Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 03:30 AM EDT

PDB ID	:	3M4O
Title	:	RNA polymerase II elongation complex B
Authors	:	Wang, D.; Zhu, G.; Huang, X.; Lippard, S.J.
Deposited on	:	2010-03-11
Resolution	:	3.57 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 (i) 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 (1)) were used in the production of this report:

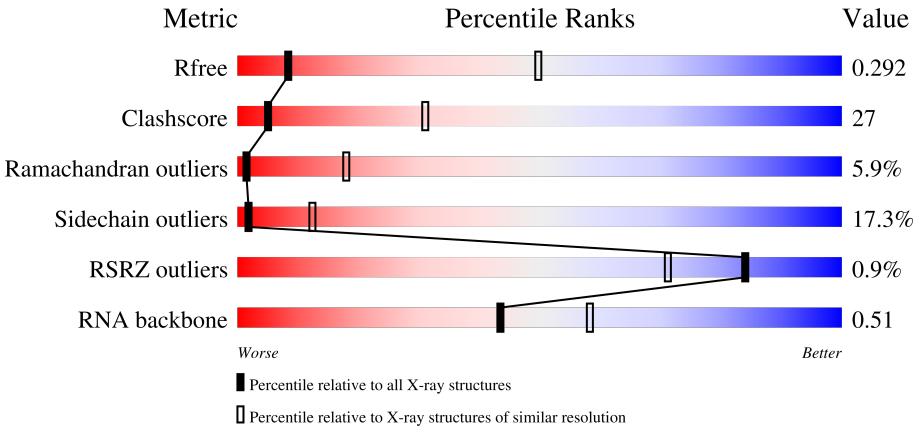
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 3.57 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.



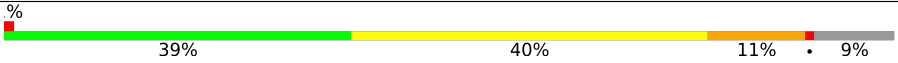
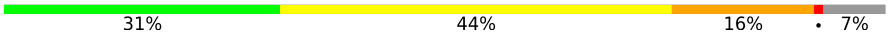
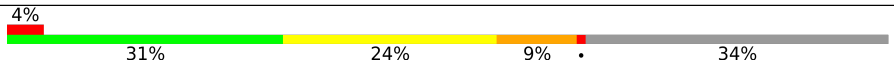
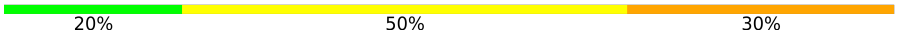
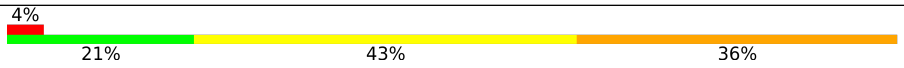
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)
RNA backbone	3102	1008 (4.10-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1733	38% 34% 8% • 20%
2	B	1224	41% 38% 10% • 10%
3	C	318	38% 36% 9% • 16%
4	E	215	2% 55% 38% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	10	
12	T	28	
13	N	14	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29227 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1395	10969	6917	1923	2068	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1106	8792	5568	1538	1631	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	214	1752	1111	309	321	11	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	84	679	434	115	127	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	133	1068	673	180	211	4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	10	Total	C	N	O	P	0	0	0
			220	99	47	65	9			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			553	265	92	168	28			

- Molecule 13 is a DNA chain called DNA (5'-D(P*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			296	140	55	87	14			

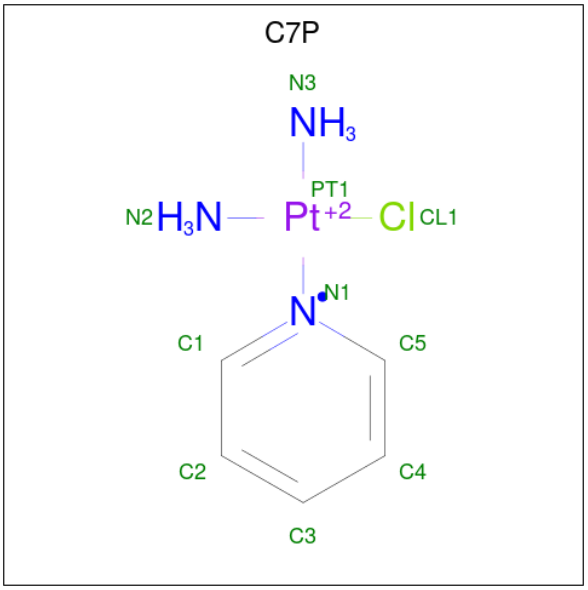
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	2	Total Zn 2 2	0	0
14	B	1	Total Zn 1 1	0	0
14	C	1	Total Zn 1 1	0	0
14	I	2	Total Zn 2 2	0	0
14	J	1	Total Zn 1 1	0	0
14	L	1	Total Zn 1 1	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0

- Molecule 16 is cis-diammine(pyridine)chloroplatinum(II) (three-letter code: C7P) (formula: $C_5H_{11}ClN_3Pt$).



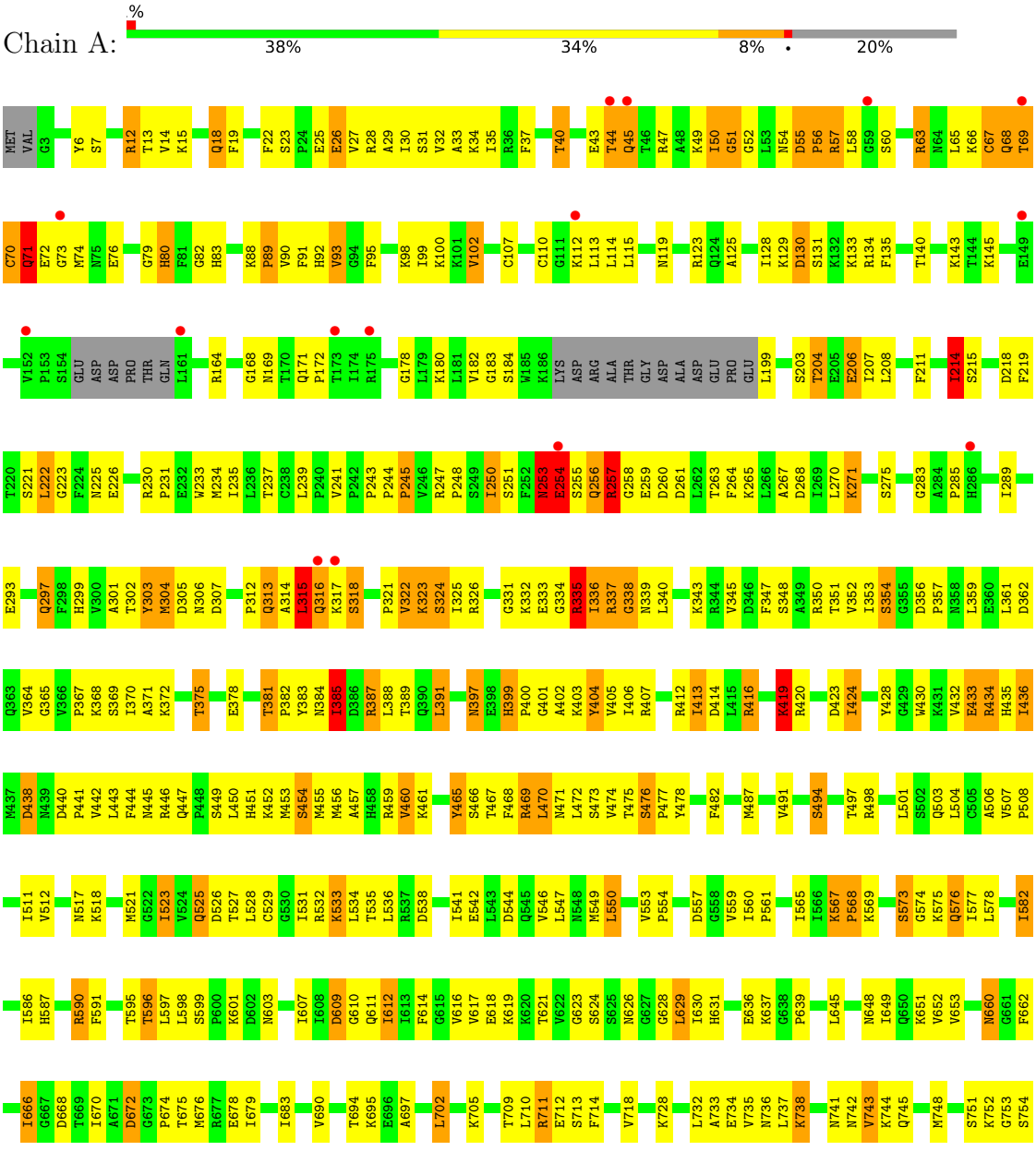
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	T	1	Total C N Pt 9 5 3 1	0	0

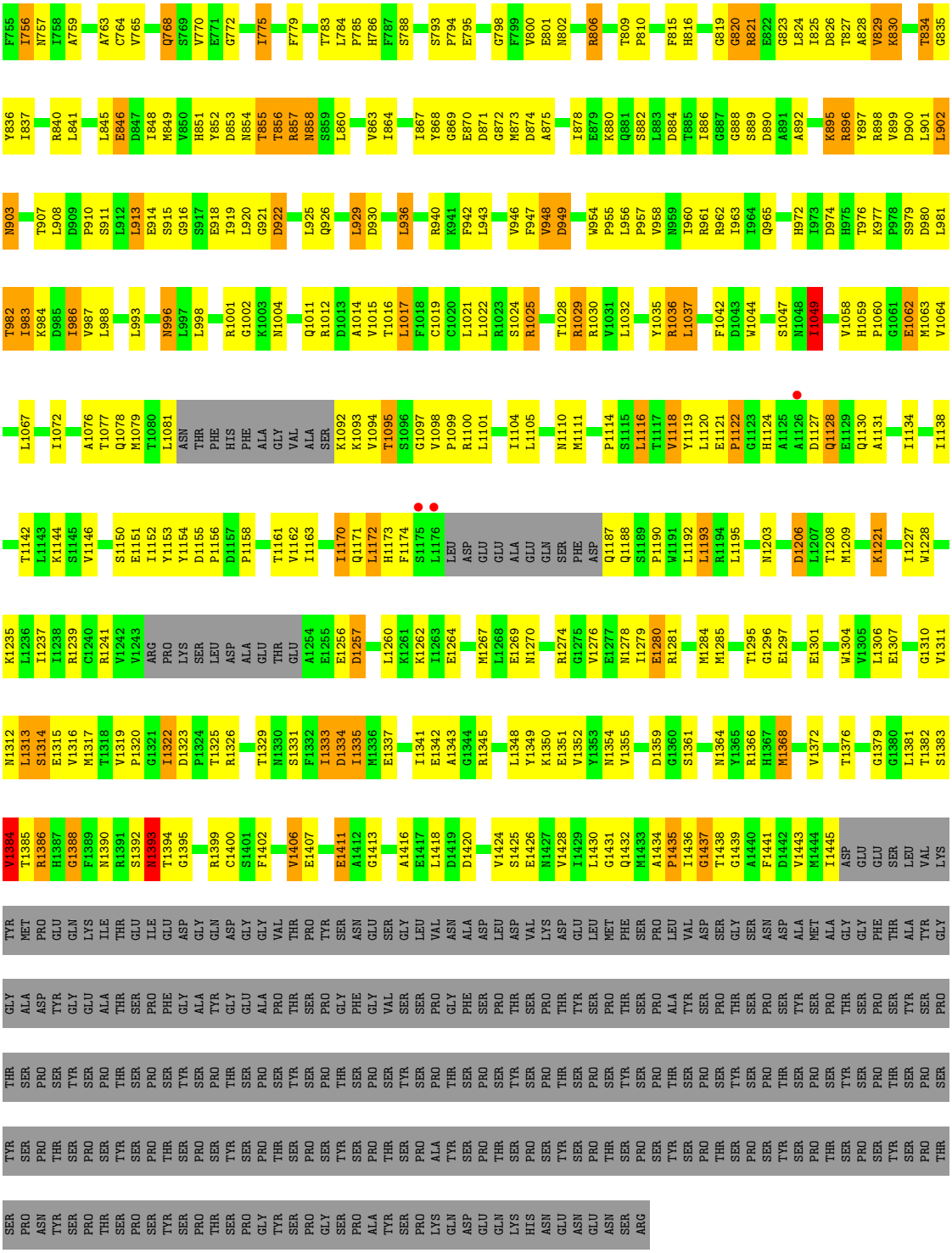
3 Residue-property plots (i)

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

• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

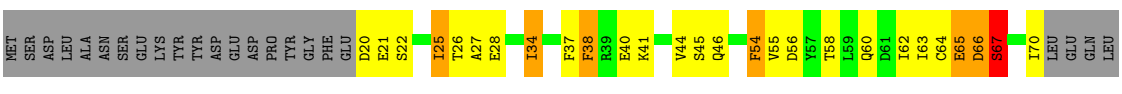
Chain A:

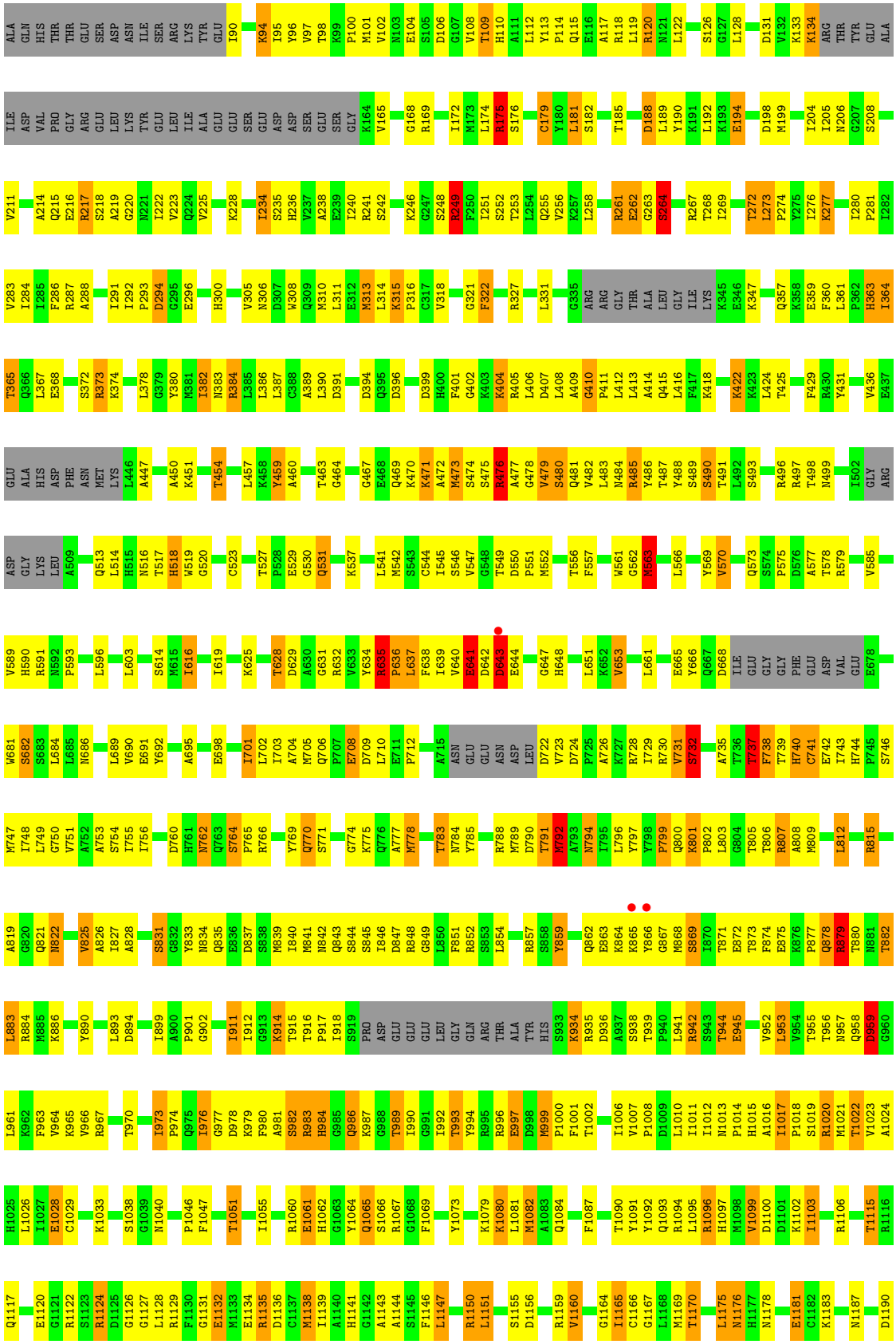


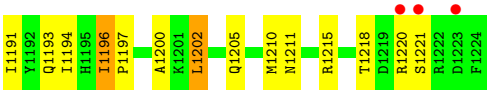


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

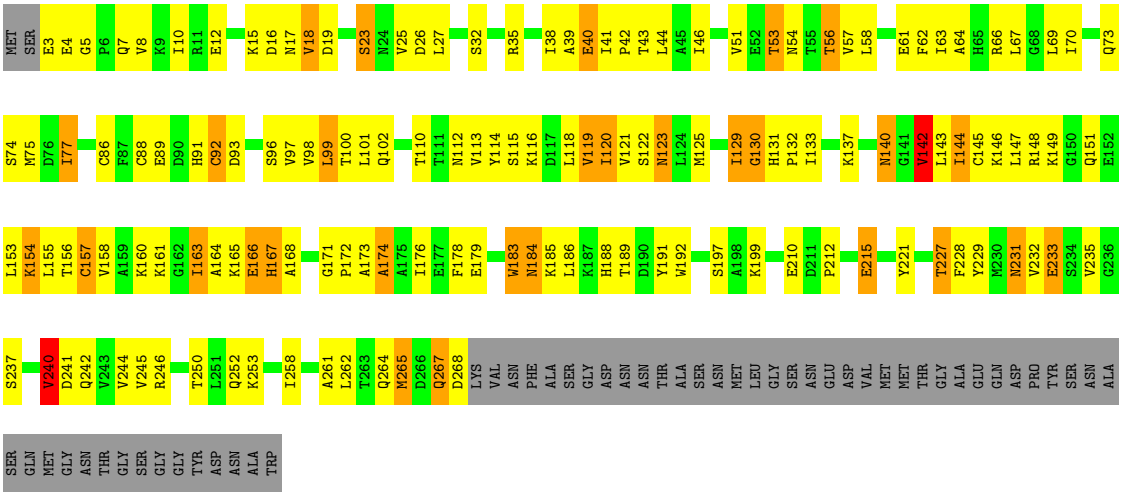






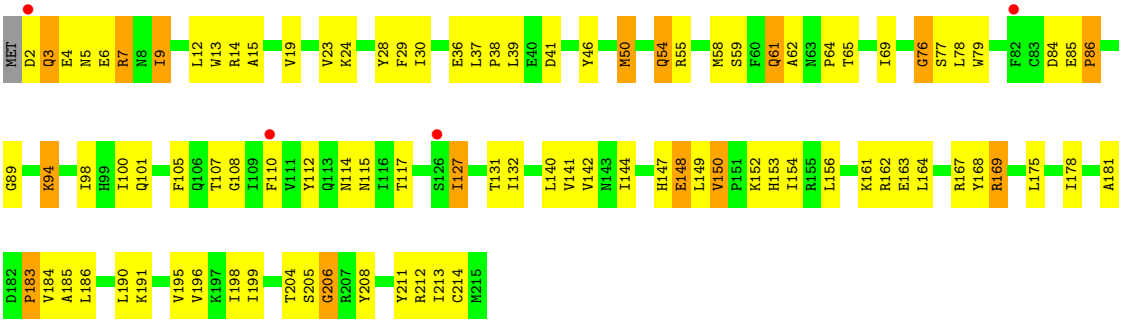
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



