEU:CD2	2.38	0.53
3:D:978:TYR:O	3:D:981:GLY:N	2.40	0.53
3:D:1487:VAL:HG12	4:E:85:LEU:HD11	1.91	0.53
2:C:292:ARG:HD3	2:C:299:LYS:HB2	1.89	0.53
2:C:974:LEU:HD22	2:C:987:ILE:CB	2.38	0.53
2:C:1099:VAL:HG22	3:D:10:ILE:HG13	1.90	0.53
3:D:64:LYS:O	3:D:65:ARG:HG3	2.08	0.53
3:D:116:LEU:HD12	3:D:118:LEU:HD12	1.89	0.53
3:D:409:VAL:CG2	3:D:435:VAL:HG21	2.39	0.53
3:D:700:VAL:C	3:D:701:LEU:HD23	2.29	0.53
3:D:936:TYR:C	3:D:936:TYR:CD2	2.82	0.53
5:F:127:ILE:O	5:F:131:VAL:HG23	2.09	0.53
1:A:152:PRO:O	1:A:155:LYS:HB3	2.09	0.53
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:542:VAL:HG12	2:C:543:ASN:N	2.24	0.53
2:C:682:TYR:CE1	2:C:851:LYS:HD3	2.44	0.53
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.44	0.53
3:D:33:ASN:N	3:D:38:LYS:O	2.32	0.53
5:F:155:THR:HA	5:F:158:GLU:HB2	1.90	0.53
1:A:41:ARG:HG3	1:A:177:VAL:CG1	2.37	0.53
1:A:122:ILE:O	1:A:125:PRO:HD3	2.09	0.53
1:B:101:LEU:HD11	1:B:109:VAL:HG11	1.90	0.53
1:B:205:VAL:HG22	1:B:206:THR:N	2.23	0.53
2:C:683:ASN:HB3	2:C:872:ASN:CB	2.33	0.53
3:D:565:ILE:HD11	5:F:189:GLU:OE1	2.09	0.53
3:D:789:LEU:HD23	3:D:938:GLY:HA2	1.91	0.53
3:D:957:PRO:HG3	3:D:1007:VAL:HG22	1.91	0.53
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.91	0.53
2:C:129:ILE:HG22	2:C:129:ILE:O	2.09	0.53
2:C:150:PRO:HD3	2:C:322:VAL:CG2	2.39	0.53
2:C:831:ARG:NE	2:C:1002:GLU:OE1	2.42	0.53
2:C:880:MET:HE3	3:D:1037:GLN:HB2	1.91	0.53
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.39	0.53
3:D:44:LEU:O	3:D:525:ARG:NH2	2.42	0.53
3:D:767:HIS:CB	3:D:924:MET:HE1	2.39	0.53
3:D:851:LEU:HD11	3:D:855:HIS:CE1	2.44	0.53
3:D:1495:ILE:HA	4:E:88:GLU:OE2	2.09	0.53
1:B:58:ILE:HG22	1:B:61:VAL:CG2	2.39	0.53
2:C:29:ALA:O	2:C:44:ILE:HB	2.09	0.53
2:C:524:VAL:HG22	2:C:528:GLU:HB2	1.91	0.53
2:C:808:ARG:HG3	2:C:814:GLU:HA	1.91	0.53
4:E:37:ASN:HA	4:E:93:TYR:CE2	2.44	0.53
5:F:374:GLY:N	5:F:378:GLY:HA2	2.24	0.53
1:A:149:GLY:O	1:A:171:PHE:HB2	2.09	0.52
1:B:120:VAL:O	1:B:120:VAL:HG12	2.08	0.52
2:C:102:HIS:ND1	2:C:105:THR:HG23	2.25	0.52
2:C:884:GLN:HB2	2:C:992:MET:HE3	1.92	0.52
3:D:135:LEU:HD11	3:D:463:GLN:HG2	1.89	0.52
3:D:698:LYS:HB2	3:D:756:GLN:OE1	2.09	0.52
3:D:1263:PHE:HA	3:D:1375:MET:CE	2.39	0.52
3:D:1431:THR:HG23	3:D:1433:SER:H	1.73	0.52
1:A:6:LEU:HD21	1:A:27:PRO:HG2	1.91	0.52
3:D:116:LEU:HD12	3:D:118:LEU:CD1	2.40	0.52
3:D:204:LEU:HD11	3:D:445:ARG:HE	1.74	0.52
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:699:VAL:HB	3:D:716:PHE:O	2.10	0.52
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.90	0.52
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.90	0.52
2:C:974:LEU:HD22	2:C:987:ILE:HB	1.92	0.52
3:D:955:VAL:HG22	3:D:1011:PHE:CE1	2.44	0.52
5:F:113:ILE:CD1	5:F:128:ARG:HG3	2.38	0.52
5:F:210:LEU:O	5:F:213:ILE:N	2.42	0.52
2:C:880:MET:HE3	3:D:1037:GLN:CB	2.39	0.52
3:D:728:LEU:HD12	3:D:729:HIS:N	2.24	0.52
5:F:94:LEU:HD11	5:F:187:LEU:HD12	1.92	0.52
1:A:42:ARG:NH2	1:B:31:GLY:O	2.35	0.52
2:C:74:GLY:O	2:C:93:PRO:HD2	2.10	0.52
2:C:140:ILE:CD1	2:C:331:ARG:HH11	2.20	0.52
2:C:200:LEU:HD13	2:C:300:ASP:CB	2.29	0.52
2:C:239:PHE:HE2	2:C:246:ASP:HB3	1.74	0.52
2:C:540:PHE:CD1	2:C:544:THR:HG21	2.45	0.52
2:C:1047:HIS:O	2:C:1051:GLU:HG3	2.10	0.52
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.40	0.52
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.25	0.52
3:D:806:PHE:O	3:D:829:VAL:HG13	2.10	0.52
3:D:879:ARG:HB3	3:D:902:LEU:HD12	1.91	0.52
1:A:216:GLU:OE1	1:A:219:ARG:NH2	2.42	0.52
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.45	0.52
3:D:798:GLU:HG2	3:D:824:ASN:HB2	1.89	0.52
3:D:1277:ILE:HD13	3:D:1278:ASP:O	2.09	0.52
5:F:413:SER:HA	5:F:416:ARG:NH2	2.25	0.52
1:A:88:ARG:HB3	1:A:123:MET:CE	2.20	0.52
1:B:7:LYS:HE3	1:B:186:LEU:CD2	2.39	0.52
1:B:58:ILE:HD11	1:B:140:MET:SD	2.50	0.52
1:B:97:VAL:CG1	1:B:99:LEU:HD12	2.39	0.52
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.90	0.52
2:C:196:LEU:HD22	2:C:196:LEU:C	2.30	0.52
2:C:280:LYS:HE3	2:C:309:TYR:CE1	2.45	0.52
2:C:328:LEU:HD11	2:C:438:ILE:HD13	1.91	0.52
2:C:596:TYR:C	2:C:655:LEU:HD13	2.29	0.52
3:D:405:ASP:N	3:D:423:ASP:OD1	2.39	0.52
3:D:626:SER:HA	3:D:747:VAL:O	2.10	0.52
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.09	0.52
3:D:1038:LEU:O	3:D:1060:SER:OG	2.27	0.52
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.91	0.52
5:F:88:ILE:HD11	5:F:192:LEU:CD1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HG12	1:A:98:THR:N	2.24	0.52
1:B:96:THR:O	1:B:97:VAL:HG23	2.10	0.52
1:B:188:GLN:HG2	3:D:685:ASP:OD2	2.09	0.52
3:D:171:LEU:HD12	3:D:171:LEU:O	2.10	0.52
3:D:181:ASP:N	3:D:205:TYR:CE1	2.78	0.52
3:D:367:ILE:HB	3:D:377:VAL:HG22	1.90	0.52
3:D:546:ARG:O	3:D:550:ARG:HG3	2.09	0.52
3:D:566:ILE:HG22	3:D:567:ILE:N	2.24	0.52
3:D:798:GLU:HG3	3:D:824:ASN:CB	2.36	0.52
1:A:221:HIS:ND1	1:A:224:TYR:HE2	2.07	0.52
2:C:253:ALA:O	2:C:257:VAL:HG22	2.09	0.52
2:C:422:ARG:NH2	7:H:13:DT:H5'	2.24	0.52
2:C:550:LEU:HD23	2:C:906:PHE:HE1	1.75	0.52
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.92	0.52
2:C:1037:VAL:HG13	2:C:1049:LEU:CD1	2.38	0.52
3:D:314:PRO:HD2	3:D:317:VAL:HG11	1.92	0.52
3:D:709:HIS:C	3:D:711:LEU:H	2.13	0.52
3:D:916:TYR:CZ	3:D:920:LEU:HD11	2.44	0.52
1:A:58:ILE:O	1:A:61:VAL:HB	2.10	0.52
2:C:281:LEU:O	2:C:283:ILE:HG23	2.10	0.52
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.25	0.52
3:D:42:ASP:N	3:D:46:ASP:OD2	2.38	0.52
3:D:767:HIS:HE1	4:E:3:GLU:HB2	1.73	0.52
3:D:968:ASP:N	3:D:968:ASP:OD1	2.37	0.52
4:E:47:LYS:NZ	4:E:56:ASP:OD1	2.32	0.52
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.91	0.51
1:B:14:ARG:HB3	1:B:14:ARG:NH1	2.25	0.51
3:D:41:ARG:HH21	3:D:48:ARG:NH1	2.09	0.51
3:D:86:LYS:HB2	3:D:523:ASP:OD2	2.11	0.51
3:D:462:GLN:O	3:D:466:LYS:HB2	2.10	0.51
3:D:657:LEU:HG	3:D:661:MET:HE2	1.91	0.51
3:D:729:HIS:CE1	3:D:730:PRO:HD2	2.45	0.51
3:D:1263:PHE:CE1	3:D:1352:ILE:HD13	2.44	0.51
5:F:366:ALA:O	5:F:370:LYS:HB2	2.10	0.51
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.92	0.51
1:A:167:VAL:HG12	1:A:168:ASP:N	2.26	0.51
1:B:20:TYR:CZ	1:B:22:GLU:HG2	2.46	0.51
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.92	0.51
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	1.92	0.51
3:D:1431:THR:HG23	3:D:1432:LYS:N	2.25	0.51
3:D:1445:HIS:O	3:D:1449:GLU:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:193:ARG:HG2	7:H:7:DG:H5'	1.92	0.51
2:C:236:ILE:CG2	2:C:248:PRO:HB2	2.40	0.51
2:C:690:ILE:HG13	2:C:852:ILE:CG2	2.25	0.51
2:C:704:HIS:HD2	2:C:831:ARG:HD2	1.69	0.51
2:C:915:LYS:HD3	2:C:968:LEU:HB3	1.90	0.51
3:D:499:VAL:HG12	3:D:503:LEU:CD1	2.40	0.51
3:D:1019:PRO:O	3:D:1023:MET:HE2	2.10	0.51
3:D:1207:TYR:HA	3:D:1213:ARG:O	2.09	0.51
3:D:1394:VAL:HG22	3:D:1420:LEU:CD2	2.40	0.51
3:D:1487:VAL:O	4:E:74:VAL:HG23	2.10	0.51
2:C:498:GLN:HE21	3:D:1068:LEU:HD12	1.76	0.51
3:D:122:GLU:HG2	3:D:152:LEU:CD1	2.38	0.51
3:D:832:ARG:H	3:D:832:ARG:NE	2.08	0.51
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.93	0.51
2:C:693:GLU:HG2	2:C:855:VAL:HB	1.91	0.51
2:C:974:LEU:CD2	2:C:987:ILE:HG21	2.41	0.51
3:D:236:TYR:HB3	3:D:313:MET:HG3	1.91	0.51
3:D:811:GLU:O	3:D:814:ALA:HB3	2.10	0.51
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.46	0.51
3:D:1192:LEU:CD1	3:D:1345:GLU:HB3	2.40	0.51
3:D:1489:GLN:NE2	3:D:1492:LEU:HB3	2.25	0.51
4:E:39:VAL:CG2	4:E:72:ARG:HB3	2.39	0.51
5:F:186:HIS:ND1	5:F:186:HIS:O	2.44	0.51
1:B:54:THR:HG23	1:B:143:ARG:HG2	1.93	0.51
2:C:709:GLU:OE2	2:C:824:ARG:HD3	2.11	0.51
3:D:343:LYS:CD	3:D:345:TYR:HE2	2.24	0.51
3:D:343:LYS:NZ	3:D:380:GLU:OE2	2.42	0.51
3:D:422:ALA:O	3:D:427:VAL:HG12	2.10	0.51
3:D:554:LEU:HD12	3:D:570:GLU:HB3	1.90	0.51
3:D:803:GLY:HA2	3:D:826:PRO:O	2.10	0.51
1:A:9:PRO:HB2	1:A:26:GLU:C	2.31	0.51
2:C:6:PHE:CG	2:C:909:ALA:HB2	2.46	0.51
2:C:461:VAL:HG23	2:C:461:VAL:O	2.10	0.51
2:C:613:VAL:HG23	2:C:613:VAL:O	2.09	0.51
3:D:62:LYS:HB3	3:D:63:TYR:HD2	1.71	0.51
3:D:661:MET:SD	3:D:677:LEU:HD21	2.50	0.51
1:B:54:THR:HG21	1:B:145:ASP:OD1	2.11	0.51
2:C:340:MET:HB2	2:C:385:PHE:CE2	2.45	0.51
3:D:1216:SER:HB3	4:E:15:SER:HA	1.93	0.51
2:C:707:ARG:CB	2:C:707:ARG:HH11	2.23	0.51
2:C:752:GLY:HA3	3:D:679:ARG:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:156:VAL:O	5:F:160:ASP:HB2	2.11	0.51
5:F:167:PRO:HD2	5:F:170:HIS:HB2	1.91	0.51
1:B:7:LYS:HE3	1:B:186:LEU:HD21	1.91	0.51
2:C:390:GLN:NE2	2:C:414:GLY:HA2	2.26	0.51
2:C:1015:LEU:HD11	5:F:333:ILE:CG2	2.40	0.51
3:D:63:TYR:CD2	3:D:73:CYS:HB2	2.46	0.51
3:D:916:TYR:CZ	3:D:920:LEU:HD21	2.46	0.51
3:D:1263:PHE:HE2	3:D:1371:VAL:HG11	1.74	0.51
3:D:1376:MET:HE2	3:D:1376:MET:HA	1.92	0.51
1:A:201:THR:HG21	1:A:206:THR:HA	1.93	0.50
2:C:767:PRO:CG	2:C:782:ALA:CB	2.88	0.50
2:C:892:LEU:HD13	2:C:989:VAL:O	2.12	0.50
3:D:1442:ASN:ND2	6:G:11:DT:H4'	2.25	0.50
5:F:383:LEU:HD12	5:F:384:GLU:HG3	1.93	0.50
1:A:131:THR:C	1:A:132:LEU:HD12	2.30	0.50
2:C:124:ASP:HA	2:C:592:LEU:CD1	2.39	0.50
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.93	0.50
2:C:422:ARG:CZ	7:H:13:DT:H5'	2.42	0.50
3:D:112:ILE:HG12	3:D:512:MET:SD	2.51	0.50
3:D:231:VAL:HG13	3:D:242:LEU:C	2.32	0.50
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.93	0.50
3:D:792:ILE:HD13	3:D:941:PHE:CE2	2.46	0.50
3:D:1047:LYS:CG	3:D:1048:PRO:HD2	2.40	0.50
