Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2024 – 07:21 AM EST

PDB ID	:	4LLG
Title	:	Crystal Structure Analysis of the E.coli holoenzyme/Gp2 complex
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2013-07-09
Resolution	:	3.79 Å(reported)

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

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

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

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

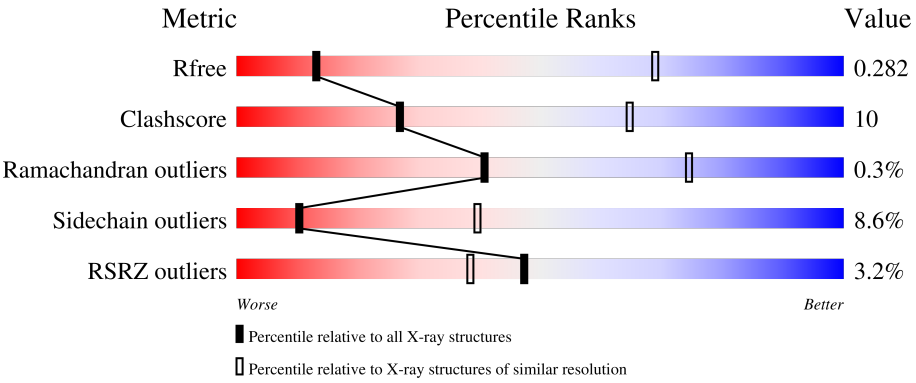
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.79 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.



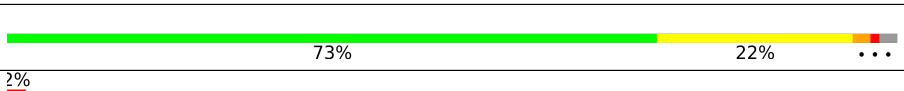
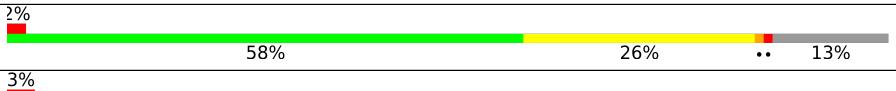
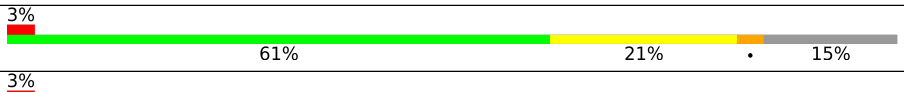
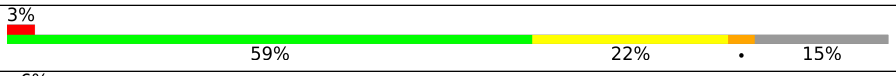
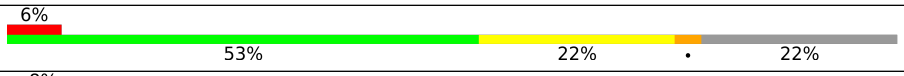
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	239	63% 26% 5% 6%
1	B	239	7% 58% 31% • 8%
1	G	239	% 64% 27% • 5%
1	H	239	3% 59% 29% • 9%
2	C	1342	2% 71% 27% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	
6	M	64	
6	N	64	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 59147 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP C9QXI7
A	236	VAL	-	expression tag	UNP C9QXI7
A	237	LEU	-	expression tag	UNP C9QXI7
A	238	PHE	-	expression tag	UNP C9QXI7
A	239	GLN	-	expression tag	UNP C9QXI7
B	235	GLU	-	expression tag	UNP C9QXI7
B	236	VAL	-	expression tag	UNP C9QXI7
B	237	LEU	-	expression tag	UNP C9QXI7
B	238	PHE	-	expression tag	UNP C9QXI7
B	239	GLN	-	expression tag	UNP C9QXI7
G	235	GLU	-	expression tag	UNP C9QXI7
G	236	VAL	-	expression tag	UNP C9QXI7
G	237	LEU	-	expression tag	UNP C9QXI7
G	238	PHE	-	expression tag	UNP C9QXI7
G	239	GLN	-	expression tag	UNP C9QXI7
H	235	GLU	-	expression tag	UNP C9QXI7
H	236	VAL	-	expression tag	UNP C9QXI7
H	237	LEU	-	expression tag	UNP C9QXI7
H	238	PHE	-	expression tag	UNP C9QXI7
H	239	GLN	-	expression tag	UNP C9QXI7