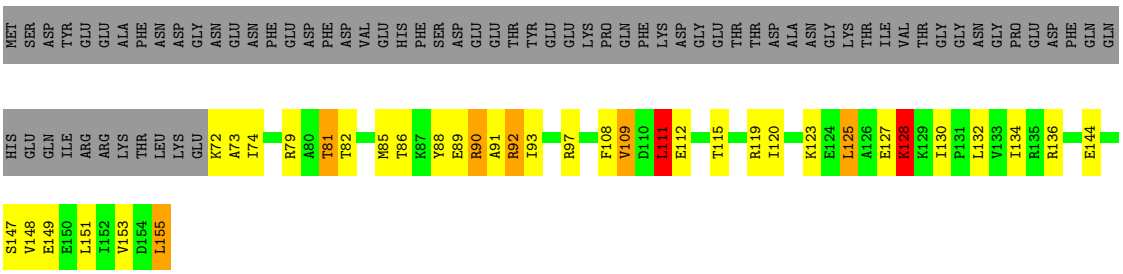
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



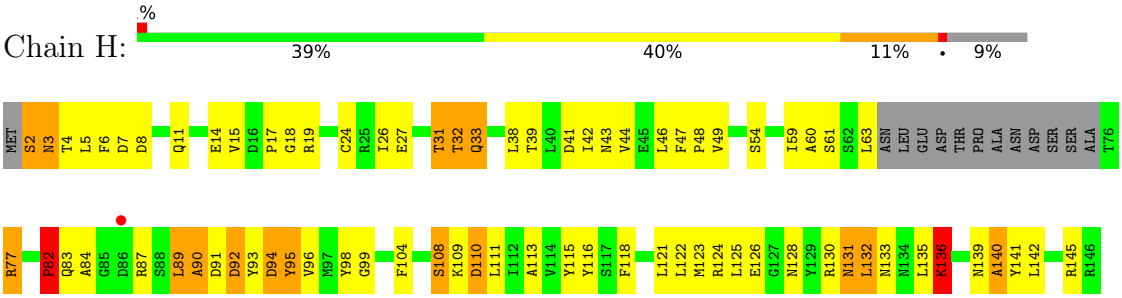
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



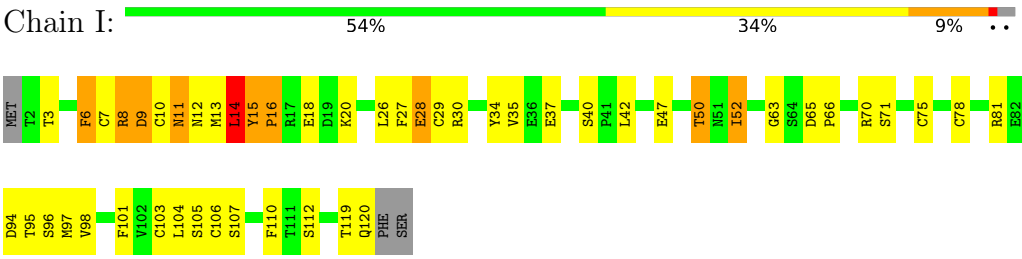
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



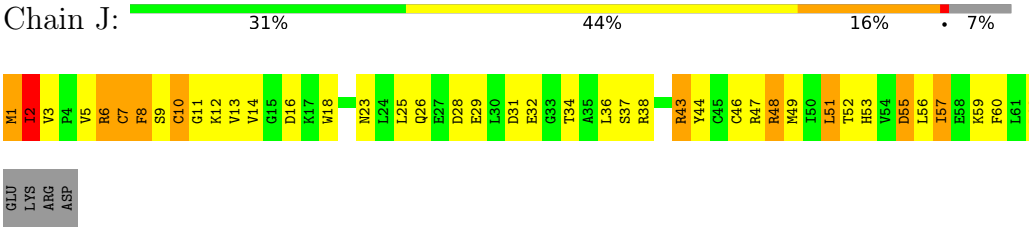
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



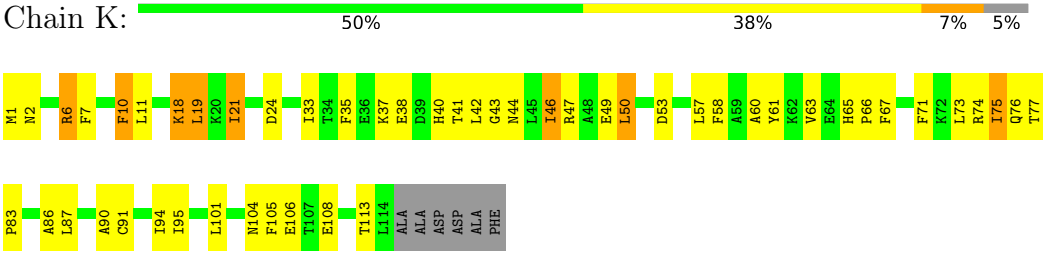
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



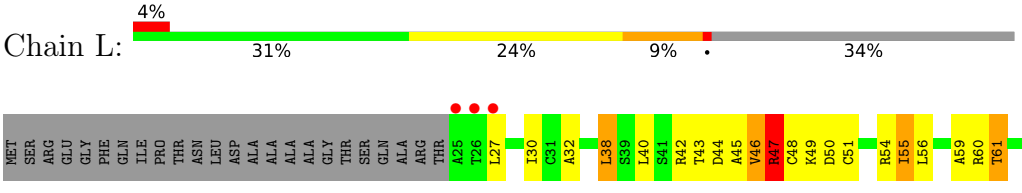
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:



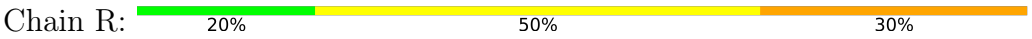
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

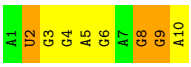
Chain L:



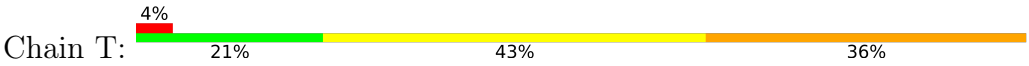
• Molecule 11: RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*A)-3')

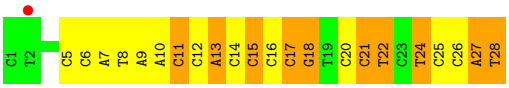
Chain R:



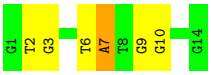


• Molecule 12: DNA (28-MER)





• Molecule 13: DNA (5'-D(P*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP*GP*TP*AP*G)-3')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.11Å 222.13Å 191.78Å 90.00° 100.99° 90.00°	Depositor
Resolution (Å)	40.00 – 3.57 39.79 – 3.57	Depositor EDS
% Data completeness (in resolution range)	90.5 (40.00-3.57) 90.5 (39.79-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.241 , 0.292 0.248 , 0.292	Depositor DCC
R_{free} test set	3681 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	85.0	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 100.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	29227	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: ZN, C7P, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	0/11163	0.75	5/15091 (0.0%)
2	B	0.64	1/8963 (0.0%)	0.78	3/12086 (0.0%)
3	C	0.59	0/2133	0.74	0/2891
4	E	0.49	0/1788	0.66	1/2406 (0.0%)
5	F	0.51	0/691	0.76	0/933
6	H	0.47	0/1086	0.76	0/1470
7	I	0.55	0/989	0.76	1/1331 (0.1%)
8	J	0.66	0/541	0.88	1/727 (0.1%)
9	K	0.57	0/937	0.72	0/1265
10	L	0.59	0/365	0.87	0/485
11	R	0.71	0/248	1.27	2/387 (0.5%)
12	T	1.06	3/615 (0.5%)	2.00	23/941 (2.4%)
13	N	0.74	0/332	1.31	1/513 (0.2%)
All	All	0.60	4/29851 (0.0%)	0.83	37/40526 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	H	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	DG	C8-N7	7.66	1.35	1.30
12	T	18	DG	C6-N1	-6.66	1.34	1.39
12	T	18	DG	N7-C5	-5.70	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1029	CYS	CB-SG	-5.32	1.73	1.81

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	18	DG	N3-C4-C5	-18.97	119.12	128.60
12	T	18	DG	C2-N3-C4	16.08	119.94	111.90
12	T	18	DG	C5-C6-N1	13.88	118.44	111.50
12	T	18	DG	N3-C4-N9	12.76	133.65	126.00
12	T	18	DG	C5-C6-O6	-10.72	122.17	128.60
12	T	21	DC	O4'-C4'-C3'	-8.29	101.03	106.00
12	T	27	DA	O4'-C4'-C3'	-7.70	101.38	106.00
12	T	11	DC	O4'-C1'-N1	6.92	112.85	108.00
2	B	476	ARG	CB-CA-C	-6.91	96.57	110.40
8	J	51	LEU	CA-CB-CG	6.61	130.50	115.30
12	T	25	DC	O4'-C1'-N1	6.61	112.63	108.00
12	T	28	DT	O4'-C4'-C3'	-6.49	101.90	104.50
12	T	24	DT	O4'-C4'-C3'	-6.24	102.01	104.50
12	T	15	DC	P-O3'-C3'	6.21	127.16	119.70
12	T	17	DC	O4'-C1'-C2'	-6.08	101.03	105.90
12	T	13	DA	P-O3'-C3'	6.08	126.99	119.70
12	T	18	DG	C6-N1-C2	-5.93	121.54	125.10
12	T	22	DT	C4'-C3'-C2'	-5.80	97.88	103.10
12	T	28	DT	O4'-C1'-N1	5.72	112.00	108.00
1	A	936	LEU	CA-CB-CG	5.72	128.45	115.30
12	T	17	DC	C6-N1-C2	-5.69	118.03	120.30
11	R	2	U	O4'-C1'-N1	5.41	112.52	108.20
1	A	253	ASN	N-CA-C	5.40	125.58	111.00
12	T	22	DT	N3-C4-O4	5.33	123.10	119.90
12	T	27	DA	C4'-C3'-C2'	-5.32	98.32	103.10
11	R	8	G	C4'-C3'-C2'	-5.25	97.35	102.60
12	T	17	DC	C5-C6-N1	5.25	123.62	121.00
2	B	476	ARG	N-CA-C	5.19	125.02	111.00
12	T	26	DC	O4'-C1'-N1	5.19	111.63	108.00
1	A	1393	ASN	N-CA-C	5.19	125.00	111.00
1	A	1116	LEU	CA-CB-CG	5.18	127.21	115.30
4	E	175	LEU	CA-CB-CG	5.14	127.12	115.30
12	T	11	DC	P-O3'-C3'	5.13	125.86	119.70
2	B	637	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	1313	LEU	CA-CB-CG	5.08	126.97	115.30
13	N	7	DA	O4'-C1'-N9	5.02	111.51	108.00
7	I	14	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1172	LEU	Peptide
6	H	136	LYS	Peptide
6	H	82	PRO	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	10969	0	11071	670	0
2	B	8792	0	8824	560	0
3	C	2095	0	2052	152	0
4	E	1752	0	1776	70	0
5	F	679	0	701	31	0
6	H	1068	0	1040	63	0
7	I	971	0	929	33	0
8	J	532	0	543	62	0
9	K	919	0	929	54	0
10	L	363	0	387	18	0
11	R	220	0	110	12	0
12	T	553	0	315	24	0
13	N	296	0	160	3	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	T	9	0	5	5	0
All	All	29227	0	28842	1570	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 27.