3:D:1310:ARG:CB	3:D:1327:ARG:HD2	2.42	0.50
5:F:415:THR:OG1	5:F:415:THR:O	2.28	0.50
1:A:34:VAL:O	1:A:36:LEU:N	2.45	0.50
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.38	0.50
1:A:225:PHE:HA	1:B:11:PHE:CD2	2.47	0.50
2:C:376:ARG:N	2:C:376:ARG:HD2	2.27	0.50
2:C:886:LEU:HD11	3:D:951:ILE:CD1	2.38	0.50
2:C:1113:GLU:O	2:C:1115:LEU:HD12	2.11	0.50
3:D:956:ILE:HD13	3:D:1039:CYS:O	2.12	0.50
5:F:362:SER:O	5:F:366:ALA:HB3	2.10	0.50
1:A:182:GLU:HG3	1:A:194:LYS:CE	2.41	0.50
1:B:143:ARG:HD3	1:B:158:ILE:CD1	2.41	0.50
2:C:55:GLU:O	2:C:359:MET:HE1	2.11	0.50
2:C:666:LEU:HD11	2:C:668:LEU:CD2	2.41	0.50
2:C:738:ASP:OD2	2:C:742:VAL:HB	2.11	0.50
2:C:1088:LEU:HG	2:C:1088:LEU:O	2.11	0.50
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.47	0.50
3:D:162:ARG:O	3:D:414:ARG:NH2	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:601:ARG:NH1	3:D:606:ILE:HA	2.26	0.50
3:D:876:SER:OG	3:D:879:ARG:HG3	2.12	0.50
3:D:1352:ILE:CG2	3:D:1368:ILE:HD13	2.42	0.50
5:F:198:ILE:HD12	5:F:243:ILE:HG21	1.92	0.50
1:B:20:TYR:OH	1:B:22:GLU:HG2	2.11	0.50
1:B:26:GLU:OE2	1:B:194:LYS:HE3	2.11	0.50
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.93	0.50
1:B:58:ILE:CG2	1:B:61:VAL:HG21	2.41	0.50
2:C:230:ARG:HB2	2:C:233:GLU:HG3	1.93	0.50
3:D:499:VAL:HG12	3:D:503:LEU:HD12	1.94	0.50
3:D:644:LEU:HD11	3:D:648:MET:HE2	1.94	0.50
3:D:703:ASN:HA	3:D:712:GLY:O	2.11	0.50
3:D:805:GLU:HA	3:D:828:LYS:O	2.12	0.50
3:D:885:ILE:HG23	3:D:937:TYR:HE1	1.71	0.50
1:A:62:LEU:HA	1:A:163:ASN:CB	2.34	0.50
2:C:875:GLY:O	2:C:879:ARG:HD3	2.11	0.50
2:C:1006:HIS:ND1	2:C:1007:ALA:N	2.58	0.50
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.93	0.50
3:D:1150:ALA:O	3:D:1151:ARG:HD2	2.10	0.50
5:F:191:ASN:OD1	7:H:6:DT:N3	2.34	0.50
5:F:247:ILE:CG2	5:F:251:ILE:HD12	2.42	0.50
2:C:148:PHE:CZ	2:C:309:TYR:HB3	2.47	0.50
2:C:459:ALA:C	2:C:460:ARG:HG3	2.32	0.50
2:C:693:GLU:CD	2:C:696:LYS:HD2	2.32	0.50
2:C:988:VAL:HG23	3:D:948:THR:HG21	1.94	0.50
3:D:135:LEU:CD1	3:D:463:GLN:HG2	2.42	0.50
3:D:566:ILE:HD11	5:F:192:LEU:HD22	1.92	0.50
3:D:921:ARG:O	3:D:922:LEU:HD23	2.11	0.50
3:D:982:PHE:C	3:D:983:LEU:HG	2.32	0.50
3:D:1485:GLN:O	4:E:75:PHE:HA	2.12	0.50
5:F:167:PRO:O	5:F:169:GLU:N	2.44	0.50
2:C:328:LEU:HD11	2:C:438:ILE:CD1	2.42	0.50
3:D:116:LEU:O	3:D:118:LEU:HG	2.12	0.50
3:D:486:ARG:HG3	3:D:489:ARG:HH22	1.72	0.50
3:D:1333:HIS:HE1	3:D:1421:LEU:O	1.95	0.50
3:D:1444:THR:O	3:D:1447:LEU:N	2.44	0.50
7:H:13:DT:H2"	7:H:14:DG:OP1	2.11	0.50
1:A:78:ILE:O	1:A:82:LEU:HG	2.12	0.50
2:C:9:ILE:HD11	2:C:500:ASN:HB3	1.94	0.50
2:C:422:ARG:HH22	7:H:13:DT:C4'	2.25	0.50
2:C:502:PRO:C	2:C:503:LEU:HD23	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:LEU:O	3:D:135:LEU:HD23	2.12	0.50
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.92	0.50
3:D:315:ARG:HG2	3:D:316:GLN:N	2.27	0.50
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.93	0.50
3:D:767:HIS:HB3	3:D:924:MET:HE1	1.94	0.50
5:F:95:THR:H	5:F:98:GLU:CG	2.15	0.50
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.66	0.49
2:C:211:LEU:HB2	2:C:218:VAL:HG13	1.94	0.49
2:C:272:ALA:HA	2:C:464:LEU:HD13	1.93	0.49
2:C:391:LEU:N	2:C:391:LEU:HD23	2.26	0.49
2:C:724:ARG:O	2:C:724:ARG:HG2	2.12	0.49
2:C:783:ARG:HG3	2:C:784:ASP:N	2.27	0.49
2:C:911:GLU:O	2:C:914:ILE:HG23	2.12	0.49
3:D:116:LEU:HD11	3:D:465:LEU:HD13	1.93	0.49
3:D:206:ARG:HG2	3:D:392:SER:O	2.12	0.49
5:F:395:GLU:HB3	5:F:398:ARG:HH12	1.77	0.49
2:C:626:ARG:O	2:C:639:GLN:HB2	2.12	0.49
2:C:697:ARG:HG3	2:C:699:PHE:CD1	2.48	0.49
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.25	0.49
3:D:97:THR:HG21	3:D:571:LYS:CD	2.42	0.49
4:E:18:ARG:O	4:E:22:VAL:HG23	2.11	0.49
5:F:126:LEU:HD12	5:F:126:LEU:O	2.12	0.49
5:F:367:MET:CE	5:F:368:VAL:HG13	2.42	0.49
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.94	0.49
2:C:773:LEU:O	2:C:777:ILE:HD12	2.12	0.49
3:D:46:ASP:OD1	3:D:48:ARG:HG3	2.12	0.49
3:D:135:LEU:HD13	3:D:455:ARG:NH1	2.27	0.49
3:D:298:VAL:HG12	3:D:302:GLN:OE1	2.12	0.49
3:D:704:ARG:HG2	3:D:705:ALA:N	2.27	0.49
5:F:369:LEU:HD23	5:F:372:ARG:CB	2.38	0.49
2:C:140:ILE:HG22	2:C:412:ALA:HA	1.92	0.49
2:C:157:ARG:HH22	2:C:178:PRO:HA	1.76	0.49
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.94	0.49
2:C:1092:LEU:HD12	2:C:1099:VAL:HG21	1.93	0.49
3:D:191:LEU:HB2	3:D:195:VAL:HG12	1.94	0.49
3:D:1264:GLU:HG3	3:D:1266:ARG:CZ	2.43	0.49
3:D:1310:ARG:O	3:D:1327:ARG:HG2	2.12	0.49
4:E:68:LEU:HD12	4:E:73:LEU:HD12	1.94	0.49
5:F:270:LYS:HG2	5:F:273:ARG:NH2	2.28	0.49
3:D:96:ALA:CB	3:D:554:LEU:HD23	2.40	0.49
3:D:208:PRO:HG2	3:D:353:VAL:HG11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:215:TYR:O	3:D:340:THR:HG22	2.12	0.49
3:D:221:ALA:HB2	3:D:281:THR:HG22	1.94	0.49
3:D:222:GLY:HA2	3:D:333:LEU:O	2.11	0.49
3:D:489:ARG:HD2	3:D:1391:GLU:OE1	2.12	0.49
3:D:672:ALA:HB2	5:F:420:ASP:OD1	2.13	0.49
5:F:153:PRO:CA	5:F:156:VAL:HG12	2.41	0.49
5:F:387:GLY:HA3	5:F:394:ARG:HG2	1.94	0.49
5:F:400:ILE:HD13	5:F:403:LYS:HB2	1.95	0.49
1:B:50:GLY:HA3	1:B:173:PRO:HD3	1.95	0.49
2:C:45:GLN:OE1	2:C:71:TYR:CE2	2.66	0.49
2:C:55:GLU:HG3	2:C:56:GLU:N	2.28	0.49
2:C:351:LEU:HD12	2:C:374:ASN:O	2.13	0.49
2:C:910:LYS:HD2	2:C:910:LYS:N	2.27	0.49
3:D:185:VAL:HG13	3:D:189:GLN:CD	2.32	0.49
3:D:367:ILE:CD1	3:D:379:ALA:HB2	2.24	0.49
3:D:500:ARG:NH2	3:D:1388:ARG:HG3	2.28	0.49
2:C:148:PHE:CD2	2:C:160:ALA:HB2	2.48	0.49
2:C:860:HIS:CE1	2:C:975:TYR:HB2	2.47	0.49
3:D:181:ASP:H	3:D:205:TYR:HE1	1.61	0.49
3:D:394:LEU:CG	3:D:396:VAL:HG23	2.41	0.49
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.42	0.49
1:A:91:ASN:OD1	1:A:93:SER:N	2.46	0.49
2:C:214:TYR:CD2	2:C:218:VAL:CG2	2.95	0.49
3:D:394:LEU:HD21	3:D:396:VAL:CG2	2.42	0.49
3:D:448:GLU:O	3:D:449:SER:OG	2.29	0.49
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.94	0.49
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.48	0.49
3:D:930:LEU:CD1	3:D:934:LEU:CD1	2.91	0.49
3:D:1031:ASN:HB2	3:D:1032:PRO:HD2	1.95	0.49
2:C:443:THR:OG1	2:C:444:PRO:CD	2.60	0.49
2:C:513:VAL:HG21	2:C:529:VAL:CG2	2.42	0.49
2:C:902:ILE:O	2:C:902:ILE:HG22	2.13	0.49
2:C:988:VAL:HG23	3:D:948:THR:OG1	2.13	0.49
3:D:236:TYR:HB2	3:D:319:ALA:CB	2.43	0.49
3:D:923:GLY:O	3:D:927:THR:OG1	2.22	0.49
3:D:1444:THR:O	3:D:1445:HIS:C	2.51	0.49
6:G:18:DA:N6	6:G:19:DG:C2	2.81	0.49
1:B:179:PHE:CB	1:B:197:LEU:HD13	2.41	0.49
2:C:297:GLU:HG3	2:C:299:LYS:NZ	2.28	0.49
2:C:889:HIS:HE1	2:C:988:VAL:HG13	1.77	0.49
3:D:119:SER:HB3	3:D:122:GLU:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.94	0.49
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.47	0.48
1:B:105:GLY:O	1:B:132:LEU:HB2	2.12	0.48
2:C:3:ILE:HD12	2:C:900:ARG:HB2	1.95	0.48
2:C:86:LYS:O	2:C:88:LEU:HD23	2.12	0.48
2:C:109:LYS:HD2	2:C:110:GLU:N	2.21	0.48
2:C:176:VAL:HG22	2:C:182:VAL:CG1	2.43	0.48
2:C:492:ASP:CB	2:C:518:LYS:HG2	2.43	0.48
2:C:700:TYR:HB3	2:C:833:LEU:HD22	1.96	0.48
3:D:134:VAL:HG22	3:D:151:GLN:H	1.78	0.48
3:D:986:ARG:HB2	3:D:986:ARG:CZ	2.43	0.48
3:D:1087:ARG:NH1	3:D:1236:LEU:O	2.46	0.48
6:G:6:DA:H2'	6:G:7:DT:C7	2.42	0.48
1:A:49:PRO:O	1:A:173:PRO:HG3	2.13	0.48
1:A:101:LEU:HD12	1:A:114:PHE:CE1	2.47	0.48
1:B:195:LEU:HD12	1:B:196:THR:N	2.28	0.48
2:C:317:VAL:HB	2:C:320:HIS:HD2	1.76	0.48
2:C:385:PHE:HD2	2:C:386:PHE:CE1	2.32	0.48
2:C:557:ARG:HA	2:C:560:MET:HG3	1.95	0.48
3:D:808:THR:OG1	3:D:811:GLU:HG2	2.12	0.48
3:D:1155:VAL:HB	3:D:1177:ALA:HB1	1.94	0.48
1:A:10:VAL:HG12	1:A:26:GLU:O	2.13	0.48
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.96	0.48
2:C:211:LEU:CB	2:C:218:VAL:HG13	2.44	0.48
2:C:766:GLU:CG	2:C:767:PRO:HD2	2.25	0.48
2:C:861:LEU:CB	2:C:862:PRO:HD2	2.40	0.48
3:D:231:VAL:HG22	3:D:231:VAL:O	2.12	0.48
3:D:686:GLU:H	3:D:686:GLU:CD	2.16	0.48
3:D:1087:ARG:HD3	3:D:1234:THR:O	2.14	0.48
3:D:1088:THR:HG21	6:G:14:DG:C6	2.48	0.48
6:G:7:DT:H3	7:H:21:DA:H61	1.61	0.48
1:A:219:ARG:CG	1:B:219:ARG:HG3	2.43	0.48
2:C:195:LEU:HD12	2:C:195:LEU:O	2.13	0.48
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.14	0.48
2:C:715:THR:HG22	2:C:716:LYS:N	2.28	0.48
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.27	0.48
3:D:1347:TYR:CE2	3:D:1351:GLU:HG3	2.48	0.48
4:E:88:GLU:OE1	4:E:91:ARG:NH2	2.46	0.48
5:F:286:PRO:HB2	5:F:291:ILE:CD1	2.42	0.48
1:B:205:VAL:HG22	1:B:206:THR:H	1.78	0.48
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:ARG:HB2	2:C:739:GLU:O	2.12	0.48
2:C:734:LEU:HD23	2:C:737:LEU:CD1	2.28	0.48
2:C:974:LEU:HD22	2:C:987:ILE:HG21	1.95	0.48
3:D:206:ARG:HB2	3:D:392:SER:O	2.13	0.48
3:D:629:SER:HB3	3:D:726:ILE:HG13	1.94	0.48
3:D:1066:THR:OG1	3:D:1069:GLU:HB2	2.13	0.48
3:D:1168:MET:HE3	3:D:1172:HIS:CD2	2.49	0.48
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.45	0.48
5:F:128:ARG:HB3	5:F:128:ARG:CZ	2.43	0.48
1:B:93:SER:O	1:B:95:GLN:HG3	2.13	0.48
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.48	0.48
3:D:185:VAL:HG12	3:D:186:VAL:N	2.28	0.48
3:D:1041:LEU:O	3:D:1041:LEU:HD23	2.12	0.48
3:D:1444:THR:O	3:D:1448:THR:HG23	2.13	0.48
1:A:9:PRO:HD2	1:B:224:TYR:CD2	2.48	0.48
1:A:109:VAL:O	1:A:129:ILE:HB	2.14	0.48
1:B:42:ARG:HH21	2:C:981:GLU:HG2	1.78	0.48
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.95	0.48
2:C:915:LYS:CE	2:C:968:LEU:O	2.61	0.48
3:D:93:ILE:HD11	3:D:548:ILE:CD1	2.44	0.48