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1345	Total	C	N	O	S	0	0	0
			10447	6560	1864	1974	49			
3	J	1325	Total	C	N	O	S	0	0	0
			10295	6470	1831	1945	49			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	521	Total	C	N	O	S	0	0	0
			4161	2609	735	791	26			
5	L	519	Total	C	N	O	S	0	0	0
			4155	2605	733	791	26			

- Molecule 6 is a protein called Bacterial RNA polymerase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	50	Total	C	N	O	S	0	0	0
			406	264	63	78	1			
6	N	48	Total	C	N	O	S	0	0	0
			389	253	60	75	1			

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

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

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

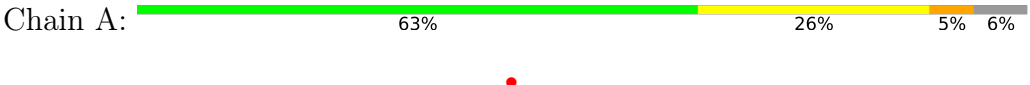
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	2	Total Zn 2 2	0	0
8	J	2	Total Zn 2 2	0	0

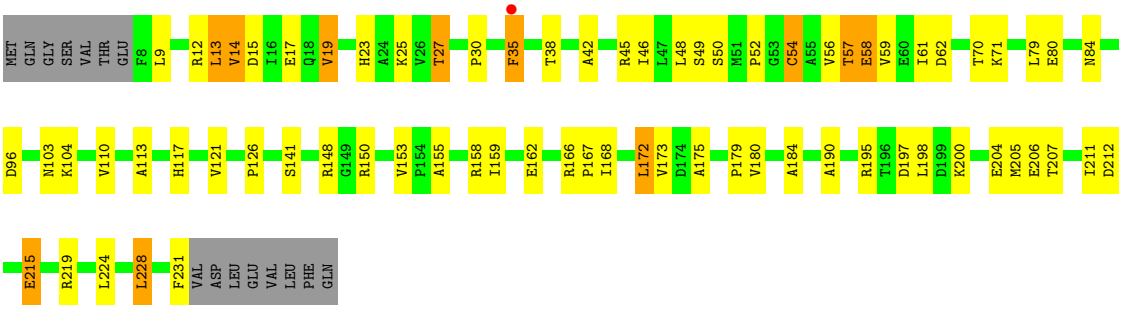
3 Residue-property plots (i)

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 subunit alpha

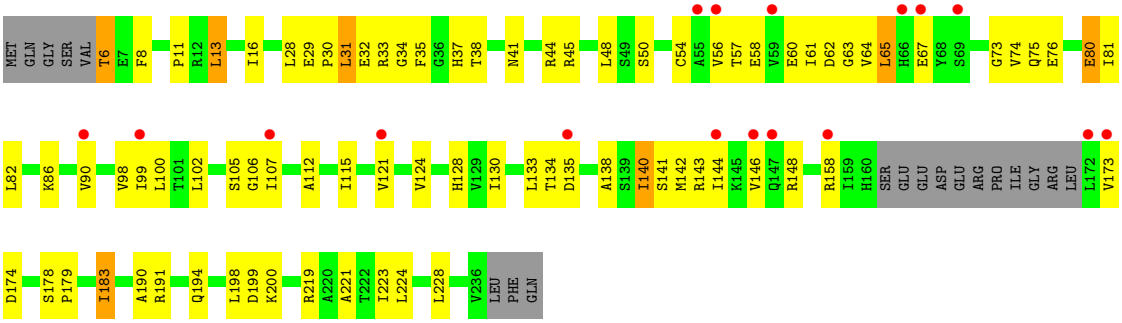
Chain A:





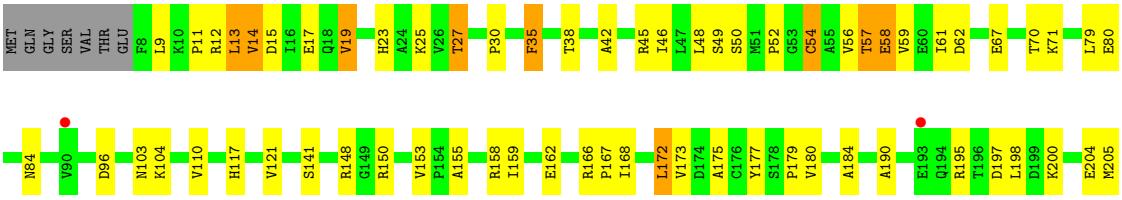
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



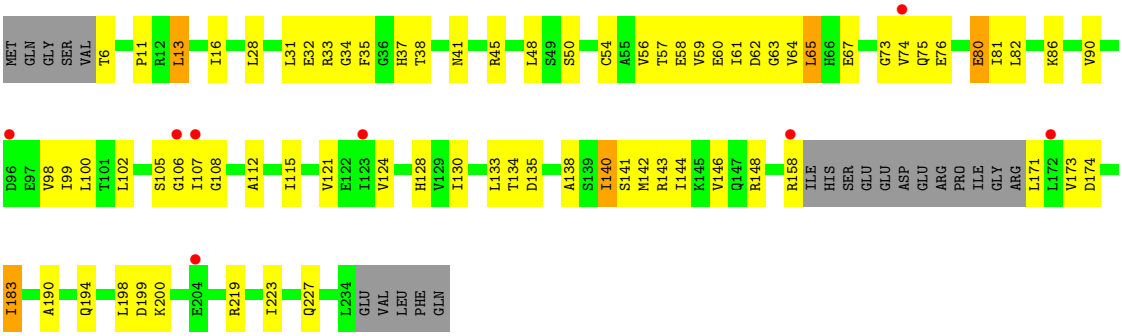
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



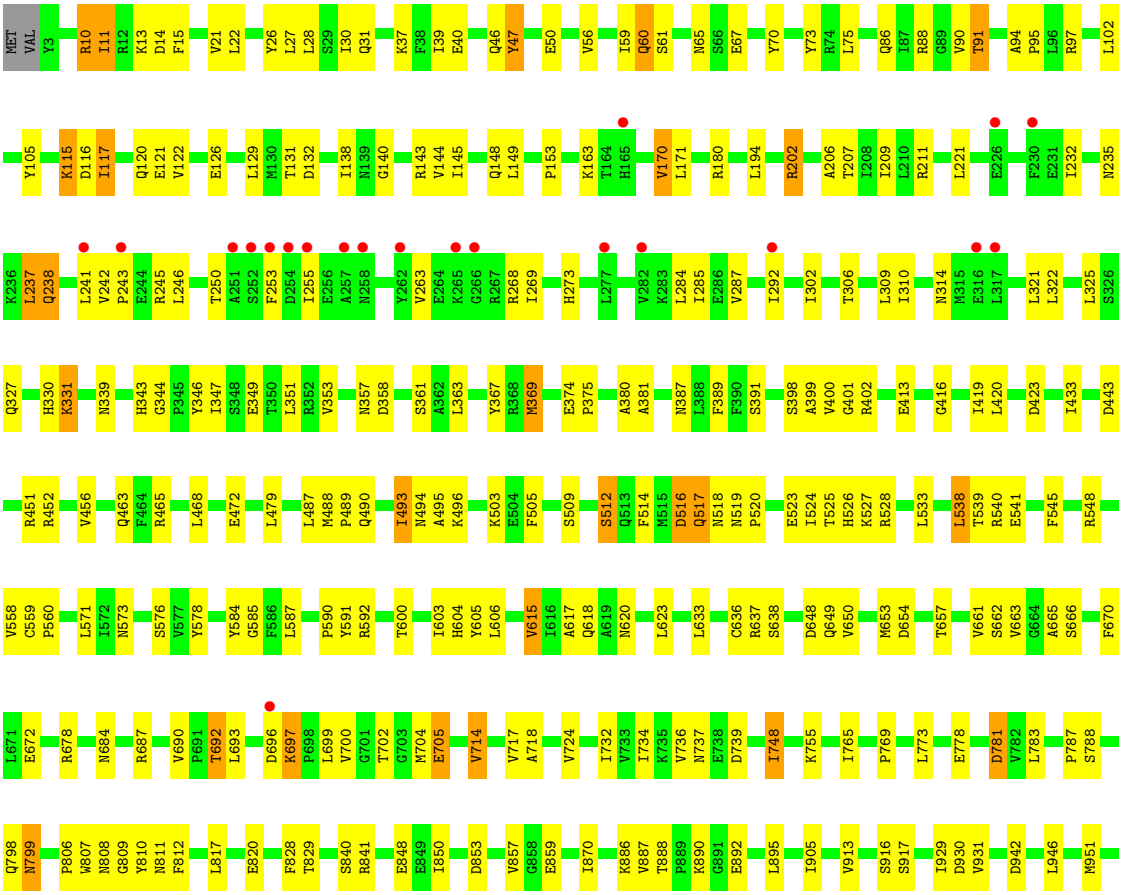
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H:



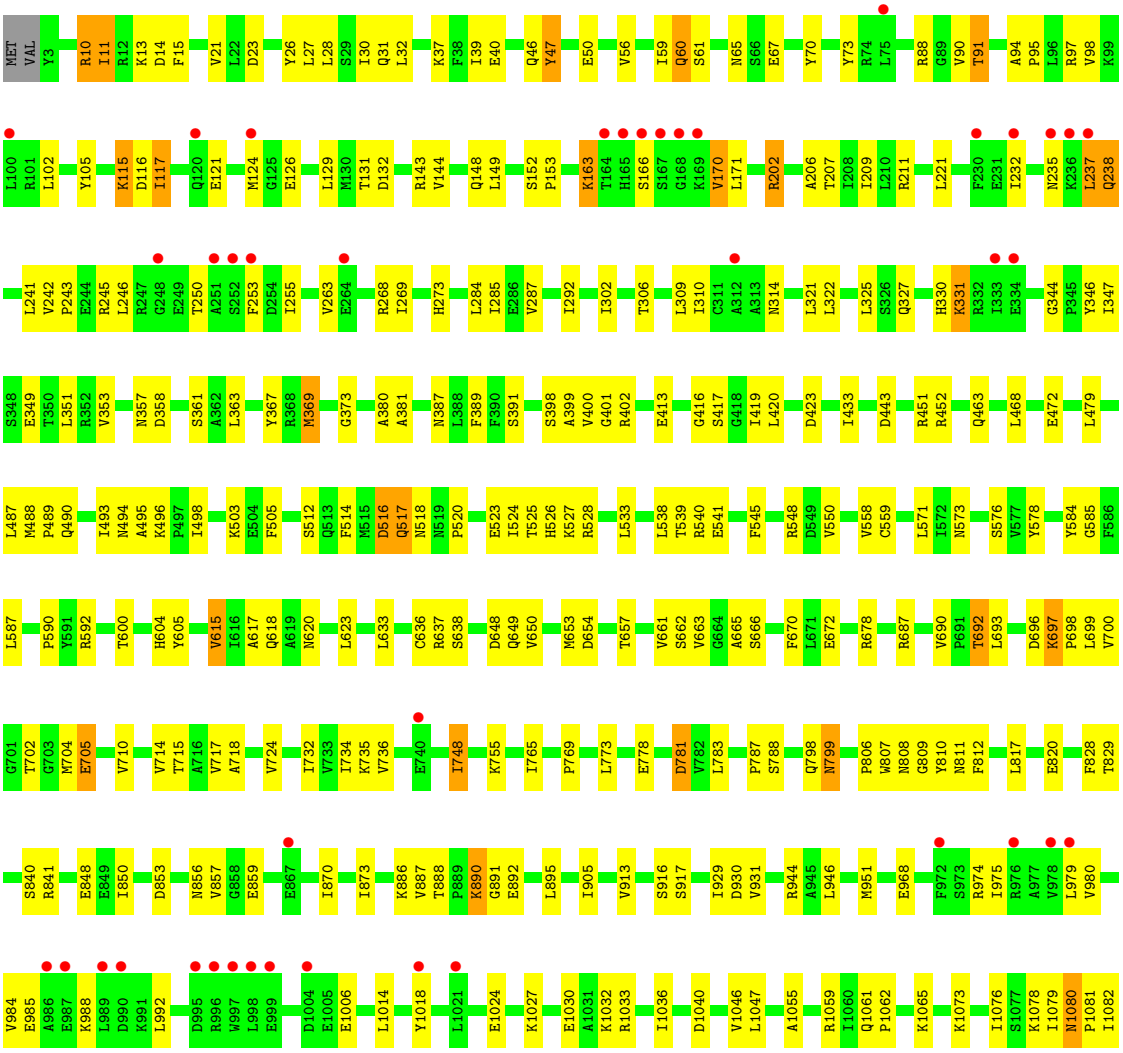
• Molecule 2: DNA-directed RNA polymerase subunit beta