All (1570) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.31	1.13
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.79	1.10
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.82	1.09
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.18	1.08
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.14	1.07
2:B:635:ARG:HB2	2:B:636:PRO:CD	1.82	1.07
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.53	1.06
2:B:635:ARG:HB2	2:B:636:PRO:HD3	1.09	1.05
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.39	1.05
1:A:401:GLY:C	1:A:435:HIS:HD2	1.59	1.05
2:B:956:THR:HB	10:L:46:VAL:HG21	1.37	1.05
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.39	1.04
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.21	1.03
3:C:56:THR:HG23	3:C:147:LEU:HD23	1.39	1.03
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.06	1.02
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.35	1.01
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.25	1.00
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.41	0.98
2:B:65:GLU:HG3	2:B:66:ASP:H	1.29	0.97
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	1.80	0.97
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.48	0.96
1:A:868:TYR:CE2	1:A:1366:ARG:HD3	2.00	0.96
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.29	0.95
2:B:175:ARG:HH11	2:B:175:ARG:CG	1.79	0.94
1:A:869:GLY:O	4:E:204:THR:HG21	1.66	0.94
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.29	0.94
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.47	0.94
1:A:567:LYS:HB3	6:H:96:VAL:H	1.32	0.94
2:B:636:PRO:HB2	2:B:637:LEU:CA	1.96	0.93
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.49	0.93
2:B:744:HIS:HD2	2:B:746:SER:OG	1.53	0.92
5:F:111:LEU:HD12	5:F:111:LEU:H	1.33	0.91
1:A:261:ASP:HB3	1:A:323:LYS:HD2	1.49	0.91
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.50	0.91
1:A:1342:GLU:HG2	4:E:212:ARG:HH12	1.33	0.91
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.51	0.91
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.84	0.91
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.36	0.91
3:C:56:THR:HG23	3:C:147:LEU:CD2	2.01	0.91
1:A:851:HIS:CD2	1:A:857:ARG:HG3	2.06	0.90
1:A:315:LEU:CB	1:A:316:GLN:HA	2.00	0.90
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.00	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.06	0.89
1:A:404:TYR:HB2	1:A:433:GLU:HG3	1.54	0.89
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.03	0.88
1:A:90:VAL:HG13	1:A:297:GLN:NE2	1.89	0.88
2:B:479:VAL:O	2:B:480:SER:HB3	1.72	0.88
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.54	0.87
2:B:474:SER:HA	2:B:476:ARG:HG3	1.55	0.87
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.57	0.86
2:B:981:ALA:O	2:B:982:SER:O	1.93	0.85
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.54	0.85
1:A:401:GLY:C	1:A:435:HIS:CD2	2.49	0.85
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.16	0.85
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.04	0.85
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.58	0.85
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.25	0.85
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.56	0.85
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.12	0.85
2:B:986:GLN:NE2	2:B:1020:ARG:HD2	1.92	0.85
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.58	0.84
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.58	0.84
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.40	0.84
2:B:485:ARG:HH11	2:B:485:ARG:CG	1.90	0.84
2:B:614:SER:H	2:B:632:ARG:HH12	1.26	0.84
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.59	0.84
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.57	0.84
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.93	0.83
2:B:176:SER:O	2:B:182:SER:HB3	1.78	0.83
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.79	0.83
2:B:40:GLU:OE1	2:B:682:SER:HB2	1.78	0.83
7:I:71:SER:H	7:I:83:ASN:HD21	1.26	0.82
1:A:901:LEU:H	1:A:926:GLN:HE21	1.26	0.82
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.12	0.82
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.44	0.82
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.19	0.82
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.27	0.81
3:C:56:THR:HG21	3:C:145:CYS:SG	2.20	0.81
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	1.96	0.81
3:C:231:ASN:HD22	3:C:231:ASN:C	1.82	0.81
2:B:744:HIS:CD2	2:B:746:SER:OG	2.34	0.81
2:B:126:SER:OG	2:B:172:ILE:HD11	1.79	0.81
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.16	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:HIS:HD2	1:A:857:ARG:HG3	1.43	0.80
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.45	0.80
1:A:134:ARG:HD2	1:A:221:SER:O	1.81	0.80
1:A:765:VAL:CG2	1:A:800:VAL:HB	2.12	0.80
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.47	0.80
1:A:913:LEU:HD12	1:A:915:SER:H	1.47	0.79
2:B:843:GLN:HB2	2:B:993:THR:HB	1.64	0.79
8:J:25:LEU:O	8:J:29:GLU:HA	1.82	0.79
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.80	0.79
3:C:74:SER:O	3:C:77:ILE:HB	1.83	0.79
3:C:91:HIS:CE1	3:C:158:VAL:HG21	2.18	0.78
1:A:49:LYS:O	1:A:50:ILE:HG12	1.82	0.78
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.48	0.78
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.65	0.78
2:B:976:ILE:HG23	2:B:977:GLY:N	1.99	0.78
1:A:23:SER:O	1:A:27:VAL:HG23	1.82	0.78
2:B:474:SER:CA	2:B:476:ARG:HG3	2.12	0.78
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.66	0.78
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.63	0.78
2:B:639:ILE:HA	2:B:740:HIS:HB3	1.65	0.78
6:H:104:PHE:CZ	6:H:136:LYS:HA	2.19	0.78
1:A:351:THR:HG23	2:B:1103:ILE:CD1	2.13	0.77
1:A:1101:LEU:O	1:A:1105:LEU:HD12	1.83	0.77
2:B:638:PHE:O	2:B:740:HIS:HB2	1.84	0.77
2:B:706:GLN:O	2:B:710:LEU:HB2	1.83	0.77
8:J:56:LEU:HB3	8:J:60:PHE:HE2	1.49	0.77
2:B:384:ARG:HH12	2:B:579:ARG:HH21	1.32	0.77
2:B:955:THR:HG22	2:B:956:THR:N	1.98	0.77
1:A:752:LYS:HD2	2:B:1015:HIS:O	1.85	0.76
2:B:249:ARG:HG3	2:B:251:ILE:HD11	1.66	0.76
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.30	0.76
1:A:351:THR:CG2	2:B:1103:ILE:HD12	2.15	0.76
2:B:698:GLU:O	2:B:701:ILE:HD13	1.86	0.76
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.15	0.76
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.50	0.76
1:A:90:VAL:HG13	1:A:297:GLN:HE21	1.49	0.76
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.20	0.76
2:B:120:ARG:HB3	2:B:955:THR:HG21	1.66	0.76
3:C:46:ILE:HD12	3:C:157:CYS:HB2	1.67	0.76
2:B:701:ILE:HG13	2:B:740:HIS:CE1	2.20	0.76
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	2.00	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ARG:O	2:B:936:ASP:HB3	1.85	0.75
2:B:1138:MET:HE3	2:B:1138:MET:HA	1.67	0.75
11:R:9:G:C2	12:T:21:DC:O2	2.39	0.75
2:B:589:VAL:HG12	2:B:590:HIS:H	1.50	0.75
1:A:315:LEU:HB2	1:A:316:GLN:CA	2.09	0.75
1:A:1077:THR:HB	1:A:1078:GLN:HE21	1.50	0.75
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.01	0.75
3:C:165:LYS:O	9:K:6:ARG:NH1	2.20	0.74
1:A:559:VAL:HG12	1:A:559:VAL:O	1.87	0.74
3:C:56:THR:CG2	3:C:147:LEU:HD23	2.14	0.74
2:B:640:VAL:HG12	2:B:640:VAL:O	1.87	0.74
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.69	0.74
2:B:408:LEU:HD22	2:B:545:ILE:HD12	1.67	0.74
2:B:422:LYS:HA	2:B:425:THR:HG22	1.69	0.74
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.17	0.74
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.15	0.73
2:B:459:TYR:HD2	2:B:459:TYR:C	1.92	0.73
1:A:304:MET:HG2	2:B:1210:MET:HG3	1.70	0.73
2:B:578:THR:OG1	2:B:593:PRO:HG3	1.88	0.73
2:B:916:THR:HG23	2:B:916:THR:O	1.88	0.73
3:C:133:ILE:HD12	3:C:237:SER:HA	1.69	0.73
8:J:8:PHE:H	8:J:49:MET:HE3	1.53	0.73
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.70	0.73
3:C:3:GLU:HG3	3:C:4:GLU:H	1.53	0.73
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.71	0.73
1:A:347:PHE:HB2	2:B:1150:ARG:HH22	1.53	0.73
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.71	0.73
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.71	0.73
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.71	0.73
11:R:4:G:H2'	11:R:5:A:H8	1.54	0.73
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.70	0.72
2:B:459:TYR:C	2:B:459:TYR:CD2	2.63	0.72
1:A:69:THR:O	1:A:71:GLN:HG3	1.88	0.72
4:E:15:ALA:O	4:E:19:VAL:HG23	1.89	0.72
6:H:89:LEU:O	6:H:91:ASP:N	2.20	0.72
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.03	0.72
1:A:759:ALA:O	1:A:763:ALA:HB3	1.90	0.72
1:A:351:THR:HG22	1:A:352:VAL:O	1.89	0.72
2:B:957:ASN:O	2:B:959:ASP:N	2.23	0.72
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.87	0.72
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.16	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.72	0.72
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.20	0.72
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.24	0.72
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.19	0.71
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.88	0.71
1:A:218:ASP:O	1:A:222:LEU:HD11	1.90	0.71
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.36	0.71
2:B:1106:ARG:HD2	2:B:1126:GLY:O	1.90	0.71
1:A:809:THR:HG21	2:B:730:ARG:HG3	1.71	0.71
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.55	0.71
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.73	0.71
3:C:43:THR:HG22	3:C:44:LEU:H	1.55	0.71
3:C:66:ARG:NH2	8:J:3:VAL:O	2.23	0.71
1:A:826:ASP:O	1:A:830:LYS:N	2.20	0.71
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.26	0.71
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.56	0.71
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.03	0.71
1:A:271:LYS:O	1:A:275:SER:HB2	1.91	0.70
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.72	0.70
2:B:65:GLU:HG3	2:B:66:ASP:N	2.06	0.70
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.57	0.70
1:A:568:PRO:HD3	6:H:94:ASP:O	1.89	0.70
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.73	0.70
1:A:457:ALA:O	1:A:507:VAL:HG23	1.92	0.70
1:A:573:SER:O	1:A:576:GLN:HB2	1.92	0.70
1:A:626:ASN:O	1:A:631:HIS:CD2	2.45	0.70
2:B:1082:MET:HA	3:C:189:THR:HA	1.73	0.70
16:T:29:C7P:H6	16:T:29:C7P:N3	2.05	0.70
1:A:55:ASP:O	1:A:57:ARG:N	2.24	0.70
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.22	0.70
1:A:596:THR:O	1:A:598:LEU:N	2.24	0.70
2:B:34:ILE:HG23	2:B:542:MET:HE3	1.72	0.70
2:B:175:ARG:HG3	2:B:175:ARG:NH1	2.05	0.70
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.53	0.70
1:A:399:HIS:O	1:A:401:GLY:N	2.24	0.70
2:B:955:THR:HG23	10:L:54:ARG:O	1.92	0.70
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.73	0.69
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.06	0.69
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.57	0.69
1:A:1319:VAL:HG12	1:A:1320:PRO:O	1.92	0.69
2:B:986:GLN:HE22	2:B:1016:ALA:HB1	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:CG2	1:A:352:VAL:N	2.55	0.69
1:A:901:LEU:HA	1:A:907:THR:HG23	1.75	0.69
2:B:542:MET:HG3	2:B:747:MET:HE2	1.75	0.69
2:B:912:ILE:O	2:B:938:SER:HB3	1.92	0.69
8:J:10:CYS:SG	8:J:43:ARG:CD	2.80	0.69
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.07	0.69
1:A:49:LYS:NZ	1:A:60:SER:HA	2.07	0.69
1:A:567:LYS:CB	1:A:568:PRO:CD	2.53	0.69
1:A:783:THR:HG21	1:A:815:PHE:HE2	1.55	0.69
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.08	0.69
7:I:71:SER:H	7:I:83:ASN:ND2	1.91	0.69
2:B:292:ILE:HD11	2:B:327:ARG:HG2	1.73	0.69
1:A:129:LYS:O	1:A:130:ASP:HB2	1.91	0.68
1:A:365:GLY:O	1:A:468:PHE:HA	1.93	0.68
1:A:896:ARG:HH11	1:A:897:TYR:HE1	1.39	0.68
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.75	0.68
2:B:1081:LEU:O	3:C:189:THR:HG23	1.93	0.68
2:B:310:MET:O	2:B:313:MET:HB2	1.92	0.68
5:F:132:LEU:O	5:F:148:VAL:HG23	1.94	0.68
9:K:21:ILE:HG13	9:K:33:ILE:HG23	1.75	0.68
3:C:242:GLN:O	3:C:246:ARG:HB2	1.94	0.68
1:A:404:TYR:HA	1:A:413:ILE:O	1.93	0.68
1:A:806:ARG:NH2	2:B:729:ILE:HD11	2.08	0.68
2:B:976:ILE:HG23	2:B:977:GLY:H	1.56	0.68
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.58	0.68
1:A:630:ILE:HD12	1:A:630:ILE:H	1.59	0.68
4:E:19:VAL:O	4:E:23:VAL:HG23	1.94	0.68
1:A:335:ARG:HH11	2:B:1202:LEU:CD1	2.06	0.68
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.76	0.68
2:B:37:PHE:O	2:B:38:PHE:HB2	1.94	0.68
2:B:174:LEU:HD13	2:B:204:ILE:HD12	1.74	0.68
9:K:7:PHE:O	9:K:11:LEU:HB2	1.94	0.68
2:B:986:GLN:HE21	2:B:1020:ARG:HD2	1.59	0.68
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.59	0.68
1:A:107:CYS:HB2	1:A:114:LEU:HD21	1.76	0.67
1:A:662:PHE:O	2:B:828:ALA:HA	1.94	0.67
2:B:807:ARG:CG	2:B:807:ARG:HH11	2.08	0.67
2:B:841:MET:HE3	2:B:990:ILE:HD11	1.75	0.67
3:C:123:ASN:HD22	3:C:125:MET:H	1.43	0.67
1:A:438:ASP:HA	1:A:460:VAL:O	1.95	0.67
2:B:58:THR:O	2:B:62:ILE:HG12	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:O	2:B:1013:ASN:HB2	1.94	0.67
6:H:89:LEU:HD13	6:H:91:ASP:OD1	1.95	0.67
1:A:351:THR:HG22	1:A:352:VAL:N	2.08	0.67
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.75	0.67
1:A:1279:ILE:HG22	1:A:1279:ILE:O	1.94	0.67
4:E:144:ILE:O	4:E:150:VAL:HG21	1.93	0.67
1:A:553:VAL:HG22	1:A:652:VAL:HG22	1.75	0.67
7:I:71:SER:N	7:I:83:ASN:HD21	1.92	0.67
2:B:642:ASP:O	2:B:644:GLU:N	2.28	0.67
1:A:19:PHE:O	1:A:1416:ALA:HA	1.94	0.67
1:A:436:ILE:HD11	1:A:491:VAL:CG1	2.25	0.67
1:A:535:THR:HG21	1:A:617:VAL:H	1.60	0.67
1:A:858:ASN:C	1:A:858:ASN:HD22	1.97	0.67
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.29	0.67
2:B:635:ARG:CB	2:B:636:PRO:CD	2.67	0.66
1:A:436:ILE:CD1	1:A:491:VAL:HG11	2.25	0.66
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.77	0.66
2:B:211:VAL:CG2	2:B:483:LEU:HG	2.25	0.66
1:A:1017:LEU:HB2	4:E:206:GLY:N	2.09	0.66
1:A:826:ASP:HA	1:A:829:VAL:HG12	1.78	0.66
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.59	0.66
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.60	0.66
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.77	0.66
1:A:1025:ARG:HG3	1:A:1030:ARG:NH1	2.11	0.66
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.61	0.66
6:H:31:THR:O	6:H:32:THR:OG1	2.14	0.66
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.16	0.66
1:A:783:THR:CG2	1:A:815:PHE:HE2	2.09	0.65
2:B:955:THR:HG22	2:B:956:THR:H	1.59	0.65
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.77	0.65
1:A:1436:ILE:O	1:A:1437:GLY:C	2.35	0.65
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.78	0.65
1:A:354:SER:O	1:A:469:ARG:HA	1.96	0.65
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.32	0.65
2:B:168:GLY:N	2:B:450:ALA:HB1	2.12	0.65
1:A:575:LYS:HB3	1:A:612:ILE:CD1	2.26	0.65
3:C:142:VAL:HG21	8:J:5:VAL:HG13	1.79	0.65
2:B:705:MET:H	2:B:710:LEU:HD12	1.61	0.65
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.62	0.65
2:B:791:THR:O	2:B:792:MET:HB2	1.96	0.65
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:82:PRO:C	6:H:84:ALA:H	2.00	0.65
1:A:541:ILE:HG21	1:A:549:MET:CE	2.26	0.65
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.79	0.65
2:B:169:ARG:H	2:B:454:THR:HG23	1.60	0.65
3:C:38:ILE:HG12	3:C:176:ILE:HD12	1.77	0.65
4:E:199:ILE:O	4:E:199:ILE:HG22	1.96	0.65
11:R:4:G:H2'	11:R:5:A:C8	2.32	0.65
1:A:913:LEU:HD11	1:A:981:LEU:O	1.96	0.65
2:B:863:GLU:O	2:B:864:LYS:HG2	1.97	0.65
4:E:77:SER:HB3	4:E:105:PHE:CD2	2.32	0.65
1:A:744:LYS:O	1:A:748:MET:HG3	1.97	0.65
1:A:573:SER:H	1:A:576:GLN:HG3	1.60	0.65
8:J:1:MET:H1	8:J:56:LEU:HB2	1.62	0.65
1:A:413:ILE:CD1	1:A:413:ILE:H	2.10	0.64
1:A:837:ILE:HG22	1:A:841:LEU:HD12	1.79	0.64
2:B:641:GLU:HG2	2:B:643:ASP:OD2	1.96	0.64
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.79	0.64
3:C:43:THR:HG22	3:C:44:LEU:N	2.11	0.64
3:C:133:ILE:CD1	3:C:237:SER:HA	2.26	0.64
1:A:343:LYS:HD2	2:B:1151:LEU:HG	1.80	0.64
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.79	0.64
8:J:1:MET:N	8:J:56:LEU:HB2	2.13	0.64
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.11	0.64
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.31	0.64
1:A:942:PHE:C	1:A:942:PHE:CD2	2.69	0.64
2:B:701:ILE:HG13	2:B:740:HIS:HE1	1.60	0.64
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.79	0.64
4:E:86:PRO:HB3	4:E:114:ASN:HD22	1.63	0.64
2:B:976:ILE:O	2:B:990:ILE:HB	1.97	0.64
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.08	0.64
2:B:702:LEU:HD23	2:B:737:THR:HG22	1.79	0.64
3:C:15:LYS:O	3:C:240:VAL:HG22	1.97	0.63
1:A:942:PHE:CD2	1:A:942:PHE:O	2.50	0.63
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.80	0.63
2:B:493:SER:OG	2:B:497:ARG:NH2	2.31	0.63
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.62	0.63
6:H:139:ASN:O	6:H:140:ALA:HB2	1.98	0.63
1:A:889:SER:HB2	1:A:892:ALA:H	1.63	0.63
2:B:255:GLN:HB2	2:B:272:THR:OG1	1.98	0.63
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.31	0.63
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:O	1:A:435:HIS:HD2	1.80	0.63
2:B:485:ARG:HG2	2:B:485:ARG:NH1	2.04	0.63
2:B:479:VAL:O	2:B:480:SER:CB	2.46	0.63
1:A:131:SER:HB3	1:A:223:GLY:CA	2.28	0.63
1:A:630:ILE:HD12	1:A:630:ILE:N	2.13	0.63
8:J:43:ARG:HG2	8:J:46:CYS:HB2	1.81	0.63
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.81	0.63
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.12	0.63
2:B:64:CYS:O	2:B:65:GLU:HB3	1.98	0.63
1:A:547:LEU:HD22	9:K:58:PHE:HD1	1.63	0.62
2:B:992:ILE:HD12	9:K:67:PHE:HE2	1.64	0.62
9:K:19:LEU:HD22	9:K:35:PHE:CE2	2.34	0.62
8:J:9:SER:OG	8:J:48:ARG:NH2	2.33	0.62
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.80	0.62
2:B:273:LEU:HB3	2:B:276:ILE:HD12	1.81	0.62
2:B:976:ILE:CG2	2:B:977:GLY:H	2.12	0.62
7:I:50:THR:HG22	7:I:52:ILE:HG22	1.82	0.62
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.99	0.62
1:A:1436:ILE:O	1:A:1439:GLY:N	2.28	0.62
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.82	0.62
1:A:1077:THR:HB	1:A:1078:GLN:NE2	2.15	0.62
2:B:749:LEU:HD22	2:B:753:ALA:HB1	1.80	0.62
2:B:801:LYS:O	2:B:801:LYS:HG3	2.00	0.62
2:B:864:LYS:HB3	2:B:871:THR:HA	1.81	0.62
1:A:649:ILE:O	1:A:653:VAL:HG23	2.00	0.61
2:B:1066:SER:O	2:B:1067:ARG:HD3	2.00	0.61
10:L:46:VAL:HG12	10:L:47:ARG:H	1.65	0.61
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.81	0.61
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.31	0.61
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.61	0.61
6:H:2:SER:O	6:H:3:ASN:HB2	1.98	0.61
7:I:8:ARG:O	7:I:9:ASP:HB2	2.00	0.61
1:A:67:CYS:O	1:A:70:CYS:HB3	2.00	0.61
1:A:293:GLU:O	1:A:297:GLN:HB3	2.00	0.61
1:A:1390:ASN:O	1:A:1399:ARG:HD2	2.01	0.61
3:C:142:VAL:CG2	8:J:5:VAL:HG13	2.30	0.61
7:I:83:ASN:C	7:I:83:ASN:HD22	2.04	0.61
2:B:614:SER:H	2:B:632:ARG:NH1	1.98	0.61
5:F:125:LEU:HB2	5:F:130:ILE:HD11	1.83	0.61
2:B:628:THR:O	2:B:628:THR:CG2	2.48	0.61
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ALA:N	1:A:435:HIS:HD2	1.99	0.61
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.26	0.61
1:A:214:ILE:HG23	1:A:215:SER:H	1.65	0.61
1:A:1119:TYR:HD1	1:A:1326:ARG:HB3	1.65	0.61
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.48	0.61
2:B:708:GLU:HG3	2:B:709:ASP:H	1.65	0.61
2:B:976:ILE:CG2	2:B:977:GLY:N	2.63	0.61
8:J:43:ARG:CG	8:J:46:CYS:HB2	2.31	0.61
1:A:44:THR:O	1:A:45:GLN:HB2	2.01	0.61