3:D:134:VAL:CG2	3:D:151:GLN:H	2.27	0.48
3:D:274:ARG:O	3:D:275:GLU:C	2.52	0.48
3:D:481:MET:O	3:D:489:ARG:HG3	2.13	0.48
3:D:544:TYR:O	3:D:547:LEU:N	2.46	0.48
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.95	0.48
3:D:860:LEU:HD22	3:D:878:GLY:HA2	1.95	0.48
3:D:1404:ASN:O	3:D:1408:ILE:HG13	2.13	0.48
2:C:103:LYS:O	2:C:103:LYS:HD3	2.13	0.48
2:C:148:PHE:HD2	2:C:160:ALA:HB2	1.78	0.48
2:C:462:ASP:CB	2:C:468:ARG:HH11	2.27	0.48
2:C:886:LEU:CD1	3:D:951:ILE:HD13	2.39	0.48
2:C:1073:GLY:HA2	3:D:659:LYS:HD3	1.95	0.48
3:D:569:ASN:ND2	5:F:84:TYR:CD2	2.82	0.48
3:D:1107:VAL:HG23	3:D:1221:VAL:HG13	1.95	0.48
3:D:1109:GLU:C	3:D:1217:ILE:HD11	2.34	0.48
1:A:34:VAL:CG2	1:B:42:ARG:NE	2.77	0.48
1:A:65:PHE:HE2	2:C:703:ILE:CG2	2.26	0.48
1:A:143:ARG:O	1:A:143:ARG:HD3	2.13	0.48
1:A:206:THR:HG23	1:A:208:LEU:H	1.79	0.48
1:B:40:LEU:N	1:B:40:LEU:HD23	2.29	0.48
1:B:180:GLN:HB3	1:B:196:THR:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:836:GLY:HA3	2:C:1001:VAL:HG22	1.96	0.48
2:C:841:ASN:HD22	2:C:992:MET:HE1	1.79	0.48
2:C:1093:GLN:HB3	3:D:90:MET:HE2	1.95	0.48
3:D:1259:VAL:HG23	3:D:1355:VAL:HG11	1.96	0.48
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.27	0.48
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.13	0.48
1:B:58:ILE:HG22	1:B:61:VAL:HG23	1.95	0.48
1:B:124:ASN:HD22	1:B:127:LEU:HD12	1.79	0.48
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.96	0.48
2:C:204:GLN:HG2	2:C:227:PHE:CE1	2.48	0.48
2:C:748:GLU:HA	2:C:799:ILE:CD1	2.44	0.48
2:C:983:ILE:HG22	2:C:985:GLY:H	1.78	0.48
3:D:648:MET:CE	3:D:747:VAL:HG21	2.43	0.48
3:D:778:LEU:O	3:D:778:LEU:HD23	2.14	0.48
3:D:1013:GLU:C	3:D:1014:ASN:OD1	2.53	0.48
5:F:94:LEU:HG	5:F:190:ALA:HB1	1.96	0.48
5:F:198:ILE:CD1	5:F:243:ILE:HG21	2.44	0.48
5:F:300:ASP:O	5:F:304:VAL:HG12	2.14	0.48
1:A:35:THR:OG1	1:B:42:ARG:CD	2.59	0.47
1:A:227:ASN:HD22	1:A:227:ASN:C	2.16	0.47
2:C:15:LEU:HD12	2:C:15:LEU:HA	1.70	0.47
2:C:405:ARG:HG3	2:C:543:ASN:OD1	2.14	0.47
2:C:1083:GLU:OE1	2:C:1086:ARG:HD2	2.14	0.47
3:D:1275:SER:O	3:D:1322:GLY:N	2.43	0.47
3:D:1495:ILE:HG12	4:E:88:GLU:HB3	1.96	0.47
4:E:37:ASN:OD1	4:E:37:ASN:N	2.47	0.47
5:F:159:ILE:O	5:F:163:LEU:HD12	2.14	0.47
1:B:224:TYR:N	1:B:224:TYR:HD1	2.12	0.47
2:C:436:GLY:HA2	2:C:538:GLN:O	2.14	0.47
2:C:683:ASN:CG	2:C:872:ASN:HB2	2.34	0.47
2:C:693:GLU:OE1	2:C:696:LYS:HD2	2.13	0.47
2:C:720:GLU:HG2	2:C:760:SER:OG	2.14	0.47
2:C:880:MET:CE	3:D:1061:PHE:HE2	2.23	0.47
3:D:1121:PRO:O	3:D:1135:ARG:HD3	2.14	0.47
5:F:413:SER:HA	5:F:416:ARG:CZ	2.44	0.47
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.96	0.47
2:C:73:LEU:HD22	2:C:92:ALA:CB	2.43	0.47
2:C:73:LEU:CD2	2:C:92:ALA:HB3	2.43	0.47
2:C:602:GLU:HG2	2:C:603:VAL:N	2.29	0.47
2:C:767:PRO:HG3	2:C:782:ALA:CB	2.42	0.47
2:C:815:LEU:HD12	2:C:819:VAL:CG2	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:839:LEU:HD23	2:C:996:LYS:HA	1.96	0.47
2:C:1092:LEU:HD21	3:D:607:LEU:HD21	1.95	0.47
3:D:216:VAL:CA	3:D:340:THR:HG22	2.35	0.47
3:D:860:LEU:HD23	3:D:878:GLY:N	2.30	0.47
3:D:1034:GLN:HA	3:D:1037:GLN:HE21	1.80	0.47
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.96	0.47
2:C:20:GLU:O	2:C:24:GLU:HB2	2.14	0.47
2:C:176:VAL:HG11	2:C:217:LEU:CD1	2.44	0.47
2:C:726:ILE:HD12	2:C:726:ILE:N	2.28	0.47
3:D:170:PRO:HA	3:D:392:SER:HB2	1.95	0.47
3:D:558:LEU:CD2	3:D:567:ILE:HD12	2.44	0.47
3:D:575:GLN:HA	3:D:578:VAL:HG13	1.96	0.47
3:D:789:LEU:HD21	3:D:938:GLY:CA	2.45	0.47
3:D:916:TYR:CE1	3:D:920:LEU:HD21	2.48	0.47
4:E:50:THR:HG23	4:E:53:GLY:N	2.27	0.47
5:F:400:ILE:O	5:F:404:ALA:HB2	2.13	0.47
1:A:153:ALA:N	1:A:168:ASP:OD1	2.26	0.47
1:A:226:SER:C	1:A:228:PRO:HD3	2.34	0.47
2:C:224:GLU:C	2:C:226:VAL:N	2.68	0.47
3:D:62:LYS:HE3	3:D:74:GLU:OE2	2.14	0.47
3:D:64:LYS:O	3:D:65:ARG:CB	2.62	0.47
3:D:123:LEU:O	3:D:127:LEU:HB2	2.14	0.47
3:D:134:VAL:CG1	3:D:153:LEU:HD11	2.44	0.47
3:D:237:LYS:O	3:D:240:GLU:HB2	2.15	0.47
3:D:396:VAL:CG1	3:D:397:LYS:N	2.78	0.47
3:D:527:MET:HG3	3:D:535:PHE:HD1	1.80	0.47
3:D:1054:GLU:O	3:D:1056:PRO:HD3	2.13	0.47
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.96	0.47
3:D:1118:ILE:HD13	3:D:1190:SER:HB2	1.96	0.47
5:F:239:ALA:C	5:F:241:TRP:H	2.16	0.47
2:C:825:VAL:O	2:C:825:VAL:HG22	2.15	0.47
2:C:858:MET:HG3	2:C:867:VAL:HG23	1.97	0.47
2:C:958:THR:CG2	2:C:961:GLU:HG3	2.33	0.47
2:C:1097:LEU:HD22	3:D:1451:ALA:HB2	1.96	0.47
3:D:242:LEU:CD2	3:D:311:LEU:CD1	2.92	0.47
3:D:348:GLN:H	3:D:351:MET:HE3	1.80	0.47
3:D:508:ARG:HB3	3:D:510:GLU:HG2	1.97	0.47
1:A:97:VAL:HG12	1:A:98:THR:H	1.80	0.47
1:A:143:ARG:NH1	1:A:160:ASP:OD1	2.48	0.47
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.13	0.47
2:C:72:ARG:HG2	2:C:95:TYR:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.47	0.47
2:C:148:PHE:O	2:C:322:VAL:HG13	2.15	0.47
2:C:772:ARG:HG2	2:C:772:ARG:HH11	1.80	0.47
3:D:314:PRO:CG	3:D:317:VAL:HG11	2.45	0.47
3:D:583:ASP:OD2	3:D:586:ARG:NH1	2.48	0.47
3:D:886:VAL:HG12	3:D:896:ALA:HB1	1.97	0.47
3:D:935:LYS:HE3	3:D:935:LYS:HB3	1.62	0.47
3:D:1103:HIS:HA	3:D:1223:ILE:HD11	1.96	0.47
3:D:1234:THR:H	3:D:1235:GLN:HB3	1.79	0.47
1:A:228:PRO:HB3	1:B:13:VAL:HG23	1.97	0.47
2:C:176:VAL:HG13	2:C:182:VAL:HG12	1.97	0.47
2:C:598:GLU:N	2:C:615:TYR:OH	2.44	0.47
3:D:56:TYR:OH	3:D:82:LYS:HE2	2.15	0.47
3:D:249:TYR:O	3:D:249:TYR:CG	2.68	0.47
3:D:371:ILE:CD1	5:F:232:ARG:NH1	2.78	0.47
3:D:568:ARG:HD2	5:F:87:GLU:OE2	2.14	0.47
3:D:1289:LYS:HZ1	3:D:1304:LYS:HB2	1.78	0.47
5:F:358:LEU:HD13	5:F:366:ALA:HB1	1.97	0.47
5:F:361:LEU:CG	5:F:411:HIS:HD2	2.23	0.47
1:B:13:VAL:HG12	1:B:15:THR:HG22	1.97	0.47
2:C:45:GLN:OE1	2:C:71:TYR:HE2	1.98	0.47
2:C:399:ASN:OD1	2:C:401:LEU:N	2.48	0.47
2:C:419:THR:O	2:C:422:ARG:N	2.47	0.47
2:C:1067:TYR:CD1	2:C:1071:ILE:HD13	2.50	0.47
3:D:135:LEU:HD13	3:D:455:ARG:HH12	1.79	0.47
3:D:557:LEU:HD13	3:D:566:ILE:HG21	1.96	0.47
3:D:789:LEU:CD2	3:D:938:GLY:HA2	2.45	0.47
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.48	0.47
5:F:96:LEU:O	5:F:96:LEU:HD12	2.15	0.47
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.96	0.47
2:C:567:GLN:NE2	2:C:999:HIS:NE2	2.63	0.47
2:C:630:ARG:HD2	2:C:705:ILE:CG2	2.45	0.47
2:C:683:ASN:HB3	2:C:872:ASN:ND2	2.26	0.47
2:C:715:THR:CG2	2:C:716:LYS:N	2.78	0.47
2:C:717:LEU:N	2:C:717:LEU:HD12	2.30	0.47
2:C:949:LYS:HD2	3:D:796:ARG:NE	2.30	0.47
3:D:26:VAL:HG12	3:D:548:ILE:CD1	2.45	0.47
3:D:1304:LYS:HG2	3:D:1305:LEU:N	2.29	0.47
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.97	0.47
5:F:271:LEU:HD12	5:F:271:LEU:N	2.30	0.47
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HG2	1:B:177:VAL:CG1	2.45	0.46
1:B:44:LEU:HD13	1:B:199:ILE:HD11	1.97	0.46
1:B:143:ARG:HD3	1:B:158:ILE:HD12	1.97	0.46
1:B:219:ARG:O	1:B:222:LEU:HB2	2.14	0.46
2:C:64:LEU:N	2:C:103:LYS:CB	2.77	0.46
2:C:168:ARG:O	2:C:267:TYR:HA	2.16	0.46
2:C:539:VAL:O	2:C:539:VAL:CG1	2.62	0.46
2:C:682:TYR:HB2	2:C:689:VAL:CG2	2.45	0.46
3:D:706:PRO:HG2	10:D:1601:DCP:O2	2.14	0.46
3:D:895:VAL:O	3:D:898:GLU:N	2.43	0.46
3:D:998:GLU:O	3:D:1002:LYS:HG3	2.14	0.46
5:F:152:ASP:OD1	5:F:154:LYS:HB3	2.14	0.46
5:F:367:MET:HE3	5:F:368:VAL:HG13	1.97	0.46
1:B:162:ILE:HG13	1:B:163:ASN:HD22	1.80	0.46
2:C:534:VAL:HG12	2:C:535:SER:N	2.31	0.46
2:C:673:LEU:HD23	2:C:867:VAL:HA	1.96	0.46
2:C:712:ALA:HB3	2:C:821:GLU:HG2	1.97	0.46
2:C:741:GLY:O	2:C:756:VAL:HA	2.15	0.46
2:C:1019:GLN:CD	3:D:621:LYS:HB3	2.35	0.46
3:D:7:LYS:HD3	3:D:1456:LYS:HZ1	1.77	0.46
3:D:32:ILE:HG13	3:D:32:ILE:O	2.15	0.46
3:D:203:ALA:O	3:D:204:LEU:HG	2.14	0.46
3:D:259:VAL:CG1	3:D:270:LEU:HD21	2.33	0.46
5:F:197:SER:HA	5:F:200:LYS:HE3	1.98	0.46
5:F:288:TYR:CE2	5:F:305:GLU:HG3	2.51	0.46
1:A:117:VAL:HB	1:A:120:VAL:HG21	1.96	0.46
2:C:312:ALA:O	2:C:317:VAL:HG23	2.14	0.46
2:C:340:MET:SD	2:C:340:MET:C	2.93	0.46
2:C:695:LEU:N	2:C:695:LEU:HD23	2.30	0.46
2:C:836:GLY:C	2:C:1001:VAL:HG22	2.35	0.46
3:D:74:GLU:CD	3:D:74:GLU:H	2.18	0.46
3:D:207:PHE:CZ	5:F:101:GLU:OE2	2.68	0.46
3:D:269:PHE:CE2	3:D:283:PHE:HD1	2.34	0.46
3:D:394:LEU:CD2	3:D:396:VAL:HG23	2.45	0.46
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.49	0.46
5:F:215:GLU:O	5:F:218:GLN:HB3	2.15	0.46
1:A:180:GLN:HG3	2:C:934:PHE:HD1	1.79	0.46
1:B:110:LYS:HD2	1:B:110:LYS:N	2.29	0.46
2:C:661:SER:HA	2:C:665:PHE:O	2.16	0.46
3:D:245:LEU:CD2	3:D:307:ALA:HB3	2.45	0.46
3:D:258:VAL:O	3:D:272:LEU:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:311:LEU:HD12	3:D:311:LEU:O	2.15	0.46
3:D:411:THR:O	5:F:178:ARG:HD2	2.16	0.46
3:D:433:GLY:CA	3:D:447:VAL:O	2.63	0.46
3:D:1487:VAL:HG12	4:E:85:LEU:CD1	2.45	0.46
5:F:136:LEU:HD21	5:F:185:GLN:OE1	2.16	0.46
5:F:291:ILE:HG22	5:F:292:ALA:N	2.30	0.46
5:F:362:SER:O	5:F:366:ALA:CB	2.63	0.46
2:C:262:ALA:HB2	2:C:291:ALA:HB3	1.97	0.46
2:C:461:VAL:O	2:C:461:VAL:CG2	2.64	0.46
2:C:571:LEU:HD13	2:C:669:GLY:HA2	1.97	0.46
2:C:1097:LEU:HD22	3:D:1451:ALA:CB	2.45	0.46
3:D:284:LEU:HD13	3:D:284:LEU:N	2.31	0.46
3:D:409:VAL:CG2	3:D:409:VAL:O	2.64	0.46
5:F:369:LEU:HD12	5:F:404:ALA:HB1	1.98	0.46
1:A:5:LYS:HG2	1:A:6:LEU:O	2.15	0.46
1:A:63:HIS:HB2	2:C:799:ILE:HG21	1.98	0.46
1:B:158:ILE:O	1:B:158:ILE:HG13	2.14	0.46
2:C:168:ARG:NH2	2:C:268:ASP:HB2	2.29	0.46
2:C:396:ASP:O	2:C:402:SER:HB2	2.15	0.46
3:D:84:ILE:CD1	3:D:87:ARG:HD3	2.46	0.46