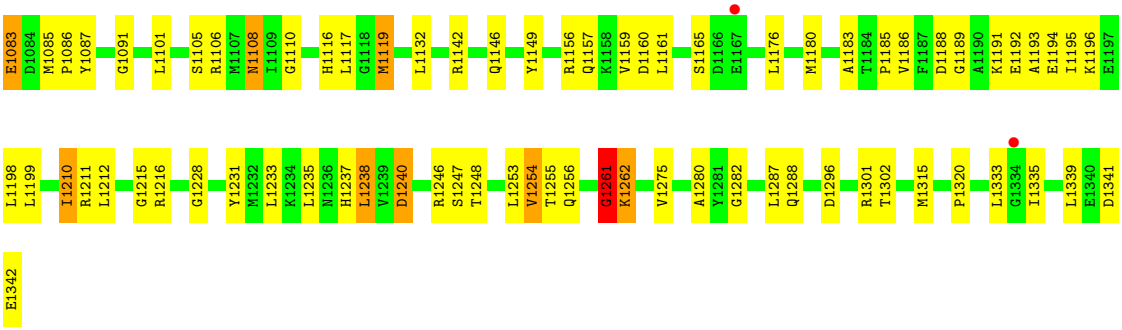
Chain C:



• Molecule 2: DNA-directed RNA polymerase subunit beta

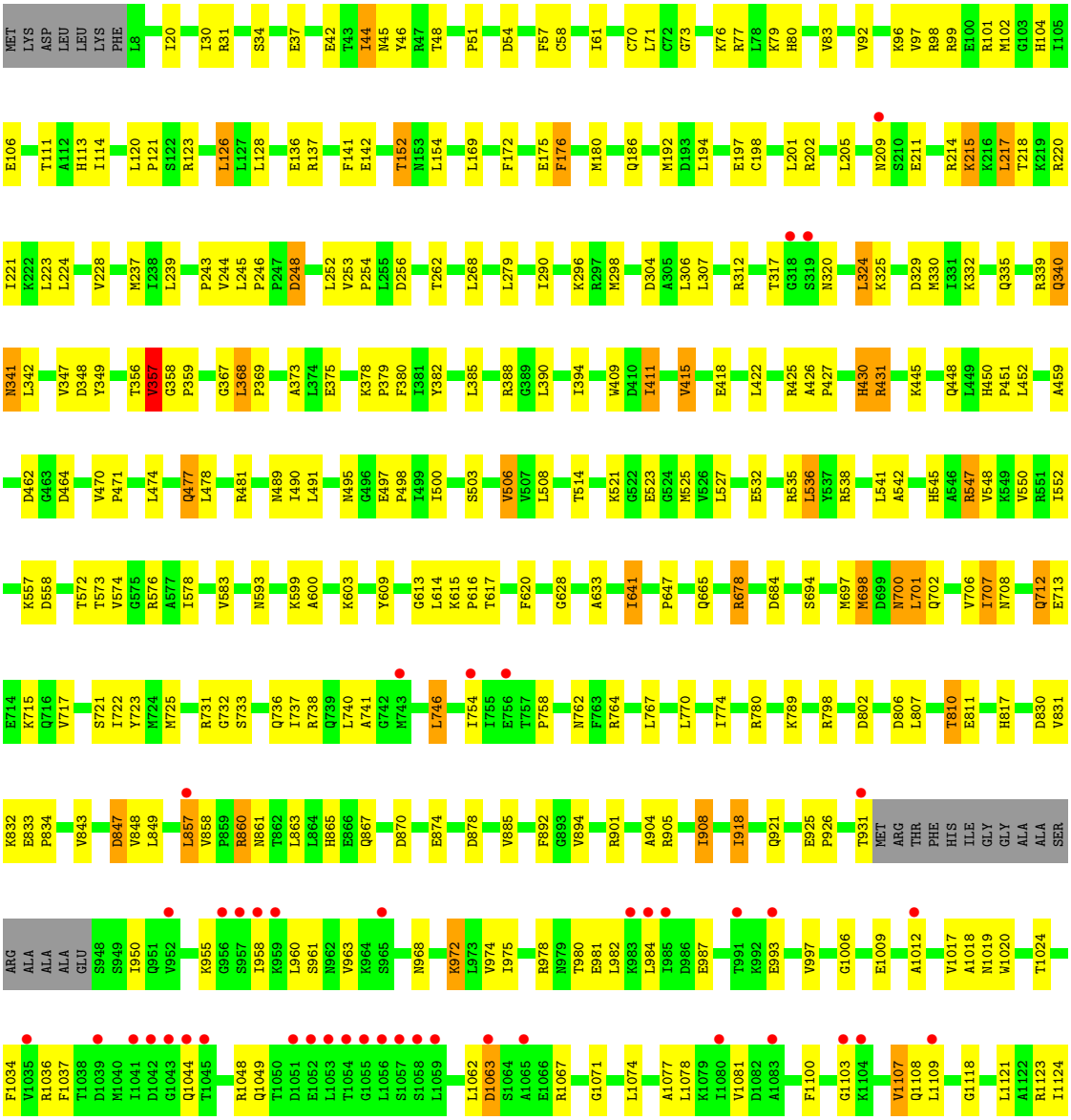