3:C:69:LEU:O	8:J:6:ARG:HD2	2.01	0.61
1:A:259:GLU:HG2	1:A:260:ASP:H	1.66	0.61
1:A:413:ILE:N	1:A:413:ILE:HD12	2.15	0.61
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.25	0.61
2:B:65:GLU:CG	2:B:66:ASP:H	2.03	0.61
2:B:464:GLY:HA2	2:B:479:VAL:O	2.01	0.61
2:B:1020:ARG:HG3	2:B:1022:THR:HG22	1.81	0.61
3:C:142:VAL:H	8:J:16:ASP:HB3	1.65	0.61
1:A:413:ILE:CD1	1:A:413:ILE:N	2.64	0.61
2:B:826:ALA:O	2:B:1011:ILE:HA	2.01	0.61
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.30	0.61
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.83	0.60
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.83	0.60
6:H:109:LYS:HB3	6:H:110:ASP:OD2	2.00	0.60
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.34	0.60
2:B:636:PRO:CB	2:B:637:LEU:HA	2.23	0.60
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.82	0.60
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.83	0.60
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.82	0.60
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.83	0.60
2:B:918:ILE:HG13	2:B:935:ARG:HH11	1.64	0.60
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.01	0.60
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.16	0.60
1:A:256:GLN:CA	1:A:257:ARG:HB3	2.20	0.60
1:A:381:THR:HG23	1:A:383:TYR:CD1	2.36	0.60
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.84	0.60
1:A:974:ASP:OD2	1:A:977:LYS:HB2	2.01	0.60
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.01	0.60
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.32	0.60
2:B:800:GLN:CB	8:J:52:THR:HG22	2.31	0.60
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.82	0.60
3:C:258:ILE:HD11	9:K:42:LEU:CD2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.82	0.60
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.66	0.60
2:B:115:GLN:HE21	2:B:119:LEU:CD1	2.15	0.60
2:B:378:LEU:O	2:B:382:ILE:HG12	2.02	0.60
2:B:589:VAL:HG12	2:B:590:HIS:N	2.17	0.60
2:B:704:ALA:HB3	2:B:741:CYS:HB2	1.83	0.60
8:J:56:LEU:HB3	8:J:60:PHE:CE2	2.35	0.60
2:B:174:LEU:O	2:B:175:ARG:CB	2.50	0.60
2:B:520:GLY:HA2	2:B:748:ILE:HA	1.83	0.60
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.84	0.60
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.83	0.59
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.84	0.59
2:B:638:PHE:O	2:B:740:HIS:CB	2.50	0.59
3:C:184:ASN:HD21	3:C:189:THR:H	1.49	0.59
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.84	0.59
1:A:1206:ASP:C	1:A:1274:ARG:HH12	2.04	0.59
2:B:174:LEU:O	2:B:175:ARG:HB2	2.02	0.59
3:C:123:ASN:HD22	3:C:125:MET:N	2.00	0.59
1:A:452:LYS:O	2:B:1141:HIS:HE1	1.85	0.59
1:A:482:PHE:O	2:B:989:THR:HG23	2.02	0.59
1:A:407:ARG:HD3	1:A:413:ILE:CD1	2.29	0.59
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.17	0.59
1:A:821:ARG:O	1:A:825:ILE:HG12	2.02	0.59
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.66	0.59
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.67	0.59
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.38	0.59
2:B:737:THR:HG23	7:I:66:PRO:HB3	1.84	0.59
5:F:128:LYS:NZ	5:F:148:VAL:O	2.27	0.59
11:R:3:G:H22	12:T:27:DA:H1'	1.67	0.59
2:B:546:SER:OG	2:B:631:GLY:N	2.24	0.59
2:B:872:GLU:HG2	2:B:916:THR:OG1	2.01	0.59
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.85	0.59
2:B:1115:THR:HB	2:B:1117:GLN:HG3	1.83	0.59
1:A:908:LEU:HD11	1:A:983:ILE:HD11	1.82	0.59
3:C:231:ASN:C	3:C:231:ASN:ND2	2.55	0.59
1:A:18:GLN:HE21	1:A:1418:LEU:HD12	1.66	0.59
2:B:749:LEU:HD22	2:B:753:ALA:CB	2.33	0.59
2:B:803:LEU:N	2:B:822:ASN:HD21	1.99	0.59
9:K:58:PHE:HE2	9:K:74:ARG:HE	1.49	0.59
10:L:48:CYS:SG	10:L:49:LYS:N	2.74	0.59
1:A:40:THR:HG21	1:A:259:GLU:OE1	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HD3	1:A:745:GLN:NE2	2.18	0.59
2:B:955:THR:CG2	2:B:956:THR:N	2.66	0.59
1:A:447:GLN:NE2	12:T:20:DC:H4'	2.18	0.59
1:A:567:LYS:HB3	6:H:96:VAL:N	2.10	0.59
1:A:1111:MET:O	1:A:1114:PRO:HD3	2.03	0.59
1:A:1392:SER:O	1:A:1394:THR:N	2.33	0.59
2:B:737:THR:HG21	7:I:66:PRO:O	2.03	0.59
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.66	0.59
1:A:332:LYS:H	1:A:337:ARG:HB3	1.68	0.59
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.03	0.58
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.85	0.58
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.36	0.58
3:C:54:ASN:CG	3:C:54:ASN:O	2.41	0.58
6:H:93:TYR:CD2	6:H:145:ARG:HB3	2.39	0.58
2:B:211:VAL:HG23	2:B:483:LEU:HG	1.86	0.58
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.85	0.58
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.85	0.58
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.85	0.58
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.36	0.58
2:B:590:HIS:HD2	2:B:596:LEU:HD22	1.68	0.58
2:B:882:THR:HG21	2:B:935:ARG:HA	1.85	0.58
4:E:3:GLN:HG3	4:E:5:ASN:H	1.67	0.58
1:A:741:ASN:HD21	1:A:743:VAL:HG23	1.68	0.58
1:A:1032:LEU:O	1:A:1036:ARG:HG2	2.04	0.58
2:B:108:VAL:HG12	2:B:109:THR:H	1.67	0.58
2:B:706:GLN:HB3	2:B:708:GLU:HG3	1.84	0.58
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.32	0.58
4:E:29:PHE:HD1	4:E:65:THR:HG22	1.69	0.58
1:A:508:PRO:HA	1:A:511:ILE:HG13	1.84	0.58
1:A:868:TYR:HE2	1:A:1366:ARG:HD3	1.64	0.58
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.85	0.58
8:J:7:CYS:HA	8:J:49:MET:HG2	1.84	0.58
1:A:265:LYS:C	1:A:267:ALA:H	2.06	0.58
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.36	0.58
1:A:626:ASN:O	1:A:631:HIS:HD2	1.85	0.58
2:B:701:ILE:CG1	2:B:740:HIS:HE1	2.16	0.58
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.86	0.58
1:A:1119:TYR:CD1	1:A:1326:ARG:HB3	2.38	0.58
2:B:408:LEU:HG	2:B:409:ALA:H	1.69	0.58
6:H:89:LEU:C	6:H:91:ASP:H	2.07	0.58
3:C:3:GLU:HB3	9:K:104:ASN:OD1	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.34	0.57
1:A:896:ARG:NH1	1:A:897:TYR:HE1	2.01	0.57
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.86	0.57
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.85	0.57
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.84	0.57
4:E:127:ILE:O	4:E:127:ILE:HG12	2.04	0.57
1:A:1349:TYR:O	1:A:1351:GLU:N	2.37	0.57
3:C:166:GLU:O	3:C:167:HIS:CB	2.52	0.57
1:A:494:SER:O	1:A:498:ARG:HG3	2.05	0.57
2:B:841:MET:CE	2:B:990:ILE:HD11	2.34	0.57
3:C:115:SER:HB3	3:C:142:VAL:HG12	1.85	0.57
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.85	0.57
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.87	0.57
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.85	0.57
2:B:1138:MET:HA	2:B:1138:MET:CE	2.32	0.57
2:B:1155:SER:OG	2:B:1156:ASP:N	2.36	0.57
1:A:214:ILE:CG2	1:A:215:SER:N	2.67	0.57
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.53	0.57
1:A:65:LEU:O	1:A:71:GLN:HA	2.03	0.57
6:H:128:ASN:O	6:H:131:ASN:ND2	2.38	0.57
1:A:960:ILE:HG12	1:A:1049:ILE:HD11	1.86	0.57
1:A:1343:ALA:HB1	4:E:149:LEU:HB2	1.87	0.57
2:B:778:MET:O	2:B:819:ALA:HB1	2.05	0.57
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.18	0.57
4:E:94:LYS:HE2	4:E:94:LYS:HA	1.86	0.57
1:A:99:ILE:HG12	1:A:234:MET:SD	2.45	0.57
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.69	0.57
1:A:508:PRO:O	1:A:511:ILE:HG13	2.05	0.57
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.21	0.57
2:B:701:ILE:CB	2:B:740:HIS:HE1	2.18	0.57
2:B:849:GLY:HA2	2:B:852:ARG:CD	2.35	0.57
2:B:879:ARG:CZ	2:B:879:ARG:H	2.17	0.57
8:J:1:MET:H1	8:J:57:ILE:H	1.53	0.57
1:A:1435:PRO:C	1:A:1436:ILE:HD12	2.25	0.57
2:B:879:ARG:H	2:B:879:ARG:NE	2.02	0.57
5:F:111:LEU:HD12	5:F:111:LEU:N	2.12	0.57
1:A:690:VAL:HG22	1:A:718:VAL:HG22	1.86	0.57
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.35	0.57
2:B:785:TYR:CE2	8:J:60:PHE:HE1	2.23	0.57
2:B:942:ARG:CB	2:B:945:GLU:HB2	2.35	0.57
3:C:67:LEU:HD23	3:C:144:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:15:ALA:HA	4:E:140:LEU:O	2.05	0.57
1:A:619:LYS:O	1:A:623:GLY:N	2.38	0.56
2:B:516:ASN:H	2:B:516:ASN:HD22	1.51	0.56
6:H:116:TYR:O	6:H:122:LEU:HA	2.05	0.56
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.86	0.56
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.87	0.56
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.54	0.56
1:A:264:PHE:CZ	1:A:317:LYS:HB2	2.39	0.56
1:A:535:THR:HG22	1:A:616:VAL:HA	1.86	0.56
1:A:1101:LEU:O	1:A:1105:LEU:CD1	2.53	0.56
2:B:590:HIS:HD2	2:B:596:LEU:CD2	2.18	0.56
3:C:40:GLU:HA	3:C:163:ILE:CG2	2.35	0.56
5:F:155:LEU:HD23	5:F:155:LEU:H	1.69	0.56
9:K:37:LYS:O	9:K:38:GLU:HG2	2.05	0.56
1:A:57:ARG:O	1:A:68:GLN:HG2	2.05	0.56
1:A:533:LYS:HD3	1:A:745:GLN:HE22	1.69	0.56
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.87	0.56
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.39	0.56
1:A:413:ILE:HG21	1:A:424:ILE:HD11	1.87	0.56
2:B:487:THR:HG22	2:B:488:TYR:N	2.20	0.56
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.40	0.56
1:A:1095:THR:HB	1:A:1100:ARG:HD3	1.87	0.56
2:B:766:ARG:NH2	2:B:1020:ARG:HB3	2.21	0.56
2:B:1187:ASN:HD21	2:B:1190:ASP:H	1.54	0.56
1:A:99:ILE:HA	1:A:102:VAL:HG23	1.87	0.56
1:A:336:ILE:H	1:A:336:ILE:HD12	1.71	0.56
1:A:382:PRO:HA	1:A:428:TYR:HE2	1.70	0.56
1:A:471:ASN:O	1:A:474:VAL:HG12	2.06	0.56
1:A:1325:THR:HG23	1:A:1326:ARG:HG3	1.87	0.56
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.06	0.56
2:B:882:THR:HG22	2:B:883:LEU:N	2.21	0.56
3:C:231:ASN:HD22	3:C:232:VAL:N	2.03	0.56
1:A:56:PRO:O	1:A:57:ARG:HB2	2.05	0.56
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.88	0.56
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.88	0.56
1:A:508:PRO:HA	1:A:511:ILE:CG1	2.36	0.56
1:A:586:ILE:HD11	1:A:637:LYS:CG	2.36	0.56
2:B:1155:SER:OG	2:B:1156:ASP:OD2	2.24	0.56
3:C:123:ASN:ND2	3:C:125:MET:H	2.04	0.56
1:A:466:SER:HB3	2:B:1103:ILE:HG13	1.87	0.56
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:THR:OG1	2:B:188:ASP:HB2	2.05	0.55
5:F:108:PHE:O	5:F:109:VAL:HG13	2.06	0.55
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.89	0.55
6:H:17:PRO:O	6:H:19:ARG:N	2.39	0.55
1:A:590:ARG:HH22	1:A:621:THR:HA	1.70	0.55
11:R:5:A:H2'	11:R:6:G:C8	2.42	0.55
1:A:102:VAL:HB	1:A:211:PHE:HZ	1.70	0.55
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.19	0.55
1:A:858:ASN:ND2	1:A:860:LEU:H	2.03	0.55
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.06	0.55
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.07	0.55
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.45	0.55
2:B:380:TYR:HE1	2:B:579:ARG:HE	1.55	0.55
4:E:64:PRO:HD3	4:E:76:GLY:O	2.06	0.55
9:K:91:CYS:O	9:K:95:ILE:HG13	2.07	0.55
11:R:5:A:H2'	11:R:6:G:H8	1.71	0.55
12:T:6:DC:H2"	12:T:7:DA:OP2	2.07	0.55
1:A:33:ALA:HB1	1:A:35:ILE:HG12	1.87	0.55
1:A:214:ILE:HG23	1:A:215:SER:N	2.21	0.55
3:C:18:VAL:O	3:C:231:ASN:HA	2.06	0.55
1:A:423:ASP:CG	1:A:424:ILE:H	2.09	0.55
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.06	0.55
2:B:363:HIS:O	2:B:365:THR:N	2.39	0.55
3:C:184:ASN:ND2	3:C:189:THR:O	2.39	0.55
10:L:60:ARG:HG3	10:L:61:THR:N	2.21	0.55
11:R:8:G:N2	12:T:22:DT:C2	2.75	0.55
1:A:449:SER:OG	2:B:1134:GLU:HG3	2.07	0.55
1:A:1257:ASP:OD2	1:A:1257:ASP:N	2.35	0.55
3:C:92:CYS:SG	3:C:93:ASP:N	2.80	0.55
3:C:129:ILE:HG23	3:C:130:GLY:N	2.22	0.55
1:A:31:SER:HB2	1:A:82:GLY:HA2	1.87	0.55
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.42	0.55
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.89	0.55
3:C:142:VAL:HG13	3:C:143:LEU:N	2.21	0.55
8:J:1:MET:N	8:J:56:LEU:H	2.04	0.55
1:A:1329:THR:HG22	1:A:1331:SER:H	1.71	0.55
2:B:286:PHE:CZ	2:B:378:LEU:HD23	2.42	0.55
1:A:542:GLU:OE1	1:A:569:LYS:NZ	2.29	0.54
12:T:18:DG:C6	16:T:29:C7P:H2	2.42	0.54
1:A:256:GLN:HA	1:A:257:ARG:CB	2.19	0.54
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLU:O	1:A:1064:VAL:HG23	2.07	0.54
1:A:182:VAL:HG12	1:A:183:GLY:N	2.22	0.54
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.71	0.54
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.38	0.54
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.88	0.54
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.89	0.54
3:C:62:PHE:O	3:C:66:ARG:HG3	2.07	0.54
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.89	0.54
12:T:20:DC:H2'	12:T:21:DC:O4'	2.07	0.54
13:N:2:DT:H72	13:N:3:DG:H1	1.72	0.54
1:A:115:LEU:HD21	1:A:145:LYS:HE3	1.89	0.54
1:A:203:SER:O	1:A:207:ILE:HG13	2.08	0.54
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.22	0.54
2:B:313:MET:HG3	2:B:390:LEU:HD21	1.89	0.54
1:A:315:LEU:CB	1:A:316:GLN:CA	2.75	0.54
2:B:784:ASN:HD21	2:B:788:ARG:HD2	1.72	0.54
9:K:46:ILE:O	9:K:50:LEU:HB2	2.06	0.54
1:A:830:LYS:HE2	1:A:1098:VAL:HB	1.90	0.54
1:A:888:GLY:O	1:A:940:ARG:NH2	2.40	0.54
1:A:1209:MET:HE3	1:A:1228:TRP:HB2	1.90	0.54
2:B:977:GLY:HA3	2:B:1099:VAL:CG1	2.37	0.54
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.40	0.54
3:C:73:GLN:CA	3:C:133:ILE:HD11	2.36	0.54
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.90	0.54
2:B:805:THR:HG22	2:B:809:MET:SD	2.48	0.54
2:B:981:ALA:CB	2:B:987:LYS:HA	2.37	0.54
3:C:4:GLU:HG3	3:C:5:GLY:N	2.23	0.54
16:T:29:C7P:N3	16:T:29:C7P:C5	2.69	0.54
1:A:367:PRO:HD3	1:A:467:THR:O	2.08	0.53
1:A:451:HIS:HB3	1:A:453:MET:N	2.23	0.53
1:A:674:PRO:O	1:A:678:GLU:HB2	2.08	0.53
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.43	0.53
3:C:183:TRP:O	3:C:185:LYS:N	2.41	0.53
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.90	0.53
6:H:113:ALA:HA	6:H:125:LEU:O	2.09	0.53
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.90	0.53
1:A:902:LEU:O	1:A:903:ASN:CB	2.56	0.53
2:B:902:GLY:O	10:L:65:VAL:HG11	2.08	0.53
2:B:955:THR:CG2	2:B:956:THR:H	2.22	0.53
3:C:43:THR:CG2	3:C:44:LEU:H	2.21	0.53
3:C:91:HIS:HB2	3:C:96:SER:CB	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:THR:OG1	2:B:777:ALA:O	2.23	0.53
3:C:102:GLN:HG2	3:C:154:LYS:HD2	1.89	0.53
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.90	0.53
6:H:24:CYS:O	6:H:41:ASP:HA	2.09	0.53
1:A:541:ILE:N	1:A:541:ILE:HD12	2.23	0.53
1:A:1434:ALA:CB	1:A:1436:ILE:HD13	2.39	0.53
2:B:234:ILE:O	2:B:234:ILE:HG12	2.09	0.53
4:E:190:LEU:HD11	4:E:196:VAL:HG13	1.90	0.53
1:A:351:THR:HG21	1:A:466:SER:O	2.09	0.53
2:B:384:ARG:HH12	2:B:579:ARG:NH2	2.04	0.53
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.89	0.53
2:B:63:ILE:HD13	2:B:95:ILE:HD12	1.91	0.53
2:B:557:PHE:O	2:B:561:TRP:HB2	2.09	0.53
2:B:801:LYS:O	8:J:52:THR:HG23	2.08	0.53
2:B:806:THR:HG22	2:B:808:ALA:H	1.74	0.53
2:B:917:PRO:HA	2:B:934:LYS:HA	1.91	0.53
3:C:98:VAL:H	3:C:122:SER:HB3	1.73	0.53
1:A:95:PHE:O	1:A:99:ILE:HG13	2.08	0.53
1:A:125:ALA:O	1:A:128:ILE:HG22	2.07	0.53
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.09	0.53
6:H:109:LYS:HB2	6:H:111:LEU:N	2.23	0.53
1:A:401:GLY:O	1:A:435:HIS:CD2	2.60	0.53
1:A:446:ARG:NH2	11:R:10:A:O2'	2.42	0.53
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.91	0.53
1:A:1349:TYR:O	1:A:1350:LYS:C	2.45	0.53
2:B:292:ILE:HD11	2:B:327:ARG:CG	2.39	0.53
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.00	0.53
8:J:56:LEU:CB	8:J:60:PHE:HE2	2.20	0.53
1:A:339:ASN:O	2:B:1117:GLN:NE2	2.40	0.53
1:A:364:VAL:O	1:A:364:VAL:HG13	2.09	0.53
2:B:857:ARG:NH2	12:T:24:DT:OP1	2.41	0.53
1:A:369:SER:HB3	9:K:2:ASN:OD1	2.09	0.52
2:B:34:ILE:HD13	2:B:542:MET:HE3	1.91	0.52
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.90	0.52
2:B:220:GLY:O	2:B:222:ILE:HG13	2.09	0.52
2:B:416:LEU:HD22	2:B:457:LEU:HD23	1.91	0.52
2:B:485:ARG:CG	2:B:485:ARG:NH1	2.60	0.52
2:B:541:LEU:HB2	2:B:747:MET:CE	2.38	0.52
4:E:89:GLY:HA2	4:E:117:THR:OG1	2.08	0.52
1:A:33:ALA:HB3	1:A:83:HIS:H	1.74	0.52
2:B:841:MET:SD	2:B:990:ILE:HD11	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:CG2	2:B:884:ARG:H	2.22	0.52
2:B:942:ARG:HB2	2:B:945:GLU:CB	2.40	0.52
5:F:92:ARG:O	5:F:92:ARG:HG3	2.08	0.52
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.42	0.52
1:A:299:HIS:HA	1:A:302:THR:HG22	1.91	0.52
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.92	0.52
2:B:542:MET:HG3	2:B:747:MET:CE	2.40	0.52
2:B:702:LEU:HD23	2:B:737:THR:CG2	2.39	0.52
2:B:791:THR:O	2:B:792:MET:CB	2.57	0.52
7:I:8:ARG:O	7:I:9:ASP:CB	2.57	0.52
9:K:43:GLY:CA	9:K:71:PHE:CE1	2.92	0.52
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.91	0.52
1:A:705:LYS:HG3	1:A:713:SER:HB2	1.90	0.52
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.09	0.52
1:A:1017:LEU:CB	4:E:205:SER:HA	2.39	0.52
1:A:1044:TRP:O	1:A:1047:SER:N	2.42	0.52
2:B:64:CYS:O	2:B:65:GLU:CB	2.57	0.52
2:B:70:ILE:O	2:B:70:ILE:HG22	2.09	0.52
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.87	0.52
1:A:567:LYS:O	1:A:569:LYS:N	2.43	0.52
2:B:840:ILE:HG12	2:B:992:ILE:CG2	2.39	0.52
2:B:1120:GLU:O	2:B:1124:ARG:HD3	2.09	0.52
3:C:173:ALA:O	3:C:174:ALA:HB3	2.09	0.52
6:H:39:THR:O	6:H:123:MET:HA	2.10	0.52
7:I:47:GLU:HB3	7:I:50:THR:HG23	1.91	0.52
1:A:134:ARG:CD	1:A:221:SER:O	2.56	0.52
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.92	0.52
1:A:816:HIS:CE1	2:B:764:SER:H	2.27	0.52
1:A:1276:VAL:HG21	1:A:1316:VAL:HG22	1.92	0.52
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.92	0.52
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.23	0.52
4:E:168:TYR:O	4:E:169:ARG:HG2	2.09	0.52
1:A:553:VAL:HG13	1:A:648:ASN:HB3	1.91	0.52
3:C:167:HIS:ND1	10:L:70:ARG:HB3	2.24	0.52
1:A:384:ASN:HB2	1:A:387:ARG:HH21	1.75	0.52
1:A:902:LEU:O	1:A:903:ASN:HB3	2.10	0.52
2:B:214:ALA:HB2	2:B:408:LEU:HD13	1.92	0.52
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.92	0.52
4:E:156:LEU:HG	4:E:195:VAL:O	2.09	0.52
12:T:18:DG:O6	16:T:29:C7P:H2	2.10	0.52
1:A:873:MET:HG2	1:A:957:PRO:CG	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.10	0.52
2:B:384:ARG:HD2	2:B:384:ARG:N	2.25	0.52
9:K:24:ASP:CG	9:K:74:ARG:HH11	2.12	0.52
1:A:567:LYS:CB	6:H:95:TYR:HA	2.40	0.51
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.92	0.51
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.46	0.51
1:A:913:LEU:HD21	1:A:981:LEU:O	2.10	0.51
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.93	0.51
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.92	0.51
2:B:484:ASN:ND2	2:B:490:SER:OG	2.24	0.51
2:B:874:PHE:CE1	2:B:964:VAL:HG23	2.45	0.51
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.25	0.51
6:H:139:ASN:O	6:H:140:ALA:CB	2.59	0.51
2:B:416:LEU:HD11	2:B:460:ALA:HB1	1.90	0.51
2:B:770:GLN:O	2:B:770:GLN:NE2	2.43	0.51
2:B:1160:VAL:HG11	2:B:1169:MET:HG2	1.92	0.51
4:E:12:LEU:HD22	4:E:55:ARG:HH21	1.73	0.51
9:K:90:ALA:O	9:K:94:ILE:HG13	2.08	0.51
1:A:304:MET:O	1:A:326:ARG:HB2	2.10	0.51
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.92	0.51
2:B:487:THR:CG2	2:B:488:TYR:N	2.72	0.51
2:B:807:ARG:HH11	2:B:807:ARG:HG3	1.76	0.51
2:B:864:LYS:HD3	2:B:871:THR:HG23	1.92	0.51
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	2.10	0.51
3:C:8:VAL:HG11	9:K:105:PHE:CD1	2.43	0.51
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.09	0.51
2:B:859:TYR:CD1	2:B:859:TYR:N	2.78	0.51
2:B:1166:CYS:SG	2:B:1167:GLY:N	2.83	0.51
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.76	0.51
1:A:765:VAL:HG13	1:A:802:ASN:O	2.11	0.51
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.93	0.51
1:A:582:ILE:HD13	1:A:629:LEU:HD11	1.92	0.51
1:A:590:ARG:CG	1:A:590:ARG:NH1	2.74	0.51
1:A:809:THR:HB	1:A:810:PRO:HD2	1.93	0.51
1:A:1334:ASP:O	1:A:1335:ILE:C	2.49	0.51