3:D:1127:GLU:HA	3:D:1130:ARG:HB3	1.96	0.46
3:D:1310:ARG:HB2	3:D:1327:ARG:CD	2.45	0.46
5:F:278:LEU:O	5:F:282:LEU:HG	2.15	0.46
6:G:6:DA:H2'	6:G:7:DT:H72	1.96	0.46
7:H:12:DC:H1'	7:H:13:DT:C6	2.51	0.46
1:A:19:GLU:O	1:A:207:PRO:CG	2.62	0.46
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.45	0.46
1:B:92:PRO:O	1:B:146:ARG:NH1	2.49	0.46
2:C:31:GLN:C	2:C:33:ASP:H	2.19	0.46
2:C:374:ASN:O	2:C:377:PRO:HD2	2.16	0.46
2:C:409:ARG:HD3	2:C:452:ILE:HG22	1.98	0.46
2:C:836:GLY:HA3	2:C:1001:VAL:HG21	1.98	0.46
2:C:1067:TYR:HE2	3:D:674:ARG:HH21	1.63	0.46
3:D:103:TRP:CE2	3:D:1444:THR:HG22	2.50	0.46
3:D:207:PHE:CE1	5:F:97:GLU:HB3	2.51	0.46
3:D:478:LEU:C	3:D:480:GLU:N	2.69	0.46
3:D:951:ILE:CD1	3:D:1062:ARG:HG3	2.45	0.46
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.97	0.46
3:D:1499:ARG:HH11	4:E:84:ARG:HG2	1.80	0.46
7:H:2:DA:H2'	7:H:2:DA:O5'	2.15	0.46
1:A:154:GLU:H	1:A:154:GLU:CD	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ASN:OD1	2:C:46:ALA:HA	2.15	0.46
2:C:211:LEU:O	2:C:213:ALA:N	2.49	0.46
2:C:757:GLY:HA2	2:C:789:SER:OG	2.16	0.46
3:D:131:LYS:HD3	3:D:152:LEU:HB3	1.98	0.46
3:D:1217:ILE:HG21	3:D:1480:PHE:CD2	2.51	0.46
5:F:79:ASP:C	5:F:79:ASP:OD1	2.53	0.46
2:C:1:MET:HB2	2:C:898:GLY:O	2.16	0.46
2:C:666:LEU:HG	2:C:668:LEU:HG	1.98	0.46
2:C:874:LEU:HD13	3:D:783:ARG:CB	2.38	0.46
3:D:396:VAL:HG12	3:D:397:LYS:N	2.31	0.46
3:D:450:TYR:CD2	3:D:450:TYR:N	2.83	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.31	0.46
3:D:1114:THR:HG23	3:D:1189:ARG:NH2	2.30	0.46
3:D:1234:THR:N	3:D:1235:GLN:HB2	2.31	0.46
3:D:1491:THR:HG21	4:E:89:MET:CG	2.45	0.46
5:F:88:ILE:HG23	5:F:193:ARG:HG3	1.98	0.46
5:F:194:LEU:HA	7:H:6:DT:O4'	2.16	0.46
1:A:206:THR:H	1:A:209:GLU:HG3	1.81	0.46
1:B:11:PHE:HE1	1:B:23:PHE:HB3	1.80	0.46
1:B:124:ASN:HD21	1:B:127:LEU:HD12	1.81	0.46
2:C:12:VAL:CG2	2:C:472:ARG:HD2	2.46	0.46
2:C:263:ASP:C	2:C:265:ARG:H	2.15	0.46
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.50	0.46
2:C:858:MET:HG2	2:C:867:VAL:O	2.15	0.46
3:D:93:ILE:CD1	3:D:548:ILE:CG1	2.93	0.46
3:D:192:ALA:HB1	3:D:193:PRO:CD	2.46	0.46
3:D:464:LEU:HA	3:D:464:LEU:HD12	1.36	0.46
3:D:974:ILE:HD11	3:D:991:GLN:OE1	2.16	0.46
3:D:1149:LEU:HD23	3:D:1149:LEU:HA	1.70	0.46
5:F:193:ARG:HB3	7:H:6:DT:O3'	2.16	0.46
7:H:3:DT:H2"	7:H:4:DA:H5'	1.98	0.46
1:A:76:VAL:O	1:A:80:LEU:HB2	2.16	0.45
1:A:195:LEU:HD12	1:A:196:THR:N	2.31	0.45
1:B:29:GLU:HG3	1:B:30:ARG:H	1.81	0.45
1:B:90:LEU:HD12	1:B:119:ASP:C	2.37	0.45
2:C:238:LEU:HD12	2:C:241:LEU:CB	2.44	0.45
2:C:250:ARG:HH11	2:C:254:VAL:HG21	1.81	0.45
3:D:314:PRO:HD2	3:D:317:VAL:HG13	1.97	0.45
3:D:643:GLY:O	3:D:726:ILE:HA	2.16	0.45
3:D:815:ALA:O	3:D:818:ARG:HB2	2.16	0.45
3:D:958:GLU:C	3:D:960:LYS:H	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1031:ASN:OD1	3:D:1034:GLN:HG3	2.16	0.45
3:D:1192:LEU:HD22	3:D:1192:LEU:HA	1.71	0.45
3:D:1312:LEU:HB2	3:D:1325:LEU:O	2.17	0.45
5:F:112:ALA:HB2	5:F:176:ILE:HG21	1.97	0.45
1:A:44:LEU:HD22	1:A:199:ILE:HD13	1.98	0.45
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.46	0.45
2:C:546:LEU:HA	2:C:546:LEU:HD23	1.63	0.45
3:D:93:ILE:HD11	3:D:548:ILE:HG12	1.98	0.45
3:D:613:ARG:HG3	3:D:618:LEU:CD2	2.47	0.45
3:D:695:ILE:HD13	3:D:720:LEU:CD1	2.47	0.45
3:D:731:LEU:HD22	3:D:780:LYS:O	2.16	0.45
3:D:957:PRO:CG	3:D:1007:VAL:HG22	2.46	0.45
3:D:958:GLU:O	3:D:960:LYS:N	2.49	0.45
3:D:1281:VAL:HA	3:D:1293:PHE:O	2.16	0.45
3:D:1330:ILE:HD12	3:D:1347:TYR:CE1	2.51	0.45
5:F:321:ILE:HG22	5:F:327:SER:OG	2.17	0.45
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.26	0.45
2:C:312:ALA:HB1	2:C:317:VAL:CG2	2.46	0.45
2:C:711:GLU:OE2	2:C:816:LYS:NZ	2.41	0.45
2:C:800:VAL:HG13	2:C:825:VAL:HG23	1.99	0.45
2:C:880:MET:HE1	3:D:1037:GLN:CD	2.36	0.45
3:D:212:ARG:HB2	3:D:344:ASP:OD1	2.15	0.45
3:D:409:VAL:HG23	3:D:409:VAL:O	2.15	0.45
3:D:1164:ARG:NH2	3:D:1170:ASP:OD1	2.49	0.45
3:D:1371:VAL:O	3:D:1372:VAL:C	2.52	0.45
5:F:396:ARG:HG3	5:F:396:ARG:O	2.15	0.45
1:A:54:THR:O	1:A:156:HIS:HE1	1.99	0.45
1:B:38:ASN:CB	1:B:39:PRO:CD	2.94	0.45
2:C:97:ARG:HG2	2:C:112:GLU:HB3	1.98	0.45
2:C:149:THR:HA	2:C:322:VAL:CG1	2.41	0.45
2:C:167:LYS:HG2	7:H:12:DC:C5	2.51	0.45
2:C:278:GLU:O	2:C:282:GLY:N	2.50	0.45
2:C:548:PRO:O	2:C:843:HIS:HE1	1.99	0.45
2:C:594:ALA:HB3	2:C:596:TYR:HE2	1.80	0.45
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.45	0.45
3:D:46:ASP:OD1	3:D:48:ARG:CG	2.65	0.45
3:D:543:LEU:CD1	3:D:581:LEU:HA	2.47	0.45
3:D:632:VAL:C	3:D:740:PHE:CE2	2.90	0.45
3:D:1312:LEU:HD21	3:D:1327:ARG:HH21	1.81	0.45
3:D:1389:LEU:C	3:D:1390:LEU:HD23	2.36	0.45
5:F:361:LEU:HD12	5:F:411:HIS:HB2	1.93	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:390:GLN:HE21	2:C:390:GLN:HB3	1.54	0.45
2:C:690:ILE:HD11	2:C:852:ILE:HG23	1.97	0.45
2:C:739:GLU:H	2:C:739:GLU:CD	2.20	0.45
2:C:860:HIS:HB2	2:C:865:THR:O	2.16	0.45
3:D:5:VAL:O	3:D:6:ARG:HG2	2.16	0.45
3:D:97:THR:HG21	3:D:571:LYS:CG	2.46	0.45
3:D:245:LEU:HD21	3:D:307:ALA:HB3	1.99	0.45
3:D:657:LEU:HG	3:D:661:MET:HE1	1.97	0.45
3:D:671:LYS:HD2	5:F:420:ASP:O	2.16	0.45
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.98	0.45
5:F:329:TYR:O	5:F:329:TYR:CD2	2.70	0.45
1:B:109:VAL:O	1:B:110:LYS:HD2	2.17	0.45
2:C:322:VAL:HG12	2:C:323:ASP:N	2.32	0.45
2:C:737:LEU:HA	2:C:742:VAL:O	2.15	0.45
2:C:745:ILE:CD1	2:C:802:ARG:HA	2.47	0.45
2:C:783:ARG:HG3	2:C:784:ASP:H	1.82	0.45
2:C:1012:PRO:HB3	5:F:334:PRO:HB3	1.99	0.45
3:D:135:LEU:O	3:D:149:LYS:CE	2.64	0.45
3:D:325:GLU:O	3:D:331:VAL:HG23	2.16	0.45
5:F:196:VAL:HG22	5:F:213:ILE:HD11	1.99	0.45
1:A:137:ARG:HG2	1:A:138:LEU:H	1.81	0.45
1:B:112:ARG:NH2	1:B:112:ARG:HB3	2.31	0.45
1:B:146:ARG:HE	1:B:146:ARG:HB2	1.62	0.45
2:C:150:PRO:CD	2:C:322:VAL:HG21	2.46	0.45
2:C:805:ARG:NH2	2:C:821:GLU:OE1	2.50	0.45
2:C:1093:GLN:HB3	3:D:90:MET:CE	2.47	0.45
3:D:363:ALA:HB2	3:D:381:ALA:HA	1.97	0.45
3:D:1151:ARG:HB3	3:D:1151:ARG:HH21	1.82	0.45
3:D:1166:LEU:N	3:D:1166:LEU:HD23	2.30	0.45
3:D:1447:LEU:HD23	3:D:1447:LEU:HA	1.79	0.45
1:B:162:ILE:HG13	1:B:163:ASN:ND2	2.32	0.45
2:C:239:PHE:HD1	2:C:253:ALA:HA	1.78	0.45
2:C:966:LEU:HD13	2:C:986:PRO:CB	2.47	0.45
2:C:1009:SER:HA	3:D:625:TYR:CD1	2.50	0.45
3:D:613:ARG:HG3	3:D:618:LEU:HD21	1.99	0.45
3:D:762:GLN:NE2	4:E:17:TYR:HD1	2.15	0.45
6:G:4:DG:H2"	6:G:5:DC:O5'	2.17	0.45
1:B:48:ILE:O	1:B:173:PRO:HD2	2.16	0.45
2:C:204:GLN:HG2	2:C:227:PHE:CE2	2.50	0.45
2:C:436:GLY:HA2	2:C:539:VAL:HA	1.98	0.45
2:C:905:ILE:CG2	2:C:906:PHE:HD1	2.26	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:930:LYS:HA	2:C:934:PHE:O	2.16	0.45
2:C:983:ILE:O	2:C:985:GLY:N	2.50	0.45
3:D:128:TYR:CZ	3:D:587:ARG:HD3	2.52	0.45
3:D:202:VAL:O	3:D:202:VAL:CG2	2.65	0.45
3:D:527:MET:HE2	3:D:527:MET:HB2	1.55	0.45
3:D:1381:VAL:HG12	3:D:1382:THR:N	2.31	0.45
5:F:163:LEU:HB3	5:F:174:LEU:CD1	2.47	0.45
5:F:170:HIS:C	5:F:172:ARG:N	2.70	0.45
1:A:75:VAL:O	1:A:75:VAL:HG12	2.17	0.45
1:A:198:ARG:C	1:A:199:ILE:HG12	2.36	0.45
1:B:101:LEU:HD11	1:B:109:VAL:HG12	1.99	0.45
2:C:64:LEU:N	2:C:103:LYS:HB2	2.32	0.45
2:C:72:ARG:NH2	2:C:95:TYR:CE1	2.85	0.45
2:C:497:ALA:HB3	2:C:532:MET:HG3	1.98	0.45
2:C:760:SER:HB2	2:C:788:THR:HG21	1.99	0.45
2:C:880:MET:HE1	3:D:1037:GLN:NE2	2.32	0.45
3:D:1305:LEU:HD12	3:D:1305:LEU:O	2.16	0.45
3:D:1448:THR:OG1	3:D:1449:GLU:N	2.50	0.45
1:B:45:LEU:HD23	1:B:174:VAL:HG11	1.98	0.44
1:B:202:ASP:OD1	1:B:204:SER:CB	2.65	0.44
2:C:168:ARG:HE	2:C:345:ARG:NH1	2.16	0.44
2:C:207:LEU:HD13	2:C:221:LEU:HD12	1.98	0.44
2:C:388:ARG:HG3	2:C:388:ARG:NH1	2.32	0.44
2:C:554:ASP:HA	3:D:1061:PHE:CZ	2.52	0.44
2:C:682:TYR:CE1	2:C:851:LYS:CD	3.01	0.44
2:C:700:TYR:CB	2:C:833:LEU:HD23	2.47	0.44
3:D:58:CYS:SG	3:D:62:LYS:N	2.90	0.44
3:D:374:GLU:O	3:D:375:GLU:HG2	2.17	0.44
3:D:1217:ILE:O	3:D:1217:ILE:HG22	2.17	0.44
5:F:88:ILE:C	5:F:90:GLN:H	2.19	0.44
5:F:148:LYS:HD3	5:F:148:LYS:HA	1.55	0.44
1:A:23:PHE:N	1:A:23:PHE:CD1	2.85	0.44
1:A:124:ASN:HD21	1:A:127:LEU:HD22	1.82	0.44
1:A:221:HIS:ND1	1:A:224:TYR:CE2	2.83	0.44
1:B:6:LEU:O	1:B:6:LEU:HD13	2.17	0.44
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.61	0.44
2:C:767:PRO:HG2	2:C:782:ALA:CB	2.46	0.44
2:C:837:ASP:OD1	2:C:1001:VAL:HG23	2.17	0.44
3:D:691:LEU:HD13	3:D:720:LEU:HD21	2.00	0.44
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.99	0.44
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD23	1:B:95:GLN:H	1.80	0.44
2:C:501:THR:HG22	2:C:514:VAL:HG23	1.98	0.44
2:C:578:VAL:HA	2:C:900:ARG:HD2	1.99	0.44
2:C:774:LEU:HD21	5:F:421:PHE:HB2	2.00	0.44
2:C:882:LEU:O	2:C:885:ILE:HB	2.17	0.44
3:D:185:VAL:CG1	3:D:186:VAL:H	2.29	0.44
3:D:478:LEU:O	3:D:480:GLU:N	2.50	0.44
3:D:554:LEU:HB2	3:D:570:GLU:CG	2.47	0.44
3:D:1103:HIS:CD2	3:D:1463:LYS:HG3	2.52	0.44
3:D:1273:VAL:HB	3:D:1326:THR:CG2	2.46	0.44
3:D:1432:LYS:HB2	3:D:1432:LYS:HE3	1.80	0.44
1:A:6:LEU:HD23	1:A:7:LYS:O	2.17	0.44
1:B:110:LYS:C	1:B:129:ILE:HD13	2.37	0.44
2:C:177:GLU:OE2	2:C:183:SER:HB3	2.16	0.44
3:D:137:PRO:HG2	3:D:147:VAL:O	2.17	0.44
3:D:211:VAL:HG23	3:D:347:VAL:CG2	2.48	0.44
3:D:761:ILE:HG21	4:E:19:LEU:HD23	2.00	0.44
3:D:762:GLN:NE2	4:E:17:TYR:CD1	2.86	0.44
3:D:1495:ILE:HG12	4:E:88:GLU:CB	2.47	0.44
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.50	0.44
1:B:58:ILE:HG12	1:B:140:MET:HB2	1.99	0.44