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.11	0.51
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.43	0.51
2:B:296:GLU:O	2:B:300:HIS:HD2	1.94	0.51
2:B:1147:LEU:O	2:B:1151:LEU:HB2	2.11	0.51
8:J:43:ARG:HD2	8:J:46:CYS:SG	2.51	0.51
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:O	1:A:848:ILE:HG12	2.10	0.51
1:A:899:VAL:CG2	1:A:1029:ARG:HG3	2.41	0.51
2:B:287:ARG:HA	2:B:291:ILE:O	2.10	0.51
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.11	0.51
4:E:112:TYR:CE1	4:E:115:ASN:HA	2.46	0.51
1:A:93:VAL:HG11	1:A:305:ASP:HB3	1.92	0.51
1:A:709:THR:HG22	1:A:710:LEU:N	2.26	0.51
1:A:834:THR:HG21	1:A:1077:THR:HA	1.92	0.51
1:A:913:LEU:HD12	1:A:914:GLU:N	2.25	0.51
1:A:1101:LEU:HG	1:A:1105:LEU:CD1	2.41	0.51
2:B:847:ASP:CB	3:C:167:HIS:CD2	2.93	0.51
2:B:986:GLN:HG2	2:B:1022:THR:HG21	1.92	0.51
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.93	0.51
1:A:709:THR:HG22	1:A:710:LEU:H	1.76	0.51
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.46	0.51
1:A:1333:ILE:HG12	1:A:1381:LEU:HD12	1.93	0.51
2:B:315:LYS:N	2:B:316:PRO:HD2	2.26	0.51
2:B:863:GLU:O	2:B:961:LEU:HD22	2.11	0.51
5:F:147:SER:O	5:F:151:LEU:HD12	2.11	0.51
1:A:335:ARG:NH1	2:B:1202:LEU:CD1	2.69	0.51
1:A:347:PHE:HB2	2:B:1150:ARG:NH2	2.25	0.51
1:A:1161:THR:HG23	1:A:1239:ARG:HH21	1.74	0.51
2:B:112:LEU:HD21	2:B:117:ALA:HB2	1.93	0.51
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.09	0.51
11:R:8:G:C2	12:T:22:DT:C2	2.99	0.51
1:A:473:SER:C	1:A:475:THR:H	2.15	0.50
2:B:915:THR:HG21	2:B:934:LYS:HE3	1.93	0.50
6:H:4:THR:HG22	6:H:5:LEU:H	1.77	0.50
1:A:361:LEU:HG	1:A:361:LEU:O	2.10	0.50
1:A:381:THR:CG2	1:A:383:TYR:CD1	2.94	0.50
1:A:456:MET:HG3	1:A:478:TYR:CZ	2.46	0.50
2:B:113:TYR:O	2:B:114:PRO:C	2.47	0.50
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.24	0.50
2:B:1097:HIS:HB3	2:B:1102:LYS:CE	2.41	0.50
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.93	0.50
2:B:62:ILE:HD12	2:B:418:LYS:HG3	1.91	0.50
2:B:942:ARG:HG3	2:B:945:GLU:OE1	2.11	0.50
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.77	0.50
1:A:76:GLU:CD	2:B:1159:ARG:HH12	2.14	0.50
1:A:648:ASN:O	1:A:652:VAL:HG23	2.11	0.50
2:B:65:GLU:CG	2:B:66:ASP:N	2.69	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:LEU:HD22	2:B:491:THR:HG23	1.93	0.50
2:B:1060:ARG:C	2:B:1062:HIS:H	2.14	0.50
5:F:89:GLU:O	5:F:93:ILE:HD12	2.11	0.50
1:A:318:SER:HA	12:T:28:DT:H4'	1.92	0.50
1:A:683:ILE:HG21	1:A:801:GLU:CG	2.41	0.50
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.93	0.50
1:A:1025:ARG:O	1:A:1035:TYR:OH	2.23	0.50
2:B:1165:ILE:O	2:B:1166:CYS:C	2.48	0.50
1:A:525:GLN:HE22	1:A:752:LYS:HE2	1.77	0.50
1:A:529:CYS:SG	1:A:662:PHE:CE2	3.04	0.50
1:A:1341:ILE:HD13	1:A:1379:GLY:O	2.11	0.50
8:J:1:MET:N	8:J:57:ILE:H	2.09	0.50
2:B:762:ASN:HD21	2:B:1022:THR:HA	1.77	0.50
2:B:977:GLY:HA3	2:B:1099:VAL:HG11	1.93	0.50
2:B:992:ILE:CD1	9:K:67:PHE:CE2	2.95	0.50
1:A:129:LYS:O	1:A:130:ASP:CB	2.58	0.50
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.24	0.50
1:A:920:LEU:HD23	1:A:921:GLY:N	2.26	0.50
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.58	0.50
2:B:731:VAL:O	2:B:732:SER:HB2	2.10	0.50
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.27	0.50
2:B:955:THR:HG22	2:B:956:THR:O	2.12	0.50
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.11	0.50
1:A:51:GLY:HA2	1:A:56:PRO:HG3	1.94	0.50
1:A:609:ASP:O	1:A:611:GLN:N	2.44	0.50
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.94	0.50
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.93	0.50
2:B:827:ILE:HG22	2:B:1014:PRO:HG3	1.94	0.50
2:B:852:ARG:HG2	2:B:973:ILE:HG23	1.94	0.50
1:A:867:ILE:HD13	1:A:1014:ALA:HB2	1.94	0.49
2:B:788:ARG:NH1	2:B:790:ASP:OD2	2.44	0.49
2:B:916:THR:O	2:B:916:THR:CG2	2.57	0.49
8:J:7:CYS:HB2	8:J:49:MET:HG2	1.93	0.49
1:A:182:VAL:HG12	1:A:183:GLY:H	1.77	0.49
1:A:672:ASP:HB3	1:A:675:THR:H	1.77	0.49
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.47	0.49
1:A:982:THR:C	1:A:984:LYS:N	2.65	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.47	0.49
2:B:365:THR:HG23	2:B:367:LEU:H	1.77	0.49
4:E:29:PHE:CD1	4:E:65:THR:HG22	2.48	0.49
1:A:568:PRO:HB3	3:C:221:TYR:CE1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.27	0.49
12:T:9:DA:H2"	12:T:10:DA:C8	2.46	0.49
12:T:16:DC:H2"	12:T:17:DC:H6	1.77	0.49
1:A:367:PRO:HB3	1:A:465:TYR:O	2.12	0.49
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.93	0.49
12:T:27:DA:H2'	12:T:27:DA:N3	2.26	0.49
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.94	0.49
2:B:764:SER:O	2:B:765:PRO:C	2.49	0.49
3:C:167:HIS:CD2	3:C:168:ALA:N	2.81	0.49
1:A:315:LEU:HD22	1:A:315:LEU:H	1.77	0.49
1:A:737:LEU:O	1:A:744:LYS:HD2	2.12	0.49
1:A:979:SER:OG	1:A:980:ASP:N	2.44	0.49
1:A:996:ASN:C	1:A:998:LEU:H	2.16	0.49
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.48	0.49
2:B:722:ASP:OD2	2:B:723:VAL:HG22	2.13	0.49
2:B:997:GLU:HG3	3:C:38:ILE:HG21	1.95	0.49
3:C:27:LEU:HD12	3:C:228:PHE:CE2	2.45	0.49
4:E:6:GLU:O	4:E:9:ILE:HG22	2.13	0.49
9:K:24:ASP:CG	9:K:74:ARG:NH1	2.65	0.49
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.28	0.49
1:A:819:GLY:O	1:A:820:GLY:C	2.51	0.49
2:B:102:VAL:CG2	2:B:110:HIS:HB3	2.42	0.49
2:B:474:SER:CB	2:B:476:ARG:HG3	2.42	0.49
2:B:1006:ILE:CG2	2:B:1007:VAL:N	2.76	0.49
5:F:111:LEU:H	5:F:111:LEU:CD1	2.07	0.49
12:T:5:DC:H2"	12:T:6:DC:OP2	2.13	0.49
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.95	0.49
1:A:1062:GLU:OE2	5:F:88:TYR:OH	2.31	0.49
1:A:1443:VAL:HG22	5:F:134:ILE:HD13	1.94	0.49
2:B:20:ASP:OD2	2:B:21:GLU:N	2.45	0.49
2:B:168:GLY:H	2:B:450:ALA:HB1	1.77	0.49
2:B:496:ARG:HH12	2:B:541:LEU:HA	1.76	0.49
2:B:882:THR:HG22	2:B:884:ARG:H	1.78	0.49
2:B:979:LYS:C	2:B:980:PHE:CD1	2.86	0.49
3:C:63:ILE:O	3:C:66:ARG:N	2.44	0.49
2:B:119:LEU:HD23	2:B:953:LEU:CD1	2.43	0.49
2:B:263:GLY:O	2:B:264:SER:C	2.50	0.49
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.95	0.49
3:C:46:ILE:HD12	3:C:157:CYS:CB	2.39	0.49
6:H:108:SER:O	6:H:109:LYS:HB2	2.12	0.49
7:I:28:GLU:HB3	7:I:35:VAL:HG22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD12	1:A:218:ASP:OD1	2.12	0.49
1:A:254:GLU:HA	1:A:255:SER:HA	1.57	0.49
1:A:874:ASP:HB2	1:A:1058:VAL:HA	1.95	0.49
1:A:1116:LEU:HD13	1:A:1329:THR:OG1	2.13	0.49
2:B:293:PRO:HB2	7:I:11:ASN:O	2.13	0.49
2:B:848:ARG:NH2	2:B:996:ARG:NH1	2.60	0.49
3:C:16:ASP:O	3:C:233:GLU:HA	2.12	0.49
3:C:250:THR:HA	3:C:253:LYS:HB2	1.95	0.49
1:A:512:VAL:O	1:A:512:VAL:HG13	2.11	0.48
2:B:523:CYS:SG	2:B:750:GLY:N	2.82	0.48
2:B:802:PRO:HA	2:B:1091:TYR:CD1	2.49	0.48
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.13	0.48
7:I:7:CYS:CB	7:I:10:CYS:SG	3.01	0.48
7:I:96:SER:HB2	7:I:98:VAL:HG23	1.94	0.48
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.95	0.48
2:B:807:ARG:HG3	2:B:807:ARG:NH1	2.28	0.48
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.59	0.48
7:I:14:LEU:HD13	7:I:27:PHE:HB3	1.95	0.48
2:B:258:LEU:HD11	2:B:267:ARG:HB3	1.94	0.48
2:B:408:LEU:O	2:B:412:LEU:HD12	2.13	0.48
3:C:91:HIS:HB2	3:C:96:SER:OG	2.13	0.48
3:C:235:VAL:HG11	8:J:6:ARG:NH2	2.28	0.48
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.94	0.48
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.96	0.48
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.49	0.48
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.93	0.48
1:A:477:PRO:HG3	1:A:521:MET:SD	2.53	0.48
1:A:541:ILE:HG21	1:A:549:MET:HE1	1.96	0.48
1:A:855:THR:CG2	1:A:857:ARG:HE	2.26	0.48
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.28	0.48
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.28	0.48
4:E:7:ARG:C	4:E:9:ILE:N	2.66	0.48
4:E:161:LYS:O	4:E:163:GLU:N	2.47	0.48
12:T:5:DC:H1'	12:T:6:DC:O5'	2.13	0.48
1:A:283:GLY:O	1:A:285:PRO:HD3	2.13	0.48
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.48	0.48
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.29	0.48
2:B:984:HIS:C	2:B:986:GLN:H	2.16	0.48
8:J:26:GLN:O	8:J:26:GLN:HG3	2.14	0.48
1:A:15:LYS:HD2	2:B:1220:ARG:NH1	2.28	0.48
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:LYS:O	1:A:1093:LYS:HG3	2.13	0.48
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.44	0.48
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.78	0.48
6:H:24:CYS:HB2	6:H:44:VAL:HG23	1.95	0.48
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.44	0.48
1:A:55:ASP:O	1:A:58:LEU:N	2.34	0.48
1:A:71:GLN:HB2	1:A:72:GLU:H	1.52	0.48
1:A:821:ARG:CG	1:A:825:ILE:HD11	2.44	0.48
2:B:102:VAL:HG23	2:B:110:HIS:HB3	1.95	0.48
6:H:115:TYR:HA	6:H:123:MET:O	2.13	0.48
6:H:124:ARG:NH1	6:H:126:GLU:OE2	2.44	0.48
1:A:322:VAL:HG12	1:A:323:LYS:HE2	1.95	0.48
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.13	0.48
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.95	0.48
2:B:956:THR:HB	10:L:46:VAL:CG2	2.27	0.48
5:F:109:VAL:HG11	5:F:127:GLU:OE1	2.14	0.48
7:I:78:CYS:SG	7:I:105:SER:HB2	2.54	0.48
1:A:251:SER:H	1:A:253:ASN:ND2	2.12	0.48
2:B:708:GLU:CG	2:B:709:ASP:H	2.27	0.48
2:B:794:ASN:N	2:B:794:ASN:HD22	2.12	0.48
7:I:103:CYS:SG	7:I:104:LEU:N	2.87	0.48
8:J:6:ARG:HA	8:J:12:LYS:O	2.14	0.48
12:T:11:DC:H2"	12:T:12:DC:OP2	2.14	0.48
1:A:919:ILE:O	1:A:922:ASP:HB2	2.14	0.47
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.96	0.47
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.95	0.47
5:F:125:LEU:HB2	5:F:130:ILE:CD1	2.43	0.47
9:K:33:ILE:HD12	9:K:73:LEU:HD23	1.95	0.47
12:T:5:DC:OP2	12:T:5:DC:H2'	2.14	0.47
1:A:135:PHE:C	1:A:135:PHE:CD2	2.86	0.47
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.49	0.47
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.96	0.47
9:K:43:GLY:HA2	9:K:71:PHE:CE1	2.50	0.47
1:A:184:SER:HA	1:A:199:LEU:HD13	1.95	0.47
1:A:353:ILE:HD13	1:A:487:MET:CE	2.44	0.47
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.79	0.47
1:A:587:HIS:HA	1:A:607:ILE:O	2.14	0.47
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.95	0.47
4:E:108:GLY:O	4:E:132:ILE:HG23	2.13	0.47
1:A:372:LYS:HD3	1:A:397:ASN:HA	1.97	0.47
3:C:229:TYR:CD1	3:C:229:TYR:N	2.82	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:91:ASP:HA	6:H:93:TYR:HD1	1.79	0.47
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.50	0.47
10:L:43:THR:HG22	10:L:43:THR:O	2.14	0.47
1:A:451:HIS:HB2	1:A:454:SER:H	1.80	0.47
2:B:839:MET:O	2:B:990:ILE:HA	2.14	0.47
3:C:144:ILE:HG22	3:C:145:CYS:N	2.28	0.47
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.96	0.47
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.96	0.47
9:K:82:ASP:OD1	9:K:83:PRO:HD2	2.15	0.47
1:A:867:ILE:HG22	1:A:872:GLY:CA	2.43	0.47
2:B:119:LEU:HD23	2:B:953:LEU:HD13	1.95	0.47
3:C:164:ALA:HB2	3:C:171:GLY:HA2	1.96	0.47
5:F:147:SER:C	5:F:149:GLU:H	2.18	0.47
1:A:756:ILE:HD13	1:A:759:ALA:HB3	1.95	0.47
1:A:836:TYR:CE1	1:A:840:ARG:HD2	2.48	0.47
1:A:899:VAL:CB	1:A:929:LEU:CD1	2.85	0.47
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.95	0.47
2:B:322:PHE:O	2:B:322:PHE:CG	2.68	0.47
2:B:956:THR:CB	10:L:46:VAL:HG21	2.27	0.47
3:C:43:THR:CG2	3:C:44:LEU:N	2.77	0.47
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.97	0.47
3:C:91:HIS:HB2	3:C:96:SER:HB3	1.97	0.47
3:C:235:VAL:HG21	8:J:6:ARG:HH21	1.79	0.47
4:E:7:ARG:C	4:E:9:ILE:H	2.17	0.47
4:E:205:SER:OG	4:E:205:SER:O	2.32	0.47
12:T:16:DC:H2"	12:T:17:DC:C6	2.49	0.47
1:A:1035:TYR:O	1:A:1037:LEU:N	2.48	0.47
2:B:530:GLY:O	2:B:531:GLN:C	2.53	0.47
1:A:1441:PHE:HE1	5:F:92:ARG:HD3	1.80	0.47
2:B:296:GLU:O	2:B:300:HIS:CD2	2.68	0.47
3:C:40:GLU:HA	3:C:163:ILE:HG21	1.96	0.47
1:A:472:LEU:HD11	2:B:835:GLN:HE22	1.80	0.47
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.45	0.47
2:B:470:LYS:O	2:B:471:LYS:HG3	2.15	0.47
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.95	0.47
1:A:385:ILE:O	1:A:388:LEU:N	2.48	0.46
1:A:783:THR:CG2	1:A:815:PHE:CE2	2.89	0.46
2:B:635:ARG:HH22	2:B:742:GLU:CD	2.17	0.46
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.15	0.46
3:C:73:GLN:HE21	3:C:75:MET:N	2.14	0.46
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:7:DA:OP2	12:T:7:DA:H2'	2.15	0.46
1:A:1154:TYR:CE1	7:I:18:GLU:HG3	2.50	0.46
2:B:65:GLU:H	2:B:67:SER:HB3	1.79	0.46
2:B:175:ARG:CG	2:B:175:ARG:NH1	2.48	0.46
2:B:236:HIS:NE2	2:B:389:ALA:HA	2.30	0.46
2:B:269:ILE:CD1	2:B:386:LEU:HD21	2.45	0.46
2:B:984:HIS:CD2	2:B:1024:ALA:HB3	2.50	0.46
3:C:10:ILE:HG12	9:K:108:GLU:HB3	1.98	0.46
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.15	0.46
1:A:440:ASP:O	1:A:459:ARG:HA	2.15	0.46
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.96	0.46
2:B:619:ILE:HG13	7:I:65:ASP:HB2	1.96	0.46
2:B:739:THR:HG1	2:B:740:HIS:N	2.13	0.46
2:B:807:ARG:CG	2:B:807:ARG:NH1	2.72	0.46
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.96	0.46
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.30	0.46
1:A:1364:ASN:ND2	1:A:1366:ARG:NH1	2.52	0.46
2:B:956:THR:HA	2:B:961:LEU:O	2.15	0.46
4:E:153:HIS:O	4:E:154:ILE:HD13	2.16	0.46
9:K:18:LYS:HE3	9:K:38:GLU:CG	2.45	0.46
1:A:92:HIS:HE1	2:B:1211:ASN:HB3	1.81	0.46
1:A:397:ASN:OD1	1:A:397:ASN:N	2.49	0.46
1:A:943:LEU:O	1:A:946:VAL:N	2.45	0.46
1:A:982:THR:C	1:A:984:LYS:H	2.18	0.46
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.16	0.46
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.46	0.46
6:H:109:LYS:NZ	6:H:111:LEU:HD12	2.30	0.46
1:A:55:ASP:H	1:A:56:PRO:HD2	1.81	0.46
1:A:345:VAL:HG11	2:B:1150:ARG:O	2.16	0.46
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.98	0.46
1:A:988:LEU:HD23	1:A:988:LEU:O	2.15	0.46
3:C:99:LEU:HD12	3:C:118:LEU:HD22	1.96	0.46
1:A:250:ILE:HB	1:A:253:ASN:HD21	1.80	0.46
1:A:384:ASN:OD1	1:A:385:ILE:N	2.49	0.46
1:A:508:PRO:HA	1:A:511:ILE:HD11	1.96	0.46
1:A:856:THR:O	1:A:856:THR:HG22	2.16	0.46
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.16	0.46
2:B:755:ILE:HD11	2:B:812:LEU:HD12	1.98	0.46
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.97	0.46
3:C:77:ILE:HD12	3:C:161:LYS:HE3	1.97	0.46
9:K:43:GLY:HA3	9:K:71:PHE:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.98	0.46
12:T:8:DT:H2"	12:T:9:DA:OP2	2.16	0.46
12:T:13:DA:H2"	12:T:14:DC:OP2	2.16	0.46
1:A:230:ARG:HD2	1:A:233:TRP:CH2	2.51	0.46
1:A:679:ILE:HD11	1:A:733:ALA:HB2	1.98	0.46
1:A:809:THR:HB	1:A:810:PRO:CD	2.45	0.46
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.97	0.46
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.81	0.46
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.16	0.46
2:B:478:GLY:O	2:B:481:GLN:HG3	2.16	0.46
2:B:636:PRO:HB3	2:B:743:ILE:HD12	1.98	0.46
8:J:1:MET:H1	8:J:57:ILE:N	2.13	0.46
1:A:445:ASN:ND2	1:A:446:ARG:N	2.64	0.46
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.98	0.46
2:B:179:CYS:O	2:B:182:SER:OG	2.26	0.46
2:B:701:ILE:HB	2:B:740:HIS:CE1	2.50	0.46
2:B:1079:LYS:O	2:B:1080:LYS:C	2.53	0.46
3:C:17:ASN:OD1	3:C:233:GLU:HG3	2.16	0.46
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.45	0.46
1:A:518:LYS:HE2	1:A:624:SER:O	2.16	0.46
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.98	0.46
2:B:411:PRO:HA	2:B:414:ALA:HB3	1.98	0.46
2:B:459:TYR:HD2	2:B:459:TYR:O	1.97	0.46
2:B:833:TYR:HH	9:K:65:HIS:CD2	2.34	0.46
2:B:978:ASP:HB2	2:B:980:PHE:HE1	1.80	0.46
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.46	0.46
8:J:1:MET:O	8:J:2:ILE:O	2.34	0.46
1:A:474:VAL:HG22	1:A:478:TYR:CE1	2.51	0.45
1:A:898:ARG:NH1	1:A:930:ASP:OD1	2.41	0.45
1:A:1279:ILE:O	1:A:1279:ILE:CG2	2.64	0.45
6:H:14:GLU:HB2	6:H:27:GLU:HB3	1.98	0.45
8:J:32:GLU:CD	8:J:32:GLU:H	2.18	0.45
1:A:371:ALA:HA	1:A:436:ILE:HG22	1.99	0.45
1:A:423:ASP:O	1:A:424:ILE:HB	2.16	0.45
1:A:697:ALA:HB2	1:A:702:LEU:HG	1.98	0.45
1:A:858:ASN:C	1:A:858:ASN:ND2	2.68	0.45
1:A:1170:ILE:HD13	1:A:1170:ILE:HA	1.88	0.45
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.97	0.45
8:J:38:ARG:HE	8:J:38:ARG:HB2	1.59	0.45
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.51	0.45
1:A:526:ASP:O	1:A:527:THR:C	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:SER:O	1:A:1151:GLU:HG3	2.16	0.45
2:B:704:ALA:H	2:B:741:CYS:HA	1.81	0.45
2:B:839:MET:HB3	2:B:1012:ILE:HG22	1.98	0.45
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.46	0.45
4:E:213:ILE:HG12	4:E:214:CYS:N	2.31	0.45
1:A:568:PRO:HB2	6:H:46:LEU:HD22	1.97	0.45
1:A:816:HIS:ND1	2:B:764:SER:HB2	2.31	0.45
1:A:828:ALA:O	16:T:29:C7P:H3	2.17	0.45
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.98	0.45
2:B:27:ALA:HB2	2:B:708:GLU:CD	2.36	0.45
2:B:459:TYR:CD2	2:B:459:TYR:O	2.69	0.45
2:B:616:ILE:HD12	2:B:625:LYS:O	2.16	0.45
2:B:801:LYS:O	2:B:801:LYS:CG	2.65	0.45
2:B:848:ARG:NH1	8:J:8:PHE:O	2.49	0.45
2:B:852:ARG:NH2	10:L:70:ARG:O	2.49	0.45
1:A:554:PRO:HG3	1:A:651:LYS:HE3	1.98	0.45
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.98	0.45
2:B:20:ASP:OD2	2:B:20:ASP:C	2.55	0.45
2:B:640:VAL:HB	2:B:739:THR:O	2.17	0.45
3:C:100:THR:HG23	3:C:155:LEU:O	2.17	0.45
3:C:116:LYS:HB2	3:C:140:ASN:HA	1.98	0.45
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.98	0.45
9:K:58:PHE:O	9:K:75:ILE:HA	2.17	0.45
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.98	0.45
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.99	0.45
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.46	0.45
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.80	0.45
2:B:681:TRP:O	2:B:684:LEU:HB2	2.16	0.45
2:B:794:ASN:N	2:B:794:ASN:ND2	2.64	0.45
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.32	0.45
6:H:6:PHE:CG	6:H:7:ASP:N	2.84	0.45
1:A:694:THR:HG1	1:A:714:PHE:HE1	1.65	0.45
1:A:954:TRP:HE3	1:A:955:PRO:HD2	1.82	0.45
1:A:993:LEU:O	1:A:996:ASN:ND2	2.50	0.45
1:A:1021:LEU:O	1:A:1024:SER:N	2.50	0.45
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.99	0.45
1:A:324:SER:O	1:A:326:ARG:N	2.50	0.45
2:B:108:VAL:HG12	2:B:109:THR:N	2.31	0.45
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.99	0.45
2:B:766:ARG:HE	2:B:1020:ARG:HB2	1.82	0.45
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.06	0.45
1:A:259:GLU:HG2	1:A:260:ASP:N	2.31	0.45
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.99	0.45
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.82	0.45
1:A:1124:HIS:CD2	1:A:1124:HIS:H	2.35	0.45
2:B:882:THR:CG2	2:B:935:ARG:HA	2.46	0.45
3:C:167:HIS:CE1	10:L:70:ARG:HB3	2.52	0.45
4:E:77:SER:CB	4:E:105:PHE:HD2	2.28	0.45
1:A:402:ALA:N	1:A:435:HIS:CD2	2.80	0.44
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.51	0.44
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.30	0.44
1:A:1119:TYR:HD1	1:A:1326:ARG:CB	2.30	0.44
1:A:1150:SER:HA	1:A:1195:LEU:HD23	1.99	0.44
2:B:280:ILE:HG22	2:B:281:PRO:O	2.18	0.44
1:A:26:GLU:O	1:A:30:ILE:HB	2.17	0.44
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.98	0.44
1:A:356:ASP:HA	1:A:357:PRO:HD2	1.72	0.44
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.99	0.44
1:A:1019:CYS:HA	1:A:1022:LEU:HB3	1.99	0.44
1:A:1313:LEU:C	1:A:1315:GLU:H	2.20	0.44
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.36	0.44
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.99	0.44
6:H:6:PHE:HD2	6:H:59:ILE:HG12	1.82	0.44
13:N:6:DT:H2"	13:N:7:DA:OP2	2.17	0.44
1:A:534:LEU:O	1:A:574:GLY:HA3	2.16	0.44
1:A:913:LEU:HD12	1:A:914:GLU:H	1.83	0.44
2:B:875:GLU:O	2:B:877:PRO:HD3	2.17	0.44
2:B:1060:ARG:HD2	2:B:1060:ARG:HA	1.65	0.44
3:C:44:LEU:HD12	3:C:160:LYS:O	2.17	0.44
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.98	0.44
1:A:849:MET:HB3	1:A:1063:MET:SD	2.58	0.44
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.52	0.44
1:A:915:SER:O	1:A:919:ILE:HG12	2.17	0.44
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	2.00	0.44
2:B:90:ILE:HA	2:B:133:LYS:O	2.17	0.44
2:B:241:ARG:HA	2:B:253:THR:HG22	1.99	0.44
2:B:1156:ASP:N	2:B:1156:ASP:OD2	2.51	0.44
2:B:1160:VAL:CG1	2:B:1169:MET:HG2	2.47	0.44
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.98	0.44
1:A:71:GLN:C	1:A:73:GLY:H	2.21	0.44
1:A:304:MET:CG	2:B:1210:MET:HG3	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.52	0.44
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	2.00	0.44
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.33	0.44
2:B:384:ARG:NH1	2:B:579:ARG:HH21	2.06	0.44
2:B:840:ILE:O	2:B:1010:LEU:HD12	2.18	0.44
3:C:44:LEU:HA	3:C:160:LYS:O	2.17	0.44
6:H:7:ASP:O	6:H:8:ASP:HB2	2.17	0.44
8:J:1:MET:N	8:J:56:LEU:N	2.65	0.44
1:A:119:ASN:O	1:A:123:ARG:HG3	2.18	0.44
1:A:259:GLU:CG	1:A:260:ASP:H	2.30	0.44
1:A:851:HIS:HD2	1:A:857:ARG:CG	2.24	0.44
2:B:205:ILE:O	2:B:206:ASN:C	2.55	0.44
3:C:8:VAL:HG21	9:K:105:PHE:HB2	2.00	0.44
7:I:15:TYR:HB3	7:I:16:PRO:CD	2.48	0.44
1:A:575:LYS:CB	1:A:612:ILE:HD11	2.37	0.44
1:A:690:VAL:HG13	1:A:718:VAL:CG2	2.48	0.44
2:B:34:ILE:HD13	2:B:542:MET:CE	2.46	0.44
2:B:60:GLN:HE22	2:B:95:ILE:H	1.65	0.44
2:B:825:VAL:CG2	2:B:1010:LEU:HB3	2.47	0.44
2:B:914:LYS:O	2:B:914:LYS:HG2	2.18	0.44
5:F:147:SER:C	5:F:149:GLU:N	2.71	0.44
6:H:5:LEU:HD22	6:H:133:ASN:O	2.18	0.44
1:A:265:LYS:HE2	1:A:303:TYR:HA	2.00	0.44
1:A:348:SER:OG	2:B:1128:LEU:HB2	2.18	0.44
1:A:508:PRO:HA	1:A:511:ILE:CD1	2.48	0.44
1:A:949:ASP:OD1	1:A:949:ASP:N	2.48	0.44
2:B:884:ARG:O	2:B:936:ASP:CB	2.63	0.44
7:I:63:GLY:HA2	7:I:104:LEU:HD21	1.98	0.44
1:A:92:HIS:CD2	1:A:92:HIS:O	2.71	0.44
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.52	0.44
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.18	0.44
2:B:189:LEU:O	2:B:192:LEU:N	2.47	0.44
2:B:785:TYR:CE2	8:J:60:PHE:CE1	3.04	0.44
6:H:92:ASP:OD2	6:H:92:ASP:N	2.51	0.44
7:I:6:PHE:HB3	7:I:12:ASN:O	2.17	0.44
1:A:482:PHE:C	2:B:837:ASP:O	2.56	0.43
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.18	0.43
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.48	0.43
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.17	0.43
2:B:800:GLN:CG	8:J:52:THR:HG22	2.48	0.43
3:C:5:GLY:O	3:C:7:GLN:NE2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:TYR:HE1	4:E:78:LEU:HD13	1.79	0.43
6:H:59:ILE:O	6:H:60:ALA:HB3	2.17	0.43
6:H:82:PRO:C	6:H:84:ALA:N	2.67	0.43
7:I:119:THR:O	7:I:120:GLN:HB2	2.17	0.43
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.99	0.43
9:K:40:HIS:HE1	9:K:63:VAL:CG2	2.31	0.43
1:A:12:ARG:HB3	2:B:1218:THR:HG23	2.00	0.43
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.48	0.43
2:B:640:VAL:CG2	2:B:741:CYS:H	2.31	0.43
2:B:857:ARG:HG2	2:B:859:TYR:CE1	2.53	0.43
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.71	0.43
10:L:60:ARG:HG3	10:L:61:THR:H	1.83	0.43
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.49	0.43
2:B:1038:SER:HA	2:B:1062:HIS:HE1	1.83	0.43
3:C:35:ARG:HD3	9:K:41:THR:HA	1.99	0.43
3:C:73:GLN:HE21	3:C:75:MET:H	1.65	0.43
6:H:42:ILE:HG21	6:H:49:VAL:HG23	2.01	0.43
1:A:872:GLY:O	1:A:1058:VAL:HG23	2.19	0.43
1:A:986:ILE:HD11	1:A:1032:LEU:HD21	2.00	0.43
2:B:90:ILE:HD13	2:B:134:LYS:HA	2.00	0.43
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.99	0.43
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.82	0.43
3:C:56:THR:HG21	3:C:145:CYS:HG	1.82	0.43
3:C:210:GLU:HG3	3:C:229:TYR:OH	2.18	0.43
6:H:44:VAL:HG12	6:H:44:VAL:O	2.18	0.43
1:A:140:THR:HA	1:A:143:LYS:HE3	2.01	0.43
1:A:452:LYS:O	2:B:1141:HIS:CE1	2.67	0.43
1:A:834:THR:O	1:A:836:TYR:N	2.51	0.43
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.83	0.43
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.21	0.43
2:B:628:THR:O	2:B:628:THR:HG22	2.16	0.43
2:B:639:ILE:HD11	2:B:691:GLU:CB	2.40	0.43
2:B:878:GLN:HE21	2:B:878:GLN:HB2	1.56	0.43
2:B:941:LEU:O	2:B:942:ARG:C	2.56	0.43
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.82	0.43
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.48	0.43
3:C:178:PHE:CD2	3:C:178:PHE:C	2.92	0.43
1:A:332:LYS:O	1:A:334:GLY:N	2.51	0.43
1:A:334:GLY:O	1:A:335:ARG:C	2.56	0.43
1:A:614:PHE:CD1	1:A:614:PHE:C	2.91	0.43
1:A:913:LEU:CD1	1:A:914:GLU:H	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:LEU:HD11	1:A:1025:ARG:NH1	2.34	0.43
2:B:25:ILE:CD1	2:B:651:LEU:HD12	2.49	0.43
2:B:737:THR:O	2:B:738:PHE:C	2.57	0.43
2:B:840:ILE:CG2	2:B:999:MET:HE1	2.48	0.43
2:B:1196:ILE:HG13	2:B:1200:ALA:HB3	2.01	0.43
4:E:24:LYS:HD2	4:E:30:ILE:HB	2.01	0.43
1:A:442:VAL:HG12	1:A:491:VAL:HG22	2.01	0.43
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.54	0.43
1:A:1206:ASP:OD2	1:A:1206:ASP:N	2.51	0.43
2:B:120:ARG:NH1	10:L:54:ARG:HD2	2.34	0.43
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.54	0.43
2:B:1060:ARG:C	2:B:1062:HIS:N	2.72	0.43
9:K:83:PRO:O	9:K:86:ALA:HB3	2.19	0.43
1:A:79:GLY:C	1:A:243:PRO:HG2	2.39	0.43
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.72	0.43
1:A:741:ASN:HD22	1:A:744:LYS:H	1.67	0.43
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.34	0.43
2:B:474:SER:C	2:B:476:ARG:N	2.72	0.43
2:B:783:THR:HB	8:J:63:TYR:OH	2.18	0.43
2:B:845:SER:HB2	8:J:8:PHE:HB3	2.00	0.43
2:B:941:LEU:O	2:B:942:ARG:O	2.37	0.43
3:C:183:TRP:O	3:C:184:ASN:C	2.57	0.43
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.99	0.43
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.46	0.43
1:A:878:ILE:HG21	1:A:955:PRO:HB2	2.01	0.43
2:B:46:GLN:OE1	2:B:408:LEU:HD21	2.17	0.43
2:B:308:TRP:HA	2:B:311:LEU:HD12	2.00	0.43
2:B:516:ASN:H	2:B:516:ASN:ND2	2.15	0.43
2:B:563:MET:O	2:B:563:MET:HG3	2.16	0.43
3:C:53:THR:O	3:C:153:LEU:HA	2.19	0.43
4:E:213:ILE:HG12	4:E:214:CYS:H	1.84	0.43
1:A:218:ASP:O	1:A:222:LEU:CD1	2.65	0.43
1:A:784:LEU:HB3	1:A:786:HIS:CD2	2.54	0.43
1:A:895:LYS:HE3	1:A:895:LYS:HB2	1.73	0.43
1:A:919:ILE:HD12	1:A:925:LEU:HD12	1.99	0.43
1:A:1037:LEU:HD22	1:A:1042:PHE:HA	2.01	0.43
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.99	0.43
1:A:1128:GLN:O	1:A:1131:ALA:HB3	2.19	0.43
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.54	0.43
2:B:408:LEU:CG	2:B:409:ALA:H	2.32	0.43
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:VAL:CG2	2:B:740:HIS:HA	2.45	0.43
2:B:884:ARG:NH1	2:B:935:ARG:HE	2.17	0.43
2:B:952:VAL:HG22	2:B:966:VAL:HG13	2.01	0.43
3:C:235:VAL:HG21	8:J:6:ARG:NH2	2.33	0.43
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.49	0.43
6:H:31:THR:O	6:H:32:THR:CB	2.67	0.43
1:A:125:ALA:O	1:A:134:ARG:HG3	2.19	0.42
1:A:381:THR:CG2	1:A:383:TYR:HD1	2.31	0.42
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	2.00	0.42
1:A:1435:PRO:O	1:A:1436:ILE:HD12	2.18	0.42
2:B:470:LYS:C	2:B:472:ALA:H	2.22	0.42
4:E:85:GLU:HA	4:E:86:PRO:HD3	1.87	0.42
1:A:44:THR:O	1:A:45:GLN:CB	2.66	0.42
1:A:49:LYS:HZ1	1:A:60:SER:HA	1.79	0.42
1:A:347:PHE:HE2	1:A:375:THR:HG22	1.83	0.42
1:A:586:ILE:HD11	1:A:637:LYS:HG3	2.01	0.42
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.67	0.42
1:A:867:ILE:HG22	1:A:872:GLY:HA2	2.01	0.42
2:B:756:ILE:HG12	2:B:770:GLN:CG	2.48	0.42
2:B:792:MET:HB2	2:B:792:MET:HE3	1.97	0.42
2:B:1079:LYS:HE3	3:C:188:HIS:ND1	2.35	0.42
4:E:13:TRP:CD2	4:E:39:LEU:HD13	2.54	0.42
1:A:335:ARG:O	1:A:336:ILE:C	2.56	0.42
1:A:709:THR:HG23	7:I:94:ASP:HA	2.01	0.42
1:A:868:TYR:CE2	1:A:1366:ARG:CD	2.88	0.42
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.19	0.42
3:C:148:ARG:HB3	3:C:151:GLN:HG3	2.01	0.42
4:E:64:PRO:HG2	4:E:69:ILE:HD11	2.01	0.42
1:A:350:ARG:HA	1:A:487:MET:O	2.19	0.42
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.59	0.42
1:A:690:VAL:HG13	1:A:718:VAL:HG21	2.01	0.42
1:A:784:LEU:C	1:A:786:HIS:H	2.23	0.42
1:A:1144:LYS:HE3	2:B:262:GLU:OE2	2.20	0.42
2:B:862:GLN:HG3	2:B:963:PHE:HD1	1.83	0.42
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.02	0.42
2:B:1106:ARG:HD3	2:B:1127:GLY:CA	2.50	0.42
4:E:199:ILE:O	4:E:199:ILE:CG2	2.66	0.42
8:J:43:ARG:HG3	8:J:46:CYS:HB2	2.02	0.42
1:A:388:LEU:O	1:A:391:LEU:N	2.52	0.42
1:A:535:THR:HG21	1:A:617:VAL:N	2.31	0.42
1:A:779:PHE:CZ	2:B:517:THR:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:VAL:HG12	1:A:1407:GLU:OE2	2.19	0.42
2:B:54:PHE:O	2:B:56:ASP:N	2.53	0.42
2:B:273:LEU:HD23	2:B:274:PRO:HD2	2.02	0.42
3:C:32:SER:HA	3:C:35:ARG:HG3	2.01	0.42
9:K:18:LYS:HE3	9:K:38:GLU:HG2	2.01	0.42
1:A:91:PHE:H	1:A:297:GLN:NE2	2.17	0.42
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.50	0.42
1:A:765:VAL:HG23	1:A:800:VAL:HB	1.97	0.42
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.01	0.42
2:B:65:GLU:N	2:B:67:SER:HB3	2.33	0.42
2:B:770:GLN:HG2	2:B:983:ARG:O	2.20	0.42
2:B:874:PHE:CE1	2:B:964:VAL:CG2	3.02	0.42
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.34	0.42
3:C:129:ILE:CG2	3:C:130:GLY:N	2.82	0.42
6:H:32:THR:HG22	6:H:33:GLN:HG2	2.01	0.42
6:H:42:ILE:HG21	6:H:49:VAL:CG2	2.50	0.42
7:I:7:CYS:SG	7:I:8:ARG:O	2.77	0.42
8:J:10:CYS:SG	8:J:43:ARG:HD3	2.59	0.42
9:K:18:LYS:C	9:K:19:LEU:HD23	2.40	0.42
11:R:3:G:N2	12:T:27:DA:H1'	2.32	0.42
1:A:423:ASP:CG	1:A:424:ILE:N	2.73	0.42
1:A:709:THR:CG2	7:I:94:ASP:HA	2.48	0.42
1:A:801:GLU:HG2	1:A:801:GLU:O	2.19	0.42
1:A:857:ARG:HB3	1:A:863:VAL:HA	2.01	0.42
2:B:277:LYS:H	2:B:277:LYS:HD2	1.84	0.42
2:B:472:ALA:O	2:B:474:SER:N	2.52	0.42
2:B:477:ALA:HB1	2:B:499:ASN:HD21	1.85	0.42
4:E:36:GLU:O	4:E:38:PRO:HD3	2.20	0.42
4:E:61:GLN:HB3	4:E:79:TRP:CE3	2.55	0.42
4:E:152:LYS:HG3	4:E:154:ILE:HD11	2.02	0.42
1:A:503:GLN:NE2	5:F:90:ARG:HH21	2.18	0.42
1:A:542:GLU:O	1:A:546:VAL:HG23	2.19	0.42
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.49	0.42
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.85	0.42
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.40	0.42
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.49	0.42
2:B:37:PHE:O	2:B:38:PHE:CB	2.66	0.42
2:B:739:THR:HG1	2:B:740:HIS:CE1	2.38	0.42
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.85	0.42
3:C:91:HIS:CG	3:C:158:VAL:HG11	2.54	0.42
4:E:55:ARG:HA	4:E:58:MET:HE3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:HE	1:A:387:ARG:HB3	1.61	0.42
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.47	0.42
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.35	0.42
1:A:705:LYS:HG3	1:A:713:SER:CB	2.50	0.42
2:B:361:LEU:O	2:B:363:HIS:O	2.38	0.42
2:B:851:PHE:HB3	2:B:1094:ARG:HD2	2.01	0.42
2:B:981:ALA:O	2:B:982:SER:C	2.57	0.42
2:B:1175:LEU:O	2:B:1176:ASN:HB3	2.20	0.42
3:C:18:VAL:HG22	3:C:240:VAL:HB	2.01	0.42
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.48	0.42
6:H:82:PRO:O	6:H:83:GLN:CB	2.68	0.42
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.87	0.42
9:K:6:ARG:HB3	9:K:6:ARG:HH11	1.85	0.42
13:N:9:DG:H2"	13:N:10:DG:C8	2.55	0.42
1:A:368:LYS:HB2	1:A:368:LYS:HE2	1.82	0.42
1:A:810:PRO:HA	2:B:1047:PHE:CE2	2.55	0.42
1:A:907:THR:HG22	1:A:908:LEU:N	2.34	0.42
2:B:44:VAL:O	2:B:45:SER:C	2.57	0.42
2:B:273:LEU:HB2	2:B:276:ILE:HD12	2.02	0.42
2:B:789:MET:HE3	2:B:965:LYS:HB3	2.02	0.42
2:B:890:TYR:O	2:B:893:LEU:HD12	2.20	0.42
3:C:261:ALA:HA	3:C:264:GLN:NE2	2.35	0.42
8:J:43:ARG:HB3	8:J:43:ARG:CZ	2.50	0.42
12:T:14:DC:H2"	12:T:15:DC:OP2	2.19	0.42
1:A:112:LYS:NZ	1:A:164:ARG:HD2	2.35	0.41
1:A:413:ILE:H	1:A:413:ILE:HD13	1.80	0.41
1:A:874:ASP:CA	1:A:1058:VAL:HG22	2.50	0.41
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.53	0.41
2:B:235:SER:HB3	2:B:261:ARG:HA	2.01	0.41
2:B:769:TYR:O	2:B:771:SER:N	2.53	0.41
3:C:131:HIS:O	3:C:132:PRO:C	2.59	0.41
4:E:62:ALA:HB3	4:E:78:LEU:HB3	2.02	0.41
1:A:261:ASP:CB	1:A:323:LYS:HD2	2.35	0.41
1:A:383:TYR:HB3	5:F:115:THR:HG22	2.03	0.41
1:A:384:ASN:O	1:A:385:ILE:C	2.59	0.41
1:A:535:THR:O	1:A:575:LYS:HE2	2.19	0.41
1:A:874:ASP:N	1:A:1058:VAL:HG22	2.36	0.41
1:A:955:PRO:O	1:A:956:LEU:HG	2.20	0.41
3:C:3:GLU:CG	3:C:4:GLU:H	2.28	0.41
8:J:5:VAL:O	8:J:6:ARG:O	2.39	0.41
9:K:38:GLU:CD	9:K:42:LEU:HD22	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:58:PHE:HE2	9:K:74:ARG:NE	2.16	0.41
9:K:63:VAL:HG23	9:K:63:VAL:O	2.20	0.41
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.55	0.41
1:A:443:LEU:HD23	1:A:444:PHE:N	2.35	0.41
1:A:855:THR:HG21	1:A:857:ARG:HE	1.85	0.41
1:A:947:PHE:CE2	1:A:954:TRP:CE2	3.07	0.41
1:A:961:ARG:O	1:A:965:GLN:HG3	2.20	0.41
1:A:986:ILE:HG21	1:A:1028:THR:HA	2.02	0.41
1:A:1131:ALA:HB1	1:A:1284:MET:SD	2.60	0.41
1:A:1438:THR:HG23	5:F:92:ARG:HD2	2.02	0.41
2:B:475:SER:O	2:B:477:ALA:N	2.53	0.41
2:B:634:TYR:CE1	2:B:692:TYR:CG	3.08	0.41
2:B:639:ILE:CD1	2:B:691:GLU:HB2	2.39	0.41
2:B:705:MET:HE3	2:B:705:MET:HA	2.01	0.41
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.86	0.41
2:B:831:SER:OG	2:B:994:TYR:OH	2.31	0.41
2:B:1097:HIS:HB3	2:B:1102:LYS:HE2	2.03	0.41
3:C:58:LEU:HD11	8:J:2:ILE:HD13	2.02	0.41
4:E:14:ARG:NH2	4:E:141:VAL:HG12	2.34	0.41
6:H:4:THR:HA	6:H:60:ALA:HA	2.01	0.41
9:K:57:LEU:HB2	9:K:76:GLN:HG2	2.01	0.41
9:K:77:THR:HG21	9:K:86:ALA:HB2	2.02	0.41
10:L:55:ILE:H	10:L:55:ILE:HG12	1.65	0.41
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.48	0.41
1:A:834:THR:O	1:A:837:ILE:N	2.54	0.41
1:A:1171:GLN:HE21	1:A:1171:GLN:HB3	1.71	0.41
1:A:1349:TYR:C	1:A:1351:GLU:N	2.71	0.41
2:B:383:ASN:HD22	2:B:384:ARG:HD2	1.84	0.41
2:B:1033:LYS:HE2	2:B:1087:PHE:O	2.20	0.41
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.50	0.41
6:H:94:ASP:N	6:H:94:ASP:OD1	2.52	0.41
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	2.03	0.41
1:A:56:PRO:O	1:A:57:ARG:CB	2.68	0.41
1:A:215:SER:HB3	1:A:218:ASP:HB2	2.02	0.41
1:A:382:PRO:CA	1:A:428:TYR:HE2	2.33	0.41
1:A:414:ASP:OD1	1:A:416:ARG:HG3	2.21	0.41
1:A:709:THR:HB	1:A:712:GLU:H	1.86	0.41
2:B:216:GLU:HB2	2:B:406:LEU:HD22	2.02	0.41
2:B:493:SER:OG	2:B:775:LYS:HE2	2.20	0.41
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.55	0.41
2:B:867:GLY:C	2:B:869:SER:H	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1100:ASP:OD1	9:K:1:MET:HB3	2.20	0.41
4:E:46:TYR:CD2	4:E:58:MET:HG2	2.55	0.41
11:R:8:G:C2'	11:R:9:G:H5'	2.51	0.41
1:A:456:MET:HB2	1:A:478:TYR:OH	2.20	0.41
1:A:770:VAL:C	1:A:772:GLY:H	2.22	0.41
1:A:947:PHE:HE2	1:A:954:TRP:CD2	2.38	0.41
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.86	0.41
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.56	0.41
5:F:85:MET:SD	5:F:153:VAL:HG22	2.60	0.41
10:L:40:LEU:HD11	10:L:49:LYS:HE2	2.03	0.41
1:A:18:GLN:HB3	2:B:1215:ARG:HD2	2.02	0.41
1:A:332:LYS:C	1:A:334:GLY:H	2.24	0.41
1:A:550:LEU:HD21	1:A:561:PRO:CD	2.50	0.41
1:A:672:ASP:HB2	1:A:736:ASN:CG	2.41	0.41
1:A:963:ILE:HD12	1:A:1049:ILE:HG13	2.02	0.41
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.54	0.41
2:B:473:MET:C	2:B:475:SER:H	2.24	0.41
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.52	0.41
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.92	0.41
3:C:119:VAL:O	3:C:121:VAL:HG23	2.19	0.41
11:R:5:A:C2	11:R:6:G:C5	3.08	0.41
1:A:265:LYS:HD2	1:A:302:THR:HG23	2.02	0.41
1:A:711:ARG:HG3	7:I:97:MET:CE	2.50	0.41
2:B:181:LEU:H	2:B:181:LEU:HG	1.53	0.41
7:I:7:CYS:O	7:I:11:ASN:HA	2.20	0.41
1:A:90:VAL:HA	1:A:204:THR:HG21	2.03	0.41
1:A:313:GLN:HB3	1:A:314:ALA:H	1.54	0.41
1:A:406:ILE:HD11	1:A:412:ARG:HH12	1.86	0.41
1:A:1158:PRO:HB3	1:A:1188:GLN:OE1	2.21	0.41
2:B:228:LYS:NZ	2:B:234:ILE:HD11	2.36	0.41
2:B:240:ILE:O	2:B:240:ILE:HG23	2.21	0.41
2:B:1023:VAL:O	2:B:1023:VAL:HG12	2.21	0.41
2:B:1028:GLU:HG2	2:B:1090:THR:HG23	2.02	0.41
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.02	0.41
3:C:120:ILE:H	3:C:120:ILE:HG12	1.57	0.41
3:C:265:MET:C	3:C:267:GLN:H	2.23	0.41
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.55	0.41
1:A:25:GLU:O	1:A:29:ALA:HB3	2.20	0.41
1:A:80:HIS:H	1:A:80:HIS:CD2	2.39	0.41
1:A:335:ARG:HB3	1:A:336:ILE:H	1.64	0.41
1:A:523:ILE:HG22	1:A:528:LEU:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:LYS:HD3	1:A:1092:LYS:HA	1.90	0.41
1:A:1337:GLU:O	4:E:183:PRO:HG3	2.21	0.41
2:B:1064:TYR:N	2:B:1064:TYR:CD1	2.89	0.41
3:C:41:ILE:HG13	3:C:172:PRO:CG	2.51	0.41
4:E:24:LYS:HB3	4:E:30:ILE:HD13	2.02	0.41
5:F:81:THR:HG1	5:F:144:GLU:CD	2.22	0.41
1:A:15:LYS:HG2	2:B:1218:THR:O	2.21	0.40
1:A:99:ILE:O	1:A:102:VAL:HG23	2.21	0.40
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.21	0.40
1:A:770:VAL:O	1:A:772:GLY:N	2.54	0.40
1:A:845:LEU:O	1:A:846:GLU:C	2.59	0.40
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	2.03	0.40
2:B:101:MET:SD	2:B:109:THR:HG23	2.60	0.40
2:B:410:GLY:O	2:B:413:LEU:N	2.52	0.40
2:B:915:THR:HB	2:B:934:LYS:CB	2.52	0.40
4:E:164:LEU:HD22	4:E:211:TYR:CD2	2.55	0.40
6:H:99:GLY:HA3	6:H:118:PHE:CD2	2.56	0.40
7:I:26:LEU:HB3	7:I:35:VAL:CG1	2.51	0.40
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.49	0.40
1:A:445:ASN:HD22	1:A:446:ARG:N	2.19	0.40
1:A:451:HIS:CB	1:A:454:SER:H	2.34	0.40
1:A:595:THR:HG1	1:A:603:ASN:HB3	1.84	0.40
1:A:1193:LEU:C	1:A:1193:LEU:HD12	2.40	0.40
1:A:1438:THR:HB	2:B:1144:ALA:HB3	2.02	0.40
2:B:408:LEU:HD22	2:B:545:ILE:CD1	2.43	0.40
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.86	0.40
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.70	0.40
3:C:241:ASP:O	3:C:245:VAL:HG23	2.22	0.40
1:A:356:ASP:CB	1:A:359:LEU:HD12	2.52	0.40
1:A:475:THR:HG22	1:A:476:SER:N	2.36	0.40
2:B:94:LYS:HD2	2:B:96:TYR:CE2	2.57	0.40
2:B:849:GLY:CA	2:B:852:ARG:HD2	2.48	0.40
4:E:147:HIS:O	4:E:148:GLU:C	2.59	0.40
10:L:38:LEU:CD2	10:L:48:CYS:HA	2.52	0.40
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.86	0.40
1:A:171:GLN:HA	1:A:172:PRO:HD3	1.84	0.40
1:A:853:ASP:OD1	1:A:855:THR:HB	2.21	0.40
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	2.01	0.40
1:A:1438:THR:HG23	5:F:92:ARG:HB2	2.03	0.40
2:B:517:THR:C	2:B:519:TRP:H	2.25	0.40
3:C:166:GLU:O	3:C:167:HIS:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:41:ASP:OD2	6:H:122:LEU:N	2.52	0.40
7:I:37:GLU:H	7:I:37:GLU:HG2	1.64	0.40
1:A:660:ASN:HD22	1:A:660:ASN:C	2.25	0.40
2:B:242:SER:OG	2:B:252:SER:O	2.27	0.40
2:B:284:ILE:HD11	2:B:321:GLY:HA2	2.02	0.40
2:B:815:ARG:H	2:B:815:ARG:HG2	1.42	0.40
2:B:848:ARG:NE	8:J:11:GLY:HA2	2.36	0.40
2:B:1131:GLY:HA3	2:B:1134:GLU:OE1	2.22	0.40
4:E:54:GLN:HA	4:E:54:GLN:HE21	1.87	0.40
6:H:98:TYR:HD1	6:H:141:TYR:CE1	2.39	0.40
9:K:40:HIS:CE1	9:K:63:VAL:HG21	2.57	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	1383/1733 (80%)	1080 (78%)	219 (16%)	84 (6%)	1 17
2	B	1088/1224 (89%)	855 (79%)	169 (16%)	64 (6%)	1 18
3	C	264/318 (83%)	213 (81%)	38 (14%)	13 (5%)	2 21
4	E	212/215 (99%)	178 (84%)	25 (12%)	9 (4%)	3 25
5	F	82/155 (53%)	65 (79%)	13 (16%)	4 (5%)	2 21
6	H	129/146 (88%)	97 (75%)	19 (15%)	13 (10%)	0 8
7	I	117/122 (96%)	87 (74%)	21 (18%)	9 (8%)	1 12
8	J	63/70 (90%)	54 (86%)	5 (8%)	4 (6%)	1 17
9	K	112/120 (93%)	94 (84%)	15 (13%)	3 (3%)	5 35
10	L	44/70 (63%)	26 (59%)	14 (32%)	4 (9%)	1 9
All	All	3494/4173 (84%)	2749 (79%)	538 (15%)	207 (6%)	1 18