1:B:96:THR:CG2	1:B:97:VAL:H	2.27	0.44
2:C:154:ARG:NH1	2:C:175:GLU:OE2	2.51	0.44
2:C:226:VAL:O	2:C:229:MET:HG3	2.17	0.44
3:D:348:GLN:N	3:D:351:MET:HE2	2.33	0.44
3:D:568:ARG:HE	3:D:568:ARG:HB2	1.56	0.44
3:D:648:MET:HE1	3:D:747:VAL:HG21	1.98	0.44
3:D:930:LEU:O	3:D:933:ALA:HB3	2.16	0.44
3:D:1280:VAL:HG12	3:D:1318:TYR:HA	2.00	0.44
5:F:154:LYS:HB3	5:F:154:LYS:HE3	1.87	0.44
5:F:387:GLY:HA2	5:F:394:ARG:HG2	1.98	0.44
1:A:79:ILE:HG23	1:A:167:VAL:HG22	1.99	0.44
1:B:37:GLY:HA2	1:B:40:LEU:HB2	1.99	0.44
1:B:123:MET:O	1:B:125:PRO:HD3	2.17	0.44
1:B:162:ILE:O	1:B:163:ASN:HB2	2.17	0.44
2:C:606:VAL:HG21	2:C:643:VAL:HG23	2.00	0.44
2:C:822:VAL:HG13	2:C:822:VAL:O	2.17	0.44
2:C:952:LEU:HB3	2:C:966:LEU:CD2	2.48	0.44
3:D:181:ASP:OD1	3:D:205:TYR:HB2	2.17	0.44
3:D:204:LEU:HA	3:D:204:LEU:HD23	1.86	0.44
3:D:702:LEU:O	3:D:713:ILE:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:832:ARG:CD	3:D:832:ARG:N	2.81	0.44
3:D:1127:GLU:HB3	3:D:1130:ARG:HH12	1.83	0.44
3:D:1292:VAL:HG13	3:D:1303:TYR:HB2	1.99	0.44
3:D:1295:GLU:HA	3:D:1300:SER:HB2	2.00	0.44
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.44	0.44
4:E:80:VAL:HG12	4:E:81:PRO:N	2.32	0.44
5:F:210:LEU:O	5:F:211:ASP:C	2.55	0.44
1:B:74:ASP:OD2	3:D:872:ARG:NH1	2.51	0.44
2:C:44:ILE:HD11	2:C:344:PHE:CD2	2.53	0.44
2:C:355:VAL:CG2	2:C:356:ARG:N	2.80	0.44
2:C:583:LEU:O	2:C:585:GLU:N	2.51	0.44
2:C:876:VAL:N	2:C:877:PRO:HD2	2.33	0.44
2:C:1048:THR:N	3:D:758:GLU:OE2	2.48	0.44
3:D:119:SER:HB3	3:D:122:GLU:CG	2.48	0.44
3:D:286:VAL:O	3:D:311:LEU:HB2	2.18	0.44
3:D:347:VAL:HA	3:D:351:MET:CE	2.48	0.44
3:D:519:VAL:HG22	3:D:544:TYR:CZ	2.53	0.44
3:D:706:PRO:HB3	3:D:708:LEU:HD21	1.99	0.44
3:D:707:THR:HG22	3:D:707:THR:O	2.16	0.44
3:D:741:ASP:OD1	3:D:741:ASP:N	2.44	0.44
3:D:958:GLU:C	3:D:960:LYS:N	2.71	0.44
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.47	0.44
3:D:1150:ALA:HB2	3:D:1189:ARG:HG2	2.00	0.44
3:D:1495:ILE:HG23	4:E:88:GLU:HG3	1.99	0.44
5:F:363:GLU:HG3	5:F:363:GLU:O	2.17	0.44
5:F:382:THR:HG22	5:F:383:LEU:CG	2.48	0.44
1:A:122:ILE:HD12	1:A:122:ILE:HA	1.85	0.44
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.33	0.44
1:A:206:THR:HG22	1:A:209:GLU:H	1.81	0.44
2:C:538:GLN:O	2:C:538:GLN:HG3	2.16	0.44
2:C:607:ASP:HB2	2:C:610:ARG:HH12	1.82	0.44
3:D:58:CYS:SG	3:D:59:ALA:N	2.91	0.44
3:D:210:ARG:NH2	3:D:212:ARG:HH21	2.15	0.44
3:D:514:LEU:HD22	3:D:517:VAL:HG22	2.00	0.44
3:D:650:LEU:CD1	3:D:657:LEU:HD22	2.43	0.44
3:D:1103:HIS:HA	3:D:1223:ILE:CD1	2.48	0.44
3:D:1145:TYR:CD1	3:D:1146:GLY:N	2.86	0.44
5:F:274:THR:O	5:F:277:GLN:HG2	2.18	0.44
1:A:23:PHE:CD2	1:A:211:LEU:CD2	3.01	0.44
1:A:153:ALA:C	1:A:155:LYS:N	2.69	0.44
1:A:216:GLU:OE1	1:A:216:GLU:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:HB2	1:B:110:LYS:NZ	2.32	0.44
2:C:88:LEU:O	2:C:131:GLY:N	2.51	0.44
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.33	0.44
2:C:799:ILE:O	2:C:801:VAL:HG23	2.17	0.44
3:D:132:TYR:HD1	3:D:454:ALA:O	2.00	0.44
3:D:229:ALA:HB1	3:D:244:GLU:O	2.18	0.44
3:D:371:ILE:HG13	3:D:372:ASP:OD1	2.18	0.44
3:D:775:GLY:CA	3:D:1209:LEU:HB3	2.47	0.44
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.81	0.44
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.85	0.44
4:E:9:LEU:HD23	4:E:9:LEU:HA	1.73	0.44
1:A:138:LEU:HD21	1:A:140:MET:HE2	2.00	0.43
2:C:905:ILE:HG23	2:C:906:PHE:CD1	2.41	0.43
3:D:187:LYS:CD	3:D:187:LYS:N	2.81	0.43
3:D:828:LYS:CE	3:D:831:GLY:H	2.21	0.43
3:D:1234:THR:CA	3:D:1235:GLN:CB	2.96	0.43
3:D:1462:LEU:CD2	3:D:1473:PRO:HD2	2.45	0.43
5:F:86:HIS:O	5:F:90:GLN:HG2	2.17	0.43
5:F:368:VAL:HG11	5:F:397:ILE:HD11	1.98	0.43
2:C:168:ARG:NE	2:C:345:ARG:NH1	2.65	0.43
2:C:494:TYR:CD2	2:C:531:PHE:CE2	3.06	0.43
3:D:63:TYR:HE2	3:D:73:CYS:HB2	1.81	0.43
3:D:247:GLU:HB2	3:D:248:PRO:CD	2.48	0.43
3:D:343:LYS:HG2	3:D:345:TYR:HE2	1.82	0.43
3:D:409:VAL:HG13	3:D:421:LEU:O	2.18	0.43
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.80	0.43
3:D:957:PRO:HG3	3:D:1007:VAL:HA	2.00	0.43
4:E:26:ARG:NH2	4:E:38:THR:HA	2.33	0.43
5:F:219:GLY:O	5:F:222:ARG:HB2	2.18	0.43
5:F:325:LYS:N	5:F:325:LYS:HD2	2.33	0.43
1:A:9:PRO:HD3	1:B:224:TYR:CE2	2.54	0.43
1:B:129:ILE:N	1:B:129:ILE:HD12	2.34	0.43
2:C:564:MET:CG	2:C:997:LEU:HD11	2.44	0.43
2:C:589:ARG:NE	2:C:596:TYR:CE1	2.87	0.43
3:D:230:TRP:CZ2	3:D:232:GLU:HG3	2.53	0.43
3:D:437:VAL:O	3:D:437:VAL:HG12	2.16	0.43
3:D:708:LEU:N	3:D:708:LEU:HD23	2.33	0.43
3:D:804:LEU:HD13	3:D:806:PHE:CZ	2.52	0.43
5:F:116:LEU:HD21	5:F:163:LEU:HD22	2.00	0.43
5:F:143:HIS:HB2	5:F:150:THR:HA	2.01	0.43
1:A:53:VAL:HG11	1:A:82:LEU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:GLN:O	2:C:33:ASP:N	2.51	0.43
2:C:261:ILE:HD12	2:C:261:ILE:N	2.34	0.43
2:C:815:LEU:N	2:C:815:LEU:HD23	2.34	0.43
2:C:890:LEU:N	2:C:914:ILE:HD11	2.32	0.43
2:C:1099:VAL:HG23	3:D:10:ILE:HG13	1.99	0.43
3:D:140:ALA:HB3	3:D:147:VAL:CG2	2.48	0.43
3:D:169:TYR:OH	3:D:198:ARG:HG2	2.17	0.43
3:D:374:GLU:O	3:D:375:GLU:CB	2.66	0.43
3:D:821:VAL:O	3:D:821:VAL:HG12	2.17	0.43
3:D:828:LYS:O	3:D:828:LYS:HD3	2.19	0.43
3:D:1209:LEU:N	3:D:1209:LEU:HD23	2.31	0.43
5:F:284:ARG:NH1	5:F:290:GLU:OE2	2.47	0.43
5:F:368:VAL:CG1	5:F:397:ILE:HD11	2.47	0.43
1:B:51:THR:HA	1:B:145:ASP:O	2.18	0.43
1:B:124:ASN:ND2	1:B:127:LEU:CD1	2.79	0.43
2:C:261:ILE:HG22	2:C:291:ALA:HB3	1.99	0.43
2:C:504:GLU:HG3	2:C:509:ALA:HB2	1.99	0.43
2:C:701:THR:HG23	2:C:831:ARG:O	2.18	0.43
3:D:870:GLY:O	3:D:871:LYS:C	2.56	0.43
3:D:907:GLU:OE1	3:D:909:ASN:N	2.43	0.43
3:D:1495:ILE:HG12	4:E:88:GLU:OE2	2.18	0.43
5:F:100:VAL:O	5:F:104:ARG:HB2	2.18	0.43
1:B:106:PRO:HG3	1:B:134:GLU:OE1	2.18	0.43
2:C:410:ILE:O	2:C:452:ILE:HA	2.17	0.43
2:C:815:LEU:HB2	2:C:819:VAL:CG2	2.49	0.43
2:C:1062:GLY:HA2	2:C:1065:ALA:HB3	2.00	0.43
3:D:230:TRP:HA	3:D:243:ALA:CB	2.49	0.43
3:D:413:ASP:N	3:D:435:VAL:HG12	2.34	0.43
3:D:613:ARG:O	3:D:618:LEU:HD23	2.19	0.43
3:D:638:LYS:HD3	3:D:640:HIS:HE1	1.84	0.43
3:D:757:ALA:O	4:E:20:THR:HG23	2.19	0.43
3:D:961:LYS:NZ	3:D:961:LYS:HB3	2.34	0.43
3:D:1093:TYR:CZ	3:D:1097:LYS:HE2	2.53	0.43
4:E:6:ILE:HD11	4:E:10:PHE:CZ	2.54	0.43
5:F:317:LEU:HD23	5:F:317:LEU:HA	1.81	0.43
5:F:403:LYS:O	5:F:407:LYS:HB2	2.19	0.43
1:A:41:ARG:CG	1:A:177:VAL:HG12	2.49	0.43
1:A:100:LEU:HB2	1:A:115:LEU:HD22	2.01	0.43
2:C:18:LEU:HD23	2:C:18:LEU:HA	1.81	0.43
2:C:215:GLY:HA2	2:C:219:GLN:HG3	2.01	0.43
2:C:293:PHE:HD1	2:C:298:PHE:CD1	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:432:ARG:HG3	2:C:519:GLY:HA3	2.00	0.43
2:C:942:GLU:CG	2:C:945:ARG:HH21	2.29	0.43
2:C:1070:ILE:HB	3:D:655:PRO:HB3	2.00	0.43
3:D:361:VAL:HB	3:D:365:ASP:HB2	2.00	0.43
3:D:416:ALA:CB	3:D:432:TYR:CE1	3.01	0.43
3:D:639:LEU:HD12	3:D:639:LEU:HA	1.65	0.43
3:D:691:LEU:O	3:D:694:VAL:N	2.51	0.43
3:D:955:VAL:O	3:D:957:PRO:CD	2.65	0.43
3:D:1192:LEU:HD11	3:D:1345:GLU:HB3	1.99	0.43
3:D:1422:MET:HE3	3:D:1426:LYS:CD	2.48	0.43
5:F:186:HIS:O	5:F:190:ALA:HB2	2.19	0.43
2:C:267:TYR:CZ	2:C:290:LEU:HG	2.54	0.43
2:C:437:ARG:HB3	2:C:467:ILE:HG21	2.01	0.43
2:C:850:ALA:HA	3:D:632:VAL:HG22	2.00	0.43
2:C:1078:GLU:HG3	2:C:1079:PRO:HD2	2.01	0.43
3:D:137:PRO:HA	3:D:452:ILE:HG13	2.00	0.43
3:D:245:LEU:N	3:D:245:LEU:HD12	2.34	0.43
3:D:352:ASN:HB3	5:F:104:ARG:NH1	2.34	0.43
3:D:1153:VAL:HG11	3:D:1183:ILE:CD1	2.49	0.43
3:D:1256:LEU:N	3:D:1257:PRO:HD2	2.34	0.43
5:F:99:GLU:OE2	5:F:234:LYS:HG2	2.18	0.43
5:F:118:GLU:OE1	5:F:118:GLU:HA	2.18	0.43
5:F:217:ASN:O	5:F:218:GLN:C	2.57	0.43
1:A:41:ARG:HG3	1:A:177:VAL:HG12	2.00	0.43
1:A:167:VAL:CG1	1:A:168:ASP:N	2.82	0.43
2:C:177:GLU:HG3	2:C:178:PRO:CD	2.29	0.43
2:C:243:ARG:NH2	7:H:9:DG:O6	2.52	0.43
2:C:941:VAL:HG23	2:C:942:GLU:N	2.33	0.43
2:C:974:LEU:HD22	2:C:987:ILE:CG2	2.48	0.43
2:C:1030:GLN:O	3:D:623:VAL:HG22	2.19	0.43
2:C:1073:GLY:CA	3:D:659:LYS:HD3	2.48	0.43
3:D:10:ILE:HG23	3:D:1451:ALA:HA	2.01	0.43
3:D:348:GLN:CB	3:D:351:MET:HG3	2.44	0.43
3:D:584:ASN:OD1	3:D:585:GLY:N	2.52	0.43
3:D:629:SER:OG	3:D:630:VAL:N	2.51	0.43
3:D:631:ILE:HG22	3:D:726:ILE:HB	2.01	0.43
3:D:783:ARG:H	3:D:783:ARG:HG2	1.57	0.43
3:D:1023:MET:HE2	3:D:1023:MET:HB2	1.75	0.43
3:D:1235:GLN:O	3:D:1236:LEU:HD23	2.19	0.43
5:F:260:ILE:CD1	5:F:265:VAL:HG22	2.48	0.43
5:F:343:ASP:O	5:F:346:THR:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:377:ASP:OD2	5:F:378:GLY:O	2.37	0.43
6:G:12:DG:H8	6:G:12:DG:H5"	1.83	0.43
1:A:159:LYS:HG2	1:A:164:ALA:O	2.19	0.43
1:B:31:GLY:N	1:B:193:ASP:OD1	2.52	0.43
1:B:47:SER:O	1:B:48:ILE:HD13	2.19	0.43
2:C:129:ILE:HG12	2:C:386:PHE:HB3	2.01	0.43
2:C:397:GLU:HG3	2:C:631:SER:HB2	2.00	0.43
2:C:644:VAL:CG2	2:C:645:VAL:H	2.30	0.43
2:C:707:ARG:HH11	2:C:707:ARG:HB3	1.84	0.43
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.34	0.43
2:C:1046:ALA:HB1	3:D:1471:LEU:HG	2.00	0.43
3:D:185:VAL:HG13	3:D:186:VAL:H	1.83	0.43
3:D:684:LYS:O	3:D:687:VAL:CG1	2.65	0.43
3:D:907:GLU:OE1	3:D:908:LYS:N	2.52	0.43
3:D:1486:VAL:HG13	3:D:1486:VAL:O	2.17	0.43
1:B:197:LEU:HD12	1:B:197:LEU:C	2.38	0.42
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.78	0.42
2:C:75:GLU:OE2	2:C:76:PRO:CD	2.67	0.42
2:C:841:ASN:OD1	2:C:841:ASN:C	2.58	0.42
2:C:879:ARG:HH21	2:C:879:ARG:HD2	1.70	0.42
3:D:207:PHE:HB2	3:D:391:ALA:CB	2.49	0.42
3:D:225:LEU:HA	3:D:249:TYR:CE2	2.54	0.42
3:D:410:SER:O	3:D:435:VAL:CG1	2.61	0.42
3:D:1479:ASP:OD1	3:D:1482:ARG:HD3	2.19	0.42
5:F:307:THR:HG22	5:F:308:LEU:N	2.33	0.42
5:F:321:ILE:HA	5:F:321:ILE:HD13	1.83	0.42
2:C:336:VAL:HG13	2:C:337:GLY:N	2.33	0.42
2:C:841:ASN:HD22	2:C:992:MET:HE2	1.83	0.42
2:C:1006:HIS:CD2	2:C:1024:LYS:HA	2.54	0.42
2:C:1092:LEU:CD2	3:D:607:LEU:HD21	2.49	0.42
3:D:245:LEU:HD23	3:D:249:TYR:HB3	2.01	0.42
3:D:954:ALA:O	3:D:1062:ARG:HD2	2.19	0.42
3:D:1463:LYS:O	3:D:1464:GLU:C	2.57	0.42
5:F:128:ARG:HE	5:F:132:ARG:NH2	2.16	0.42
1:A:74:ASP:OD1	1:A:76:VAL:HB	2.20	0.42
1:B:153:ALA:C	1:B:155:LYS:H	2.22	0.42
2:C:355:VAL:HG23	2:C:356:ARG:H	1.83	0.42
2:C:619:ARG:HH21	2:C:619:ARG:HB2	1.84	0.42
3:D:251:PHE:HE2	3:D:304:LEU:HD12	1.85	0.42
3:D:284:LEU:CA	3:D:288:MET:HE2	2.48	0.42
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1378:TYR:O	3:D:1420:LEU:HB2	2.19	0.42
1:A:117:VAL:HB	1:A:120:VAL:CG2	2.49	0.42
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.18	0.42
2:C:204:GLN:HA	2:C:227:PHE:CE1	2.55	0.42
2:C:224:GLU:C	2:C:226:VAL:H	2.21	0.42
2:C:292:ARG:NH1	2:C:301:GLU:OE2	2.52	0.42
2:C:701:THR:HG22	2:C:702:SER:N	2.34	0.42
2:C:820:ARG:HB3	2:C:820:ARG:CZ	2.49	0.42
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.45	0.42
2:C:911:GLU:HA	2:C:914:ILE:CG2	2.49	0.42
3:D:85:VAL:C	3:D:87:ARG:H	2.23	0.42
3:D:217:LYS:HZ1	3:D:262:LYS:NZ	2.17	0.42
3:D:230:TRP:CZ3	3:D:333:LEU:CD2	3.02	0.42
3:D:272:LEU:CD2	3:D:298:VAL:HG21	2.49	0.42
3:D:288:MET:HG3	3:D:307:ALA:HB2	2.02	0.42
3:D:492:ALA:O	3:D:496:LEU:HB2	2.20	0.42
3:D:514:LEU:HD22	3:D:517:VAL:CG2	2.50	0.42
3:D:697:GLY:CA	4:E:59:ASN:HD22	2.33	0.42
3:D:1379:VAL:C	3:D:1420:LEU:HD22	2.40	0.42
3:D:1380:GLU:HB2	3:D:1420:LEU:CD2	2.49	0.42
3:D:1381:VAL:CG1	3:D:1382:THR:N	2.83	0.42
3:D:1386:ASP:OD2	3:D:1412:LYS:HB3	2.19	0.42
4:E:34:GLY:O	4:E:35:PHE:HB2	2.19	0.42
5:F:113:ILE:HD13	5:F:128:ARG:HG3	2.01	0.42
5:F:240:THR:O	5:F:244:ARG:HG2	2.20	0.42
5:F:413:SER:O	5:F:414:ARG:NH1	2.52	0.42
1:A:111:ALA:CB	1:A:127:LEU:HB3	2.50	0.42
2:C:135:VAL:O	2:C:136:ILE:HD13	2.19	0.42
2:C:612:VAL:HG23	2:C:621:VAL:O	2.19	0.42
2:C:772:ARG:HG2	2:C:772:ARG:NH1	2.34	0.42
2:C:882:LEU:HA	2:C:882:LEU:HD23	1.43	0.42
3:D:56:TYR:HE1	3:D:69:GLU:OE2	2.03	0.42
3:D:296:GLU:CG	3:D:297:ILE:N	2.81	0.42
3:D:832:ARG:N	3:D:832:ARG:HD3	2.35	0.42
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.58	0.42
3:D:1342:GLU:HA	3:D:1345:GLU:HB2	2.02	0.42
3:D:1413:THR:HG22	3:D:1414:PRO:CD	2.47	0.42
3:D:1417:TRP:HE3	3:D:1418:LYS:N	2.17	0.42
5:F:102:LEU:HD22	5:F:183:ALA:HA	2.02	0.42
5:F:351:SER:HA	5:F:354:LEU:HD21	2.01	0.42
6:G:7:DT:H2"	6:G:8:DC:OP2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:CD1	1:A:21:GLY:N	2.79	0.42
1:A:51:THR:OG1	1:A:87:VAL:O	2.21	0.42
1:A:121:GLU:HB3	1:A:123:MET:CE	2.39	0.42
1:B:199:ILE:O	1:B:199:ILE:HG22	2.18	0.42
2:C:101:ILE:HG13	2:C:102:HIS:N	2.35	0.42
2:C:170:PRO:HD2	2:C:267:TYR:CD2	2.54	0.42
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.83	0.42
3:D:133:ILE:O	3:D:133:ILE:CG2	2.67	0.42
3:D:401:TYR:HH	3:D:430:ASP:HB2	1.81	0.42
3:D:711:LEU:CD2	3:D:714:GLN:HE21	2.31	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.54	0.42
3:D:1433:SER:OG	3:D:1464:GLU:HG2	2.20	0.42
5:F:87:GLU:O	5:F:90:GLN:HB2	2.20	0.42
5:F:215:GLU:HG3	5:F:250:ALA:CB	2.50	0.42
5:F:369:LEU:HD11	5:F:405:LEU:HD12	2.01	0.42
1:A:62:LEU:HD22	2:C:745:ILE:O	2.20	0.42
2:C:941:VAL:CG2	2:C:942:GLU:N	2.83	0.42
3:D:34:TYR:CE1	3:D:35:ARG:HG2	2.55	0.42
3:D:201:GLY:HA2	3:D:397:LYS:HD2	2.00	0.42
3:D:201:GLY:HA2	3:D:397:LYS:CD	2.49	0.42
3:D:348:GLN:N	3:D:351:MET:CE	2.82	0.42
3:D:975:GLU:O	3:D:975:GLU:HG3	2.18	0.42
3:D:1068:LEU:O	3:D:1068:LEU:HD23	2.20	0.42
3:D:1087:ARG:CD	3:D:1234:THR:O	2.68	0.42
3:D:1211:MET:CE	4:E:16:LYS:HD2	2.48	0.42
3:D:1238:MET:CB	3:D:1255:GLY:H	2.32	0.42
3:D:1389:LEU:HD21	3:D:1395:LEU:HD11	2.00	0.42
3:D:1395:LEU:HD23	3:D:1395:LEU:N	2.35	0.42
5:F:88:ILE:HD11	5:F:192:LEU:HD13	2.01	0.42
5:F:193:ARG:HG2	7:H:7:DG:C5'	2.50	0.42
5:F:247:ILE:HG22	5:F:251:ILE:HD12	2.02	0.42
5:F:365:GLU:HA	5:F:368:VAL:HG22	2.01	0.42
1:B:28:LEU:HD21	1:B:36:LEU:HD22	2.02	0.42
2:C:364:GLU:HG2	2:C:364:GLU:O	2.19	0.42
2:C:429:ASP:OD1	3:D:1079:LYS:HD2	2.20	0.42
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.02	0.42
2:C:571:LEU:CD1	2:C:669:GLY:HA2	2.50	0.42
2:C:997:LEU:HD23	2:C:997:LEU:HA	1.47	0.42
3:D:10:ILE:O	3:D:10:ILE:CG2	2.66	0.42
3:D:141:ILE:HG23	3:D:450:TYR:OH	2.20	0.42
3:D:421:LEU:N	3:D:421:LEU:CD1	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:433:GLY:HA2	3:D:447:VAL:O	2.20	0.42
3:D:484:PRO:C	3:D:486:ARG:H	2.22	0.42
3:D:519:VAL:CG2	3:D:544:TYR:CE1	3.02	0.42
3:D:637:LEU:HD13	3:D:642:CYS:HA	2.02	0.42
3:D:676:MET:O	3:D:682:ASP:HB2	2.20	0.42
3:D:695:ILE:HD13	3:D:720:LEU:HD11	2.02	0.42
3:D:879:ARG:HD3	3:D:902:LEU:O	2.19	0.42
3:D:1153:VAL:HG11	3:D:1183:ILE:HD11	2.01	0.42
4:E:46:PRO:HB2	4:E:57:ASP:HB3	2.02	0.42
4:E:85:LEU:HD23	4:E:85:LEU:C	2.40	0.42
5:F:231:ARG:HB3	5:F:233:PHE:CE2	2.55	0.42
5:F:235:PHE:O	5:F:236:SER:C	2.56	0.42
5:F:403:LYS:HA	5:F:406:ARG:HB2	2.02	0.42
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.55	0.42
1:B:106:PRO:HG3	1:B:134:GLU:CD	2.40	0.42
2:C:115:LEU:HA	2:C:115:LEU:HD23	1.76	0.42
2:C:164:PRO:CA	2:C:269:LEU:HD12	2.48	0.42
2:C:167:LYS:CE	7:H:12:DC:H5	2.32	0.42
2:C:726:ILE:HD11	2:C:757:GLY:HA3	2.01	0.42
2:C:1040:LEU:HD12	2:C:1049:LEU:HA	2.02	0.42
3:D:200:ASP:C	3:D:397:LYS:HD3	2.41	0.42
3:D:544:TYR:O	3:D:545:ARG:C	2.57	0.42
3:D:559:ALA:HA	5:F:144:ILE:CD1	2.50	0.42
3:D:941:PHE:HD1	3:D:941:PHE:HA	1.75	0.42
5:F:161:GLN:OE1	5:F:164:LYS:NZ	2.25	0.42
5:F:241:TRP:CE2	7:H:1:DT:H4'	2.54	0.42
5:F:372:ARG:NE	5:F:372:ARG:CA	2.83	0.42
1:B:24:VAL:CG1	1:B:196:THR:OG1	2.67	0.42
2:C:580:MET:HE2	2:C:902:ILE:HG12	2.01	0.42
2:C:682:TYR:HB2	2:C:689:VAL:HG21	2.02	0.42
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.49	0.42
3:D:207:PHE:CZ	5:F:97:GLU:HB3	2.55	0.42
3:D:553:ARG:HG2	3:D:570:GLU:OE2	2.19	0.42
3:D:1012:GLU:O	3:D:1012:GLU:HG2	2.20	0.42
5:F:88:ILE:HD12	5:F:88:ILE:HA	1.62	0.42
1:A:186:LEU:O	1:A:188:GLN:N	2.51	0.41
1:A:201:THR:HG23	1:A:202:ASP:N	2.34	0.41
2:C:96:ALA:HB3	2:C:115:LEU:HD11	2.01	0.41
2:C:134:ARG:NH1	2:C:392:SER:O	2.53	0.41
2:C:140:ILE:CG2	2:C:412:ALA:HA	2.49	0.41
2:C:214:TYR:C	2:C:216:GLU:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:OH	2:C:290:LEU:HD21	2.20	0.41
2:C:745:ILE:HD11	2:C:802:ARG:HA	2.02	0.41
2:C:999:HIS:CD2	2:C:999:HIS:N	2.88	0.41
3:D:85:VAL:C	3:D:87:ARG:N	2.72	0.41
3:D:416:ALA:HB1	3:D:432:TYR:CE1	2.55	0.41
3:D:562:ALA:HB2	5:F:221:ILE:HD11	2.02	0.41
3:D:618:LEU:CG	3:D:1467:ILE:HG23	2.50	0.41
3:D:786:ILE:HD11	3:D:1027:GLY:C	2.41	0.41
3:D:1290:LEU:HD23	3:D:1307:LYS:HA	2.01	0.41
1:A:206:THR:O	1:A:207:PRO:C	2.58	0.41
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.49	0.41
2:C:124:ASP:CA	2:C:592:LEU:HD13	2.44	0.41
2:C:203:ASP:O	2:C:206:THR:HG22	2.21	0.41
2:C:376:ARG:N	2:C:377:PRO:HD2	2.34	0.41
2:C:492:ASP:O	2:C:518:LYS:HE3	2.21	0.41
2:C:1055:LEU:HD23	2:C:1055:LEU:H	1.85	0.41
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.02	0.41
3:D:223:LEU:HD13	3:D:283:PHE:O	2.20	0.41
3:D:266:GLU:HG3	3:D:314:PRO:HB3	2.00	0.41
3:D:374:GLU:O	3:D:375:GLU:CG	2.68	0.41
3:D:423:ASP:O	3:D:425:GLY:N	2.48	0.41
3:D:610:LYS:HD3	3:D:615:ARG:NH2	2.35	0.41
3:D:780:LYS:HD2	3:D:912:LYS:HG3	2.00	0.41
3:D:1015:TYR:CD2	3:D:1015:TYR:N	2.88	0.41
3:D:1295:GLU:OE1	3:D:1300:SER:HB3	2.20	0.41
5:F:224:VAL:HG23	5:F:225:GLU:N	2.35	0.41
7:H:17:DA:C2'	7:H:18:DC:H5'	2.49	0.41
1:A:24:VAL:O	1:A:25:LEU:HD12	2.19	0.41
1:B:87:VAL:CG1	1:B:122:ILE:HD13	2.50	0.41
2:C:109:LYS:CD	2:C:110:GLU:H	2.24	0.41
2:C:729:LEU:CD2	2:C:754:ILE:HD11	2.49	0.41
2:C:1060:ILE:H	2:C:1060:ILE:HG12	1.38	0.41
3:D:219:GLU:HB2	3:D:339:TRP:HH2	1.86	0.41
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.55	0.41
3:D:955:VAL:O	3:D:955:VAL:CG2	2.68	0.41
3:D:972:LEU:HG	3:D:972:LEU:H	1.69	0.41
3:D:1191:PRO:HD2	3:D:1369:GLU:OE1	2.19	0.41
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.60	0.41
1:A:138:LEU:HD21	1:A:140:MET:CE	2.49	0.41
2:C:54:ILE:HG21	2:C:355:VAL:HG21	1.99	0.41
2:C:595:LEU:HD23	2:C:595:LEU:C	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:748:GLU:HG3	2:C:799:ILE:CD1	2.50	0.41
3:D:25:GLU:CD	3:D:94:GLU:HB3	2.41	0.41
3:D:41:ARG:HG2	3:D:48:ARG:HD3	2.02	0.41
3:D:1343:ALA:HA	3:D:1346:ARG:NH1	2.34	0.41
3:D:1486:VAL:HB	4:E:22:VAL:HG13	2.03	0.41
5:F:194:LEU:HB2	7:H:6:DT:C2	2.56	0.41
1:A:30:ARG:HD2	1:A:191:ASP:OD1	2.21	0.41
1:A:34:VAL:HG21	1:B:42:ARG:NE	2.36	0.41
1:A:65:PHE:HE2	2:C:703:ILE:HG23	1.84	0.41
1:A:221:HIS:CD2	1:B:32:PHE:CD2	3.08	0.41
1:B:29:GLU:HG3	1:B:30:ARG:N	2.36	0.41
1:B:96:THR:CG2	1:B:97:VAL:N	2.81	0.41
2:C:333:ILE:HG23	2:C:333:ILE:HD12	1.87	0.41
2:C:588:VAL:HG13	2:C:596:TYR:OH	2.20	0.41
2:C:679:PHE:N	2:C:683:ASN:OD1	2.53	0.41
2:C:939:ARG:HG3	2:C:975:TYR:CE1	2.55	0.41
3:D:101:HIS:CE1	3:D:103:TRP:HB2	2.56	0.41
3:D:142:LEU:HB2	3:D:161:LEU:HD21	2.03	0.41
3:D:150:ARG:HG2	3:D:464:LEU:HD21	2.03	0.41
3:D:201:GLY:HA3	3:D:396:VAL:O	2.21	0.41
3:D:583:ASP:O	3:D:584:ASN:C	2.58	0.41
3:D:787:LEU:HD12	3:D:787:LEU:HA	1.88	0.41