All (207) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	56	PRO
1	A	57	ARG
1	A	93	VAL
1	A	130	ASP
1	A	214	ILE
1	A	226	GLU
1	A	253	ASN
1	A	256	GLN
1	A	257	ARG
1	A	312	PRO
1	A	315	LEU
1	A	321	PRO
1	A	335	ARG
1	A	385	ILE
1	A	399	HIS
1	A	404	TYR
1	A	567	LYS
1	A	597	LEU
1	A	672	ASP
1	A	846	GLU
1	A	986	ILE
1	A	1036	ARG
1	A	1062	GLU
1	A	1280	GLU
1	A	1335	ILE
1	A	1393	ASN
2	B	55	VAL
2	B	65	GLU
2	B	249	ARG
2	B	473	MET
2	B	476	ARG
2	B	480	SER
2	B	531	GLN
2	B	563	MET
2	B	636	PRO
2	B	643	ASP
2	B	731	VAL
2	B	879	ARG
2	B	942	ARG
2	B	958	GLN
2	B	982	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1165	ILE
3	C	110	THR
3	C	142	VAL
3	C	167	HIS
3	C	184	ASN
3	C	215	GLU
4	E	3	GLN
4	E	59	SER
4	E	206	GLY
5	F	73	ALA
5	F	74	ILE
5	F	128	LYS
6	H	32	THR
6	H	61	SER
6	H	77	ARG
6	H	82	PRO
6	H	90	ALA
6	H	135	LEU
6	H	140	ALA
7	I	9	ASP
7	I	15	TYR
8	J	2	ILE
8	J	6	ARG
8	J	8	PHE
1	A	45	GLN
1	A	50	ILE
1	A	55	ASP
1	A	248	PRO
1	A	254	GLU
1	A	258	GLY
1	A	336	ILE
1	A	465	TYR
1	A	517	ASN
1	A	609	ASP
1	A	610	GLY
1	A	628	GLY
1	A	824	LEU
1	A	903	ASN
1	A	958	VAL
1	A	983	ILE
1	A	1002	GLY
1	A	1049	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1314	SER
1	A	1395	GLY
1	A	1437	GLY
2	B	100	PRO
2	B	264	SER
2	B	489	SER
2	B	575	PRO
2	B	708	GLU
2	B	737	THR
2	B	738	PHE
2	B	774	GLY
2	B	1021	MET
2	B	1103	ILE
2	B	1181	GLU
3	C	212	PRO
3	C	227	THR
4	E	162	ARG
5	F	111	LEU
6	H	3	ASN
6	H	18	GLY
6	H	108	SER
7	I	3	THR
7	I	11	ASN
7	I	16	PRO
9	K	50	LEU
10	L	45	ALA
1	A	63	ARG
1	A	66	LYS
1	A	71	GLN
1	A	89	PRO
1	A	168	GLY
1	A	178	GLY
1	A	245	PRO
1	A	419	LYS
1	A	568	PRO
1	A	835	GLY
1	A	854	ASN
1	A	972	HIS
1	A	1122	PRO
1	A	1221	LYS
1	A	1270	ASN
2	B	38	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	67	SER
2	B	318	VAL
2	B	577	ALA
2	B	712	PRO
2	B	732	SER
2	B	792	MET
2	B	869	SER
2	B	959	ASP
2	B	1046	PRO
2	B	1175	LEU
2	B	1176	ASN
3	C	197	SER
3	C	240	VAL
4	E	50	MET
6	H	43	ASN
6	H	132	LEU
7	I	20	LYS
9	K	53	ASP
10	L	47	ARG
1	A	333	GLU
1	A	424	ILE
1	A	441	PRO
1	A	823	GLY
1	A	834	THR
1	A	1388	GLY
2	B	364	ILE
2	B	394	ASP
2	B	467	GLY
2	B	518	HIS
2	B	635	ARG
2	B	641	GLU
2	B	735	ALA
2	B	770	GLN
2	B	799	PRO
2	B	842	ASN
2	B	865	LYS
2	B	901	PRO
2	B	1080	LYS
2	B	1178	ASN
3	C	267	GLN
4	E	148	GLU
4	E	183	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	131	ASN
7	I	34	TYR
7	I	42	LEU
9	K	10	PHE
10	L	56	LEU
1	A	324	SER
1	A	591	PHE
1	A	639	PRO
1	A	820	GLY
1	A	1174	PHE
2	B	54	PHE
2	B	175	ARG
2	B	363	HIS
2	B	410	GLY
2	B	648	HIS
2	B	1061	GLU
2	B	1143	ALA
3	C	174	ALA
4	E	86	PRO
1	A	578	LEU
1	A	987	VAL
3	C	88	CYS
10	L	59	ALA
2	B	1017	ILE
7	I	84	VAL
1	A	331	GLY
1	A	775	ILE
1	A	1435	PRO
2	B	436	VAL
8	J	57	ILE
1	A	51	GLY
1	A	325	ILE
1	A	338	GLY
2	B	647	GLY
4	E	76	GLY
1	A	1384	VAL
2	B	724	ASP
3	C	130	GLY
1	A	948	VAL