3:D:1111:ASP:CG	3:D:1203:LYS:HE2	2.41	0.41
4:E:14:ASP:CG	4:E:18:ARG:HH11	2.24	0.41
5:F:117:SER:O	5:F:121:GLY:N	2.52	0.41
1:A:162:ILE:HD12	1:A:162:ILE:N	2.36	0.41
1:B:58:ILE:O	1:B:61:VAL:HG23	2.21	0.41
1:B:115:LEU:HD22	1:B:115:LEU:HA	1.58	0.41
2:C:258:TYR:CE1	2:C:263:ASP:HB2	2.55	0.41
2:C:314:THR:HG22	2:C:314:THR:O	2.19	0.41
3:D:50:PHE:O	3:D:89:ARG:HD2	2.21	0.41
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.60	0.41
3:D:187:LYS:N	3:D:187:LYS:HD3	2.36	0.41
3:D:218:LYS:O	3:D:219:GLU:HG2	2.20	0.41
3:D:377:VAL:CG2	3:D:377:VAL:O	2.67	0.41
3:D:670:VAL:O	3:D:673:ALA:HB3	2.20	0.41
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	2.01	0.41
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.55	0.41
3:D:1407:LEU:HD13	3:D:1413:THR:O	2.20	0.41
5:F:114:LYS:HG3	5:F:115:LYS:N	2.36	0.41
5:F:132:ARG:HH11	5:F:184:ARG:NH1	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:152:ASP:O	5:F:154:LYS:N	2.53	0.41
1:A:79:ILE:HG23	1:A:167:VAL:CG2	2.51	0.41
1:B:7:LYS:HZ2	1:B:186:LEU:HD13	1.86	0.41
1:B:26:GLU:HB3	1:B:194:LYS:CG	2.46	0.41
1:B:129:ILE:O	1:B:130:ALA:HB2	2.20	0.41
2:C:97:ARG:HG2	2:C:112:GLU:CB	2.51	0.41
2:C:668:LEU:HD23	2:C:668:LEU:HA	1.75	0.41
2:C:700:TYR:HB3	2:C:833:LEU:CD2	2.50	0.41
3:D:32:ILE:HG13	5:F:258:ILE:HD13	2.01	0.41
3:D:100:ALA:HA	3:D:513:ILE:HG23	2.02	0.41
3:D:144:GLY:O	3:D:145:VAL:HG23	2.20	0.41
3:D:210:ARG:HH21	3:D:212:ARG:HH21	1.69	0.41
3:D:210:ARG:NH1	3:D:388:HIS:HB3	2.36	0.41
3:D:677:LEU:H	3:D:677:LEU:HG	1.43	0.41
3:D:1400:VAL:HG13	3:D:1401:GLU:N	2.36	0.41
4:E:70:THR:HB	4:E:72:ARG:NE	2.35	0.41
5:F:170:HIS:C	5:F:172:ARG:H	2.24	0.41
1:A:56:VAL:O	1:A:164:ALA:HA	2.20	0.41
1:A:86:VAL:HG21	1:A:202:ASP:CB	2.50	0.41
1:B:205:VAL:CG2	1:B:206:THR:H	2.34	0.41
1:B:205:VAL:CG2	1:B:206:THR:N	2.84	0.41
2:C:217:LEU:C	2:C:220:GLY:H	2.24	0.41
2:C:766:GLU:O	2:C:767:PRO:C	2.59	0.41
2:C:874:LEU:HA	2:C:874:LEU:HD23	1.84	0.41
2:C:954:THR:HB	2:C:957:LYS:HD2	2.03	0.41
2:C:1013:TYR:CE2	2:C:1063:ARG:NH1	2.89	0.41
3:D:141:ILE:CD1	3:D:145:VAL:N	2.83	0.41
3:D:298:VAL:HG12	3:D:302:GLN:CG	2.51	0.41
3:D:348:GLN:HB2	3:D:351:MET:CG	2.45	0.41
3:D:377:VAL:HG22	3:D:377:VAL:O	2.21	0.41
3:D:550:ARG:NH2	5:F:211:ASP:OD2	2.53	0.41
3:D:801:GLY:HA2	3:D:821:VAL:HG22	2.03	0.41
3:D:879:ARG:HB3	3:D:902:LEU:HD11	2.01	0.41
3:D:1164:ARG:HG2	3:D:1165:TYR:N	2.35	0.41
1:A:6:LEU:HD11	1:A:192:LEU:HD13	2.03	0.41
1:A:112:ARG:NH1	1:A:125:PRO:HB2	2.36	0.41
1:A:117:VAL:HG12	1:A:118:ALA:N	2.36	0.41
1:B:58:ILE:CG2	1:B:61:VAL:CG2	2.99	0.41
1:B:58:ILE:HG12	1:B:140:MET:CB	2.51	0.41
1:B:86:VAL:HG13	1:B:86:VAL:O	2.20	0.41
1:B:99:LEU:HD23	1:B:114:PHE:CG	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:HD3	1:B:164:ALA:O	2.21	0.41
2:C:39:ARG:NH1	2:C:71:TYR:CZ	2.89	0.41
2:C:224:GLU:HA	2:C:227:PHE:H	1.85	0.41
2:C:328:LEU:CD1	2:C:438:ILE:CD1	2.99	0.41
2:C:355:VAL:HG12	2:C:372:LEU:O	2.21	0.41
2:C:492:ASP:HB3	2:C:518:LYS:CG	2.50	0.41
2:C:567:GLN:HB2	2:C:997:LEU:HD22	2.03	0.41
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.02	0.41
2:C:916:GLU:O	2:C:920:GLN:HG3	2.21	0.41
2:C:952:LEU:HD22	2:C:952:LEU:N	2.35	0.41
3:D:123:LEU:O	3:D:123:LEU:HD23	2.20	0.41
3:D:144:GLY:O	3:D:145:VAL:CG2	2.69	0.41
3:D:1153:VAL:CG1	3:D:1183:ILE:HD11	2.51	0.41
3:D:1422:MET:HE2	3:D:1427:SER:HA	2.03	0.41
3:D:1422:MET:HE1	3:D:1426:LYS:HG2	2.02	0.41
4:E:83:ASP:OD2	4:E:83:ASP:N	2.41	0.41
5:F:172:ARG:HH11	5:F:172:ARG:HG3	1.86	0.41
5:F:239:ALA:C	5:F:241:TRP:N	2.75	0.41
5:F:353:GLU:HG2	5:F:356:LYS:HD2	2.03	0.41
2:C:23:VAL:CG2	2:C:24:GLU:H	2.32	0.41
2:C:97:ARG:NH2	2:C:110:GLU:OE1	2.45	0.41
2:C:735:ARG:O	2:C:735:ARG:HG3	2.20	0.41
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.56	0.41
3:D:7:LYS:CD	3:D:1456:LYS:NZ	2.82	0.41
3:D:128:TYR:CE2	3:D:587:ARG:HD3	2.55	0.41
3:D:463:GLN:O	3:D:466:LYS:N	2.54	0.41
3:D:584:ASN:OD1	3:D:590:PRO:HA	2.22	0.41
3:D:935:LYS:HG2	3:D:939:PHE:CD2	2.56	0.41
3:D:1294:VAL:O	3:D:1294:VAL:HG13	2.21	0.41
5:F:249:ARG:HE	5:F:249:ARG:HB3	1.77	0.41
1:B:43:ILE:HG22	1:B:214:ALA:CB	2.51	0.40
1:B:173:PRO:CG	1:B:205:VAL:HG12	2.51	0.40
2:C:28:ARG:HG2	2:C:28:ARG:O	2.21	0.40
2:C:409:ARG:HH22	2:C:454:SER:HB2	1.86	0.40
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.33	0.40
2:C:773:LEU:O	2:C:776:SER:HB2	2.21	0.40
3:D:85:VAL:O	3:D:87:ARG:N	2.54	0.40
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.98	0.40
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.78	0.40
3:D:610:LYS:HD3	3:D:615:ARG:HH21	1.86	0.40
5:F:94:LEU:HD22	5:F:98:GLU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:143:HIS:O	5:F:145:PRO:HD3	2.20	0.40
5:F:422:LEU:O	5:F:423:ASP:HB2	2.21	0.40
1:A:34:VAL:CG2	1:A:35:THR:N	2.83	0.40
1:A:90:LEU:N	1:A:90:LEU:HD13	2.36	0.40
1:B:157:GLY:O	1:B:158:ILE:C	2.60	0.40
2:C:10:ARG:O	2:C:10:ARG:HG2	2.21	0.40
2:C:23:VAL:CG2	2:C:24:GLU:N	2.84	0.40
2:C:172:ILE:HA	2:C:185:LYS:O	2.21	0.40
2:C:677:MET:O	2:C:678:PRO:C	2.59	0.40
3:D:38:LYS:HB3	3:D:39:PRO:CD	2.49	0.40
3:D:115:LEU:CD2	3:D:115:LEU:O	2.69	0.40
3:D:313:MET:CE	3:D:319:ALA:HB2	2.51	0.40
3:D:357:GLU:HB2	3:D:387:LEU:HD23	2.03	0.40
3:D:539:ASP:CG	3:D:598:ARG:HH22	2.23	0.40
3:D:675:ARG:HD2	3:D:675:ARG:HA	1.71	0.40
3:D:687:VAL:HG13	3:D:688:TRP:N	2.35	0.40
3:D:930:LEU:O	3:D:930:LEU:HD12	2.21	0.40
3:D:1108:ARG:HG3	3:D:1199:GLY:HA3	2.04	0.40
3:D:1394:VAL:HG13	3:D:1395:LEU:N	2.37	0.40
5:F:112:ALA:HB2	5:F:176:ILE:CG2	2.51	0.40
5:F:324:GLU:OE2	6:G:19:DG:N2	2.54	0.40
5:F:407:LYS:O	5:F:411:HIS:HB2	2.21	0.40
1:B:112:ARG:CB	1:B:112:ARG:HH21	2.35	0.40
2:C:214:TYR:HB2	2:C:218:VAL:HG23	2.02	0.40
2:C:438:ILE:HG22	2:C:439:CYS:O	2.22	0.40
2:C:626:ARG:N	2:C:639:GLN:HE21	2.18	0.40
3:D:187:LYS:CD	3:D:187:LYS:H	2.34	0.40
3:D:236:TYR:CE1	3:D:242:LEU:CB	3.02	0.40
3:D:1151:ARG:HD2	3:D:1151:ARG:HA	2.01	0.40
3:D:1208:ASP:O	3:D:1209:LEU:C	2.60	0.40
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.22	0.40
3:D:1376:MET:HE3	3:D:1376:MET:HB2	1.87	0.40
3:D:1380:GLU:HB2	3:D:1420:LEU:HD21	2.03	0.40
1:A:75:VAL:O	1:A:75:VAL:CG1	2.70	0.40
1:A:79:ILE:O	1:A:79:ILE:HG22	2.21	0.40
1:B:35:THR:HG22	1:B:36:LEU:HD12	2.04	0.40
1:B:105:GLY:HA2	1:B:134:GLU:HA	2.04	0.40
2:C:49:ARG:NE	2:C:49:ARG:HA	2.35	0.40
2:C:168:ARG:NE	2:C:345:ARG:HH11	2.20	0.40
2:C:168:ARG:HD3	2:C:345:ARG:HH11	1.86	0.40
2:C:183:SER:OG	2:C:184:MET:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1013:TYR:O	2:C:1021:LEU:HD11	2.21	0.40
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.21	0.40
4:E:48:MET:HG2	4:E:58:PRO:HD3	2.03	0.40
1:A:79:ILE:CG2	1:A:167:VAL:HG22	2.51	0.40
2:C:64:LEU:N	2:C:103:LYS:HB3	2.36	0.40
2:C:550:LEU:HD23	2:C:906:PHE:CE1	2.54	0.40
2:C:684:PHE:CD2	3:D:730:PRO:HB3	2.57	0.40
2:C:760:SER:O	2:C:786:LYS:HB2	2.22	0.40
3:D:553:ARG:HE	5:F:214:GLN:CB	2.34	0.40
3:D:625:TYR:HD2	3:D:751:LEU:HD11	1.87	0.40
3:D:695:ILE:CD1	3:D:720:LEU:CD1	2.99	0.40
3:D:1191:PRO:C	3:D:1193:THR:N	2.75	0.40
3:D:1494:ALA:HB3	4:E:92:LEU:HD11	2.00	0.40
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.57	0.40
5:F:358:LEU:N	5:F:358:LEU:HD23	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	224/315 (71%)	192 (86%)	32 (14%)	0	100	100
1	B	222/315 (70%)	192 (86%)	28 (13%)	2 (1%)	17	50
2	C	1107/1119 (99%)	960 (87%)	146 (13%)	1 (0%)	51	82
3	D	1481/1505 (98%)	1255 (85%)	218 (15%)	8 (0%)	29	63
4	E	92/99 (93%)	83 (90%)	9 (10%)	0	100	100
5	F	344/423 (81%)	291 (85%)	51 (15%)	2 (1%)	25	59
All	All	3470/3776 (92%)	2973 (86%)	484 (14%)	13 (0%)	34	67

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	GLY
3	D	276	ASP
1	B	154	GLU
5	F	168	LYS
2	C	212	GLY
3	D	710	ARG
3	D	783	ARG
3	D	1130	ARG
3	D	479	GLU
3	D	705	ALA
3	D	959	GLU
3	D	275	GLU
5	F	378	GLY

5.3.2 Protein sidechains (i)

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	199/273 (73%)	164 (82%)	35 (18%)	2 8
1	B	197/273 (72%)	171 (87%)	26 (13%)	4 16
2	C	936/941 (100%)	799 (85%)	137 (15%)	3 13
3	D	1249/1265 (99%)	1082 (87%)	167 (13%)	4 16
4	E	83/88 (94%)	73 (88%)	10 (12%)	5 19
5	F	301/371 (81%)	241 (80%)	60 (20%)	1 5
All	All	2965/3211 (92%)	2530 (85%)	435 (15%)	3 13

All (435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	15	THR
1	A	18	ARG
1	A	48	ILE
1	A	62	LEU
1	A	71	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	LYS
1	A	76	VAL
1	A	85	LEU
1	A	90	LEU
1	A	96	THR
1	A	115	LEU
1	A	122	ILE
1	A	134	GLU
1	A	138	LEU
1	A	143	ARG
1	A	145	ASP
1	A	158	ILE
1	A	163	ASN
1	A	175	ARG
1	A	182	GLU
1	A	184	THR
1	A	189	ARG
1	A	190	THR
1	A	197	LEU
1	A	199	ILE
1	A	201	THR
1	A	204	SER
1	A	205	VAL
1	A	206	THR
1	A	209	GLU
1	A	213	GLN
1	A	216	GLU
1	A	218	LEU
1	A	227	ASN
1	B	15	THR
1	B	22	GLU
1	B	24	VAL
1	B	36	LEU
1	B	39	PRO
1	B	41	ARG
1	B	47	SER
1	B	55	SER
1	B	58	ILE
1	B	67	THR
1	B	87	VAL
1	B	99	LEU
1	B	112	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	115	LEU
1	B	128	HIS
1	B	131	THR
1	B	155	LYS
1	B	156	HIS
1	B	160	ASP
1	B	183	ASP
1	B	188	GLN
1	B	196	THR
1	B	208	LEU
1	B	223	THR
1	B	226	SER
1	B	227	ASN
2	C	2	GLU
2	C	10	ARG
2	C	15	LEU
2	C	21	ILE
2	C	24	GLU
2	C	27	ARG
2	C	37	GLU
2	C	38	LYS
2	C	44	ILE
2	C	49	ARG
2	C	51	THR
2	C	73	LEU
2	C	101	ILE
2	C	105	THR
2	C	118	ILE
2	C	138	SER
2	C	141	HIS
2	C	149	THR
2	C	154	ARG
2	C	157	ARG
2	C	174	LEU
2	C	177	GLU
2	C	183	SER
2	C	190	LYS
2	C	194	VAL
2	C	196	LEU
2	C	204	GLN
2	C	209	ARG
2	C	214	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	221	LEU
2	C	224	GLU
2	C	235	LEU
2	C	237	ARG
2	C	246	ASP
2	C	269	LEU
2	C	279	GLU
2	C	284	ARG
2	C	285	LEU
2	C	292	ARG
2	C	311	PHE
2	C	328	LEU
2	C	335	THR
2	C	340	MET
2	C	342	ASP
2	C	348	LEU
2	C	351	LEU
2	C	353	ARG
2	C	356	ARG
2	C	367	LEU
2	C	376	ARG
2	C	383	ARG
2	C	384	GLU
2	C	387	SER
2	C	390	GLN
2	C	402	SER
2	C	403	SER
2	C	409	ARG
2	C	426	ASP
2	C	427	VAL
2	C	434	HIS
2	C	442	GLU
2	C	443	THR
2	C	460	ARG
2	C	475	VAL
2	C	481	ASP
2	C	493	ARG
2	C	495	THR
2	C	511	GLU
2	C	514	VAL
2	C	534	VAL
2	C	537	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	538	GLN
2	C	541	SER
2	C	542	VAL
2	C	559	LEU
2	C	562	SER
2	C	572	ILE
2	C	591	SER
2	C	599	GLU
2	C	610	ARG
2	C	617	ASP
2	C	642	ARG
2	C	649	VAL
2	C	670	GLN
2	C	672	VAL
2	C	674	VAL
2	C	677	MET
2	C	680	ASP
2	C	702	SER
2	C	703	ILE
2	C	707	ARG
2	C	723	THR
2	C	729	LEU
2	C	730	SER
2	C	755	LEU
2	C	773	LEU
2	C	780	GLU
2	C	785	VAL
2	C	796	GLU
2	C	805	ARG
2	C	807	ARG
2	C	808	ARG
2	C	815	LEU
2	C	823	VAL
2	C	825	VAL
2	C	829	GLN
2	C	833	LEU
2	C	834	GLN
2	C	851	LYS
2	C	852	ILE
2	C	853	LEU
2	C	861	LEU
2	C	879	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	880	MET
2	C	888	THR
2	C	897	LEU
2	C	900	ARG
2	C	916	GLU
2	C	930	LYS
2	C	939	ARG
2	C	946	ARG
2	C	954	THR
2	C	958	THR
2	C	959	PRO
2	C	974	LEU
2	C	1001	VAL
2	C	1005	MET
2	C	1006	HIS
2	C	1008	ARG
2	C	1014	SER
2	C	1055	LEU
2	C	1056	LYS
2	C	1060	ILE
2	C	1061	GLU
2	C	1063	ARG
2	C	1084	SER
2	C	1117	SER
3	D	10	ILE
3	D	25	GLU
3	D	31	THR
3	D	40	GLU
3	D	53	ILE
3	D	58	CYS
3	D	68	PHE
3	D	73	CYS
3	D	74	GLU
3	D	80	VAL
3	D	81	THR
3	D	97	THR
3	D	106	LYS
3	D	115	LEU
3	D	123	LEU
3	D	124	GLU
3	D	133	ILE
3	D	141	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	171	LEU
3	D	176	ASP
3	D	179	VAL
3	D	187	LYS
3	D	191	LEU
3	D	199	LEU
3	D	202	VAL
3	D	212	ARG
3	D	220	ARG
3	D	223	LEU
3	D	230	TRP
3	D	231	VAL
3	D	232	GLU
3	D	250	LEU
3	D	270	LEU
3	D	284	LEU
3	D	289	THR
3	D	298	VAL
3	D	315	ARG
3	D	316	GLN
3	D	335	LEU
3	D	353	VAL
3	D	378	ILE
3	D	385	VAL
3	D	389	GLU
3	D	399	ARG
3	D	410	SER
3	D	411	THR
3	D	415	VAL
3	D	420	VAL
3	D	434	ARG
3	D	440	VAL
3	D	446	VAL
3	D	450	TYR
3	D	459	GLU
3	D	464	LEU
3	D	471	GLU
3	D	475	LYS
3	D	478	LEU
3	D	480	GLU
3	D	486	ARG
3	D	513	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	514	LEU
3	D	517	VAL
3	D	525	ARG
3	D	534	ARG
3	D	567	ILE
3	D	578	VAL
3	D	586	ARG
3	D	592	THR
3	D	596	SER
3	D	600	LEU
3	D	608	SER
3	D	611	GLN
3	D	621	LYS
3	D	623	VAL
3	D	628	ARG
3	D	632	VAL
3	D	638	LYS
3	D	674	ARG
3	D	677	LEU
3	D	679	ARG
3	D	686	GLU
3	D	691	LEU
3	D	695	ILE
3	D	698	LYS
3	D	704	ARG
3	D	709	HIS
3	D	721	VAL
3	D	747	VAL
3	D	754	PHE
3	D	756	GLN
3	D	786	ILE
3	D	794	GLN
3	D	798	GLU
3	D	813	LEU
3	D	821	VAL
3	D	832	ARG
3	D	847	ASP
3	D	858	VAL
3	D	863	VAL
3	D	873	LEU
3	D	894	LYS
3	D	904	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	913	ASP
3	D	935	LYS
3	D	936	TYR
3	D	939	PHE
3	D	942	SER
3	D	943	THR
3	D	947	ILE
3	D	948	THR
3	D	961	LYS
3	D	968	ASP
3	D	973	GLN
3	D	975	GLU
3	D	982	PHE
3	D	995	LEU
3	D	997	THR
3	D	1004	THR
3	D	1015	TYR
3	D	1018	ASN
3	D	1034	GLN
3	D	1039	CYS
3	D	1041	LEU
3	D	1058	ARG
3	D	1065	LEU
3	D	1067	VAL
3	D	1083	ASP
3	D	1090	ASP
3	D	1100	ASP
3	D	1112	CYS
3	D	1114	THR
3	D	1116	ASN
3	D	1118	ILE
3	D	1119	SER
3	D	1129	THR
3	D	1133	ARG
3	D	1151	ARG
3	D	1183	ILE
3	D	1186	VAL
3	D	1188	VAL
3	D	1192	LEU
3	D	1208	ASP
3	D	1210	SER
3	D	1213	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1216	SER
3	D	1217	ILE
3	D	1235	GLN
3	D	1304	LYS
3	D	1310	ARG
3	D	1326	THR
3	D	1349	VAL
3	D	1363	LEU
3	D	1376	MET
3	D	1379	VAL
3	D	1394	VAL
3	D	1395	LEU
3	D	1413	THR
3	D	1420	LEU
3	D	1431	THR
3	D	1433	SER
3	D	1448	THR
3	D	1456	LYS
3	D	1468	LEU
3	D	1470	ARG
3	D	1489	GLN
3	D	1493	LYS
3	D	1496	GLU
4	E	15	SER
4	E	21	VAL
4	E	30	LEU
4	E	44	GLU
4	E	54	LEU
4	E	67	GLU
4	E	74	VAL
4	E	75	PHE
4	E	90	GLU
4	E	93	TYR
5	F	78	SER
5	F	82	ARG
5	F	83	GLN
5	F	88	ILE
5	F	98	GLU
5	F	114	LYS
5	F	122	LEU
5	F	123	ASP
5	F	126	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	140	ARG
5	F	142	ARG
5	F	148	LYS
5	F	149	GLU
5	F	155	THR
5	F	157	GLU
5	F	164	LYS
5	F	166	LEU
5	F	170	HIS
5	F	171	LYS
5	F	186	HIS
5	F	207	LEU
5	F	208	SER
5	F	209	PHE
5	F	210	LEU
5	F	211	ASP
5	F	213	ILE
5	F	218	GLN
5	F	254	GLN
5	F	270	LYS
5	F	282	LEU
5	F	291	ILE
5	F	304	VAL
5	F	306	GLU
5	F	307	THR
5	F	310	ILE
5	F	323	ASP
5	F	324	GLU
5	F	336	GLU
5	F	338	LEU
5	F	340	SER
5	F	348	SER
5	F	349	LEU
5	F	351	SER
5	F	353	GLU
5	F	358	LEU
5	F	359	SER
5	F	367	MET
5	F	369	LEU
5	F	372	ARG
5	F	376	ILE
5	F	377	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	379	ARG
5	F	380	GLU
5	F	386	VAL
5	F	398	ARG
5	F	399	GLN
5	F	401	GLU
5	F	406	ARG
5	F	415	THR
5	F	423	ASP

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

Mol	Chain	Res	Type
1	A	163	ASN
1	A	213	GLN
1	A	227	ASN
1	B	63	HIS
1	B	128	HIS
1	B	163	ASN
1	B	221	HIS
2	C	390	GLN
2	C	498	GLN
2	C	567	GLN
2	C	639	GLN
2	C	704	HIS
2	C	728	HIS
2	C	1047	HIS
2	C	1050	GLN
3	D	348	GLN
3	D	569	ASN
3	D	703	ASN
3	D	709	HIS
3	D	717	GLN
3	D	737	ASN
3	D	767	HIS
3	D	855	HIS
3	D	909	ASN
3	D	973	GLN
3	D	1031	ASN
3	D	1034	GLN
3	D	1046	GLN
3	D	1075	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1195	GLN
3	D	1235	GLN
3	D	1254	GLN
3	D	1333	HIS
3	D	1334	GLN
3	D	1359	GLN
3	D	1441	GLN
3	D	1442	ASN
3	D	1489	GLN
4	E	86	GLN
5	F	175	HIS
5	F	269	ASN
5	F	399	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/3 (66%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
10	DCP	D	1601	9	25,29,29	3.92	11 (44%)	37,45,45	1.94	12 (32%)

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
10	DCP	D	1601	9	-	9/22/34/34	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1601	DCP	C2'-C1'	-10.24	1.23	1.52
10	D	1601	DCP	O4'-C4'	-8.59	1.25	1.45
10	D	1601	DCP	O4'-C1'	8.36	1.61	1.42
10	D	1601	DCP	C6-C5	5.51	1.47	1.35
10	D	1601	DCP	C2-N3	4.47	1.45	1.36
10	D	1601	DCP	C4-N3	4.02	1.42	1.34
10	D	1601	DCP	C4-N4	3.99	1.43	1.33
10	D	1601	DCP	O2-C2	-3.90	1.16	1.23
10	D	1601	DCP	C1'-N1	-2.96	1.40	1.48
10	D	1601	DCP	O3'-C3'	-2.94	1.37	1.43
10	D	1601	DCP	C6-N1	2.80	1.44	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	1601	DCP	PB-O3B-PG	-4.36	117.88	132.83
10	D	1601	DCP	C1'-N1-C2	4.29	125.27	117.74
10	D	1601	DCP	O3G-PG-O3B	3.93	117.81	104.64
10	D	1601	DCP	C4-N3-C2	3.49	125.89	120.25
10	D	1601	DCP	C2'-C1'-N1	-3.13	106.56	113.77
10	D	1601	DCP	C1'-N1-C6	-2.96	115.71	121.55
10	D	1601	DCP	O4'-C4'-C3'	-2.88	98.95	105.67
10	D	1601	DCP	PB-O3A-PA	-2.65	123.73	132.83
10	D	1601	DCP	C5-C4-N3	-2.44	117.17	121.33
10	D	1601	DCP	N4-C4-N3	2.38	122.14	117.97
10	D	1601	DCP	C2'-C3'-C4'	2.36	107.68	102.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	1601	DCP	O4'-C4'-C5'	2.16	116.48	109.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

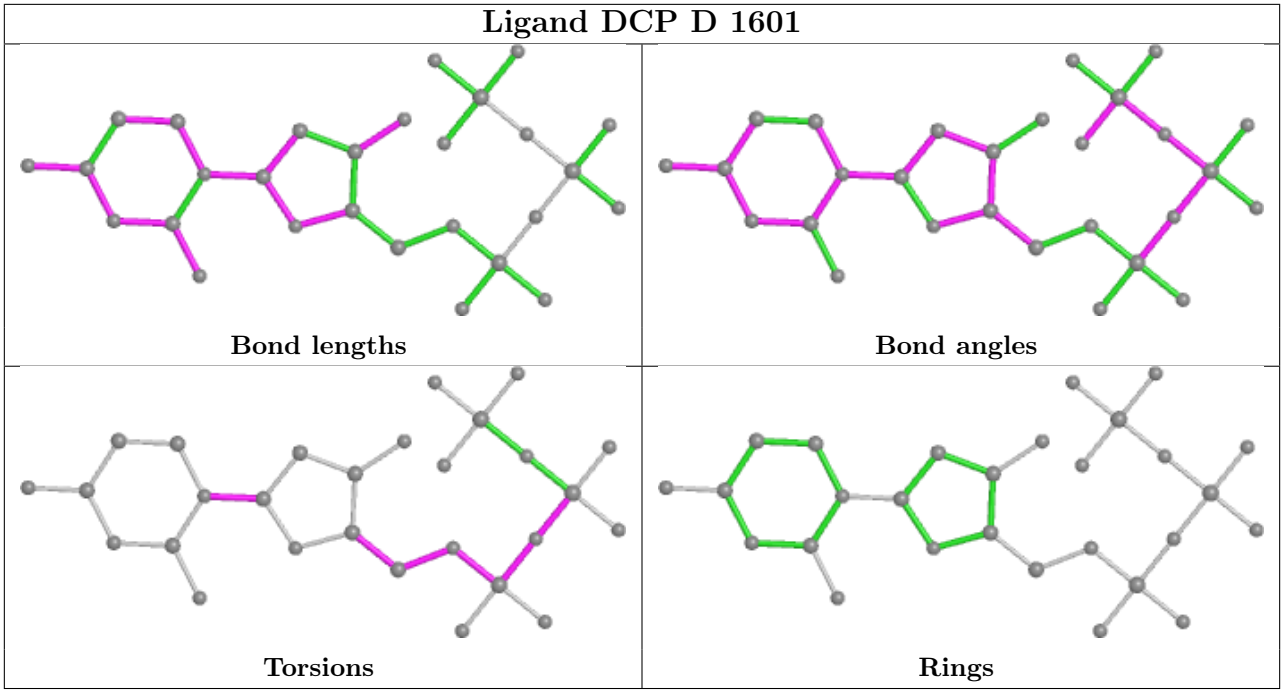
Mol	Chain	Res	Type	Atoms
10	D	1601	DCP	C5'-O5'-PA-O1A
10	D	1601	DCP	C5'-O5'-PA-O3A
10	D	1601	DCP	C2'-C1'-N1-C6
10	D	1601	DCP	PB-O3A-PA-O5'
10	D	1601	DCP	PA-O3A-PB-O1B
10	D	1601	DCP	C2'-C1'-N1-C2
10	D	1601	DCP	C4'-C5'-O5'-PA
10	D	1601	DCP	C3'-C4'-C5'-O5'
10	D	1601	DCP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1601	DCP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	226/315 (71%)	-0.39	0 100 100	73, 91, 110, 124	0
1	B	224/315 (71%)	-0.39	1 (0%) 92 86	66, 96, 121, 133	0
2	C	1111/1119 (99%)	-0.30	6 (0%) 91 83	56, 91, 138, 160	0
3	D	1485/1505 (98%)	-0.28	10 (0%) 87 77	50, 85, 138, 160	0
4	E	94/99 (94%)	-0.30	1 (1%) 80 66	64, 101, 132, 139	0
5	F	346/423 (81%)	-0.08	17 (4%) 29 14	64, 101, 153, 163	0
6	G	17/22 (77%)	0.11	0 100 100	69, 95, 169, 171	0
7	H	25/27 (92%)	-0.15	1 (4%) 38 20	90, 121, 169, 179	0
8	I	3/3 (100%)	-0.50	0 100 100	73, 73, 76, 87	0
All	All	3531/3828 (92%)	-0.28	36 (1%) 82 70	50, 91, 142, 179	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	391	GLY	4.6
3	D	1313	VAL	4.3
5	F	375	LEU	4.2
3	D	1297	GLU	4.0
5	F	389	PHE	4.0
5	F	392	VAL	3.9
5	F	381	HIS	3.6
5	F	147	LEU	3.5
5	F	149	GLU	3.3
3	D	422	ALA	3.0
2	C	212	GLY	3.0
5	F	376	ILE	2.9
2	C	188	LYS	2.8
3	D	1318	TYR	2.8
4	E	95	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	145	PRO	2.7
7	H	24	DC	2.6
5	F	390	PHE	2.5
1	B	106	PRO	2.5
5	F	382	THR	2.4
3	D	165	LYS	2.4
5	F	146	GLY	2.4
3	D	173	PRO	2.4
2	C	1	MET	2.3
5	F	360	LYS	2.3
5	F	393	THR	2.2
5	F	374	GLY	2.2
2	C	545	ASN	2.1
5	F	150	THR	2.1
2	C	219	GLN	2.1
3	D	1319	VAL	2.1
3	D	1298	GLY	2.1
3	D	384	VAL	2.1
3	D	973	GLN	2.1
2	C	1094	ALA	2.1
5	F	370	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
9	NA	C	1201	1/1	0.81	0.20	70,70,70,70	0
10	DCP	D	1601	28/28	0.91	0.18	80,93,112,115	0

Continued on next page...

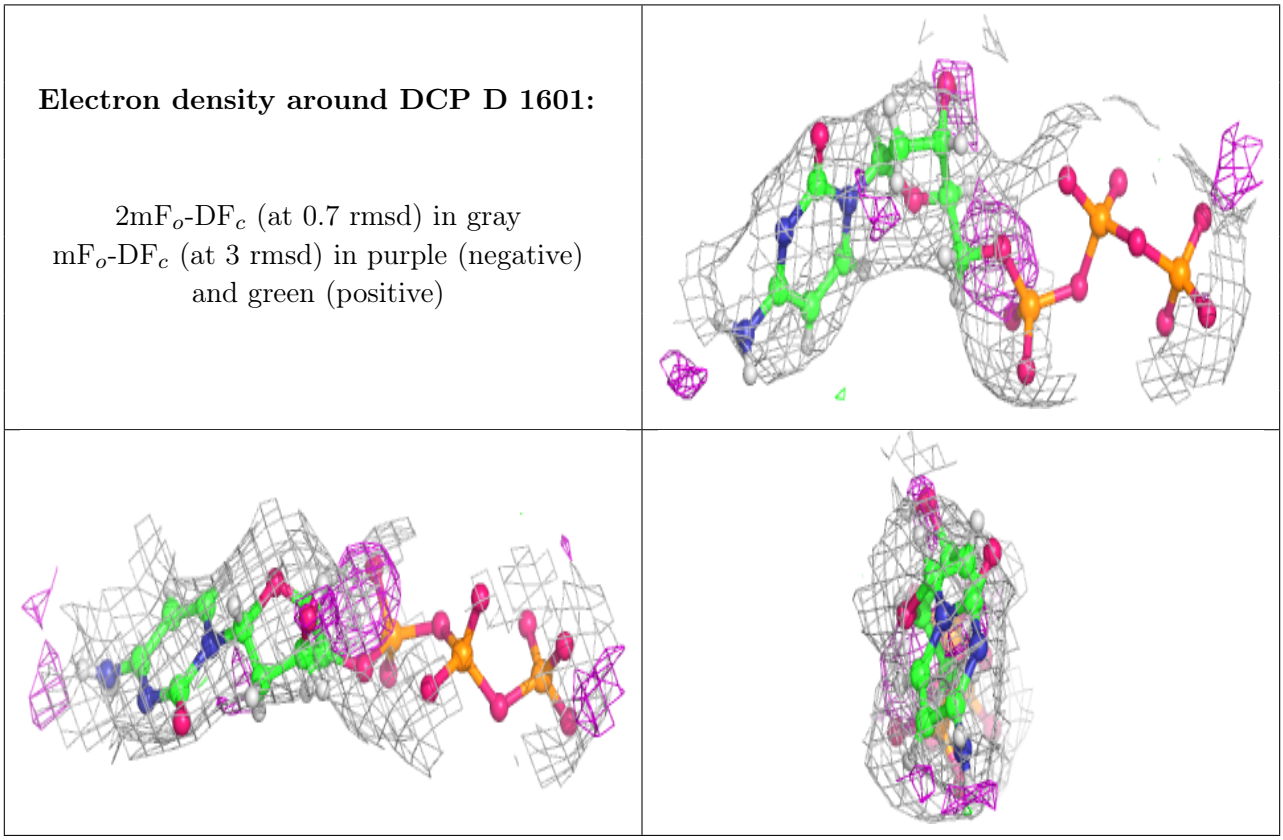
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	ZN	D	1604	1/1	0.96	0.12	120,120,120,120	0
12	ZN	D	1603	1/1	0.97	0.12	125,125,125,125	0
11	MG	D	1602	1/1	0.98	0.17	67,67,67,67	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DCP D 1601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.