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	1218/1520 (80%)	1012 (83%)	206 (17%)	2 13
2	B	960/1061 (90%)	776 (81%)	184 (19%)	1 9
3	C	234/274 (85%)	198 (85%)	36 (15%)	2 18
4	E	196/197 (100%)	175 (89%)	21 (11%)	6 33
5	F	74/137 (54%)	58 (78%)	16 (22%)	1 7
6	H	117/128 (91%)	101 (86%)	16 (14%)	3 22
7	I	113/116 (97%)	95 (84%)	18 (16%)	2 16
8	J	60/65 (92%)	45 (75%)	15 (25%)	0 4
9	K	99/102 (97%)	87 (88%)	12 (12%)	5 26
10	L	40/57 (70%)	26 (65%)	14 (35%)	0 1
All	All	3111/3657 (85%)	2573 (83%)	538 (17%)	2 12

All (538) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	22	PHE
1	A	26	GLU
1	A	28	ARG
1	A	32	VAL
1	A	34	LYS
1	A	40	THR
1	A	43	GLU
1	A	44	THR
1	A	47	ARG
1	A	63	ARG
1	A	67	CYS
1	A	68	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	THR
1	A	70	CYS
1	A	71	GLN
1	A	74	MET
1	A	80	HIS
1	A	98	LYS
1	A	100	LYS
1	A	102	VAL
1	A	110	CYS
1	A	133	LYS
1	A	169	ASN
1	A	180	LYS
1	A	204	THR
1	A	206	GLU
1	A	208	LEU
1	A	214	ILE
1	A	222	LEU
1	A	225	ASN
1	A	235	ILE
1	A	237	THR
1	A	239	LEU
1	A	247	ARG
1	A	250	ILE
1	A	254	GLU
1	A	257	ARG
1	A	263	THR
1	A	270	LEU
1	A	271	LYS
1	A	289	ILE
1	A	297	GLN
1	A	303	TYR
1	A	304	MET
1	A	306	ASN
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	318	SER
1	A	322	VAL
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	LEU
1	A	354	SER
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	387	ARG
1	A	389	THR
1	A	391	LEU
1	A	397	ASN
1	A	403	LYS
1	A	413	ILE
1	A	416	ARG
1	A	419	LYS
1	A	433	GLU
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	450	LEU
1	A	454	SER
1	A	460	VAL
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	476	SER
1	A	494	SER
1	A	501	LEU
1	A	523	ILE
1	A	525	GLN
1	A	533	LYS
1	A	536	LEU
1	A	538	ASP
1	A	550	LEU
1	A	560	ILE
1	A	573	SER
1	A	576	GLN
1	A	577	ILE
1	A	582	ILE
1	A	590	ARG
1	A	596	THR
1	A	599	SER
1	A	601	LYS
1	A	612	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	618	GLU
1	A	629	LEU
1	A	660	ASN
1	A	666	ILE
1	A	670	ILE
1	A	676	MET
1	A	695	LYS
1	A	702	LEU
1	A	711	ARG
1	A	728	LYS
1	A	732	LEU
1	A	734	GLU
1	A	735	VAL
1	A	738	LYS
1	A	743	VAL
1	A	754	SER
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	788	SER
1	A	795	GLU
1	A	806	ARG
1	A	821	ARG
1	A	827	THR
1	A	829	VAL
1	A	830	LYS
1	A	855	THR
1	A	856	THR
1	A	857	ARG
1	A	858	ASN
1	A	864	ILE
1	A	880	LYS
1	A	882	SER
1	A	884	ASP
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	911	SER
1	A	913	LEU
1	A	918	GLU
1	A	922	ASP
1	A	929	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	936	LEU
1	A	948	VAL
1	A	949	ASP
1	A	976	THR
1	A	982	THR
1	A	996	ASN
1	A	1001	ARG
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1037	LEU
1	A	1049	ILE
1	A	1067	LEU
1	A	1081	LEU
1	A	1094	VAL
1	A	1095	THR
1	A	1104	ILE
1	A	1110	ASN
1	A	1118	VAL
1	A	1128	GLN
1	A	1142	THR
1	A	1146	VAL
1	A	1170	ILE
1	A	1172	LEU
1	A	1173	HIS
1	A	1187	GLN
1	A	1193	LEU
1	A	1203	ASN
1	A	1206	ASP
1	A	1208	THR
1	A	1221	LYS
1	A	1256	GLU
1	A	1257	ASP
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1280	GLU
1	A	1281	ARG
1	A	1285	MET
1	A	1295	THR
1	A	1297	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1301	GLU
1	A	1307	GLU
1	A	1314	SER
1	A	1322	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1354	ASN
1	A	1359	ASP
1	A	1361	SER
1	A	1368	MET
1	A	1376	THR
1	A	1382	THR
1	A	1384	VAL
1	A	1386	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1406	VAL
1	A	1411	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1445	ILE
2	B	22	SER
2	B	25	ILE
2	B	26	THR
2	B	28	GLU
2	B	34	ILE
2	B	41	LYS
2	B	66	ASP
2	B	67	SER
2	B	94	LYS
2	B	97	VAL
2	B	98	THR
2	B	104	GLU
2	B	106	ASP
2	B	109	THR
2	B	120	ARG
2	B	128	LEU
2	B	131	ASP
2	B	134	LYS
2	B	165	VAL
2	B	175	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	179	CYS
2	B	181	LEU
2	B	188	ASP
2	B	194	GLU
2	B	199	MET
2	B	208	SER
2	B	217	ARG
2	B	218	SER
2	B	223	VAL
2	B	225	VAL
2	B	234	ILE
2	B	246	LYS
2	B	248	SER
2	B	249	ARG
2	B	261	ARG
2	B	262	GLU
2	B	264	SER
2	B	268	THR
2	B	272	THR
2	B	273	LEU
2	B	277	LYS
2	B	283	VAL
2	B	294	ASP
2	B	305	VAL
2	B	306	ASN
2	B	313	MET
2	B	314	LEU
2	B	315	LYS
2	B	322	PHE
2	B	347	LYS
2	B	365	THR
2	B	368	GLU
2	B	372	SER
2	B	373	ARG
2	B	382	ILE
2	B	384	ARG
2	B	387	LEU
2	B	391	ASP
2	B	396	ASP
2	B	399	ASP
2	B	404	LYS
2	B	415	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	422	LYS
2	B	424	LEU
2	B	429	PHE
2	B	451	LYS
2	B	454	THR
2	B	459	TYR
2	B	463	THR
2	B	469	GLN
2	B	471	LYS
2	B	479	VAL
2	B	482	VAL
2	B	485	ARG
2	B	490	SER
2	B	498	THR
2	B	513	GLN
2	B	527	THR
2	B	529	GLU
2	B	537	LYS
2	B	544	CYS
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	556	THR
2	B	563	MET
2	B	570	VAL
2	B	591	ARG
2	B	603	LEU
2	B	616	ILE
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
2	B	641	GLU
2	B	643	ASP
2	B	653	VAL
2	B	665	GLU
2	B	666	TYR
2	B	668	ASP
2	B	682	SER
2	B	686	ASN
2	B	701	ILE
2	B	732	SER
2	B	737	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	740	HIS
2	B	741	CYS
2	B	751	VAL
2	B	754	SER
2	B	762	ASN
2	B	764	SER
2	B	778	MET
2	B	783	THR
2	B	791	THR
2	B	792	MET
2	B	794	ASN
2	B	801	LYS
2	B	807	ARG
2	B	812	LEU
2	B	815	ARG
2	B	821	GLN
2	B	822	ASN
2	B	825	VAL
2	B	831	SER
2	B	844	SER
2	B	859	TYR
2	B	866	TYR
2	B	868	MET
2	B	873	THR
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	894	ASP
2	B	911	ILE
2	B	914	LYS
2	B	934	LYS
2	B	939	THR
2	B	944	THR
2	B	945	GLU
2	B	953	LEU
2	B	959	ASP
2	B	967	ARG
2	B	970	THR
2	B	973	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	976	ILE
2	B	983	ARG
2	B	984	HIS
2	B	986	GLN
2	B	989	THR
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1019	SER
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU
2	B	1040	ASN
2	B	1051	THR
2	B	1061	GLU
2	B	1065	GLN
2	B	1082	MET
2	B	1092	TYR
2	B	1093	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1132	GLU
2	B	1135	ARG
2	B	1138	MET
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1160	VAL
2	B	1170	THR
2	B	1181	GLU
2	B	1183	LYS
2	B	1191	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1221	SER
3	C	18	VAL
3	C	23	SER
3	C	25	VAL
3	C	26	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	40	GLU
3	C	53	THR
3	C	56	THR
3	C	77	ILE
3	C	86	CYS
3	C	89	GLU
3	C	92	CYS
3	C	99	LEU
3	C	119	VAL
3	C	120	ILE
3	C	123	ASN
3	C	129	ILE
3	C	137	LYS
3	C	140	ASN
3	C	142	VAL
3	C	144	ILE
3	C	149	LYS
3	C	154	LYS
3	C	156	THR
3	C	157	CYS
3	C	163	ILE
3	C	166	GLU
3	C	183	TRP
3	C	199	LYS
3	C	215	GLU
3	C	227	THR
3	C	231	ASN
3	C	233	GLU
3	C	240	VAL
3	C	244	VAL
3	C	265	MET
3	C	268	ASP
4	E	2	ASP
4	E	4	GLU
4	E	7	ARG
4	E	9	ILE
4	E	37	LEU
4	E	41	ASP
4	E	50	MET
4	E	54	GLN
4	E	61	GLN
4	E	84	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	94	LYS
4	E	98	ILE
4	E	101	GLN
4	E	107	THR
4	E	110	PHE
4	E	127	ILE
4	E	131	THR
4	E	150	VAL
4	E	169	ARG
4	E	184	VAL
4	E	191	LYS
5	F	72	LYS
5	F	79	ARG
5	F	81	THR
5	F	82	THR
5	F	90	ARG
5	F	92	ARG
5	F	97	ARG
5	F	109	VAL
5	F	111	LEU
5	F	112	GLU
5	F	119	ARG
5	F	120	ILE
5	F	123	LYS
5	F	125	LEU
5	F	128	LYS
5	F	155	LEU
6	H	2	SER
6	H	11	GLN
6	H	15	VAL
6	H	26	ILE
6	H	31	THR
6	H	33	GLN
6	H	54	SER
6	H	77	ARG
6	H	89	LEU
6	H	92	ASP
6	H	94	ASP
6	H	95	TYR
6	H	110	ASP
6	H	130	ARG
6	H	132	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	136	LYS
7	I	6	PHE
7	I	8	ARG
7	I	13	MET
7	I	14	LEU
7	I	28	GLU
7	I	29	CYS
7	I	30	ARG
7	I	40	SER
7	I	50	THR
7	I	52	ILE
7	I	70	ARG
7	I	81	ARG
7	I	83	ASN
7	I	84	VAL
7	I	91	ARG
7	I	95	THR
7	I	106	CYS
7	I	107	SER
8	J	1	MET
8	J	2	ILE
8	J	7	CYS
8	J	10	CYS
8	J	13	VAL
8	J	14	VAL
8	J	23	ASN
8	J	28	ASP
8	J	31	ASP
8	J	34	THR
8	J	37	SER
8	J	43	ARG
8	J	48	ARG
8	J	55	ASP
8	J	64	ASN
9	K	6	ARG
9	K	18	LYS
9	K	19	LEU
9	K	21	ILE
9	K	46	ILE
9	K	49	GLU
9	K	75	ILE
9	K	78	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	K	81	TYR
9	K	101	LEU
9	K	106	GLU
9	K	113	THR
10	L	27	LEU
10	L	30	ILE
10	L	38	LEU
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	47	ARG
10	L	50	ASP
10	L	51	CYS
10	L	55	ILE
10	L	61	THR
10	L	65	VAL
10	L	66	GLN
10	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	ASN
1	A	83	HIS
1	A	92	HIS
1	A	109	HIS
1	A	118	HIS
1	A	169	ASN
1	A	225	ASN
1	A	297	GLN
1	A	390	GLN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	503	GLN
1	A	631	HIS
1	A	660	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	851	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	858	ASN
1	A	926	GLN
1	A	965	GLN
1	A	996	ASN
1	A	1078	GLN
1	A	1110	ASN
1	A	1124	HIS
1	A	1171	GLN
1	A	1173	HIS
1	A	1232	ASN
1	A	1258	HIS
1	A	1312	ASN
1	A	1364	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	60	GLN
2	B	115	GLN
2	B	121	ASN
2	B	206	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	366	GLN
2	B	383	ASN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	573	GLN
2	B	590	HIS
2	B	657	HIS
2	B	740	HIS
2	B	744	HIS
2	B	762	ASN
2	B	794	ASN
2	B	822	ASN
2	B	862	GLN
2	B	878	GLN
2	B	986	GLN
2	B	1015	HIS
2	B	1062	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1065	GLN
2	B	1076	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1179	GLN
2	B	1187	ASN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	135	GLN
3	C	167	HIS
3	C	188	HIS
3	C	203	GLN
3	C	224	GLN
3	C	231	ASN
3	C	242	GLN
3	C	264	GLN
4	E	54	GLN
4	E	61	GLN
4	E	101	GLN
4	E	104	ASN
4	E	114	ASN
4	E	147	HIS
6	H	11	GLN
6	H	33	GLN
6	H	137	GLN
7	I	83	ASN
7	I	89	GLN
9	K	40	HIS
9	K	65	HIS
9	K	89	ASN
10	L	53	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	2	U
11	R	9	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 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	$\#\|Z\| > 2$
16	C7P	T	29	12	3,9,10	0.20	0	2,11,14	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	C7P	T	29	12	-	-	0/0/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	29	C7P	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1395/1733 (80%)	-0.37	18 (1%) 77 61	50, 115, 229, 314	0
2	B	1106/1224 (90%)	-0.48	6 (0%) 91 82	50, 103, 169, 240	0
3	C	266/318 (83%)	-0.54	0 100 100	69, 105, 142, 159	0
4	E	214/215 (99%)	-0.14	4 (1%) 66 49	91, 175, 245, 258	0
5	F	84/155 (54%)	-0.34	0 100 100	88, 118, 148, 152	0
6	H	133/146 (91%)	-0.17	1 (0%) 86 73	117, 162, 209, 217	0
7	I	119/122 (97%)	-0.22	0 100 100	104, 143, 186, 208	0
8	J	65/70 (92%)	-0.68	0 100 100	67, 86, 118, 130	0
9	K	114/120 (95%)	-0.53	0 100 100	67, 109, 139, 151	0
10	L	46/70 (65%)	-0.01	3 (6%) 18 9	78, 155, 178, 185	0
11	R	10/10 (100%)	0.72	0 100 100	183, 210, 307, 319	0
12	T	28/28 (100%)	0.68	1 (3%) 42 27	199, 326, 403, 414	0
13	N	14/14 (100%)	0.44	0 100 100	313, 367, 380, 399	0
All	All	3594/4225 (85%)	-0.38	33 (0%) 84 71	50, 116, 220, 414	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	8.5
1	A	44	THR	4.3
1	A	286	HIS	4.3
1	A	149	GLU	4.2
2	B	866	TYR	3.7
1	A	316	GLN	3.4
2	B	1223	ASP	3.3
1	A	59	GLY	3.1
1	A	161	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1175	SER	2.7
4	E	126	SER	2.7
1	A	175	ARG	2.5
2	B	865	LYS	2.5
2	B	1221	SER	2.5
1	A	173	THR	2.5
1	A	254	GLU	2.4
1	A	73	GLY	2.4
2	B	1220	ARG	2.4
1	A	152	VAL	2.4
6	H	86	ASP	2.4
4	E	2	ASP	2.4
1	A	112	LYS	2.3
1	A	45	GLN	2.3
1	A	1126	ALA	2.2
4	E	82	PHE	2.2
1	A	69	THR	2.2
10	L	26	THR	2.2
12	T	2	DT	2.2
2	B	643	ASP	2.1
4	E	110	PHE	2.1
10	L	25	ALA	2.1
1	A	317	LYS	2.1
10	L	27	LEU	2.1

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
16	C7P	T	29	9/10	0.90	0.34	314,324,360,369	1
14	ZN	A	1734	1/1	0.93	0.05	90,90,90,90	1
14	ZN	L	105	1/1	0.94	0.06	106,106,106,106	1
14	ZN	J	101	1/1	0.97	0.16	87,87,87,87	1
14	ZN	A	1735	1/1	0.97	0.08	103,103,103,103	1
14	ZN	C	319	1/1	0.97	0.03	83,83,83,83	0
14	ZN	I	203	1/1	0.98	0.08	81,81,81,81	0
14	ZN	B	1307	1/1	0.98	0.10	95,95,95,95	1
15	MG	A	2001	1/1	0.99	0.15	9,9,9,9	0
14	ZN	I	204	1/1	0.99	0.03	81,81,81,81	1

6.5 Other polymers (i)

There are no such residues in this entry.