Chain I:

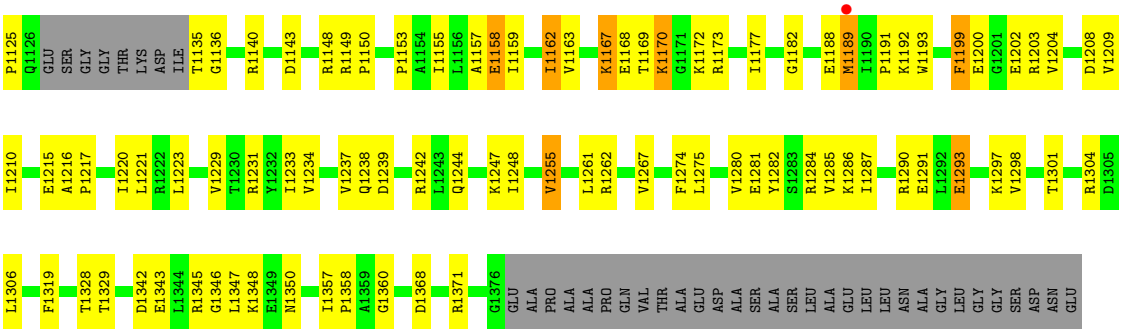




• Molecule 3: DNA-directed RNA polymerase subunit beta'

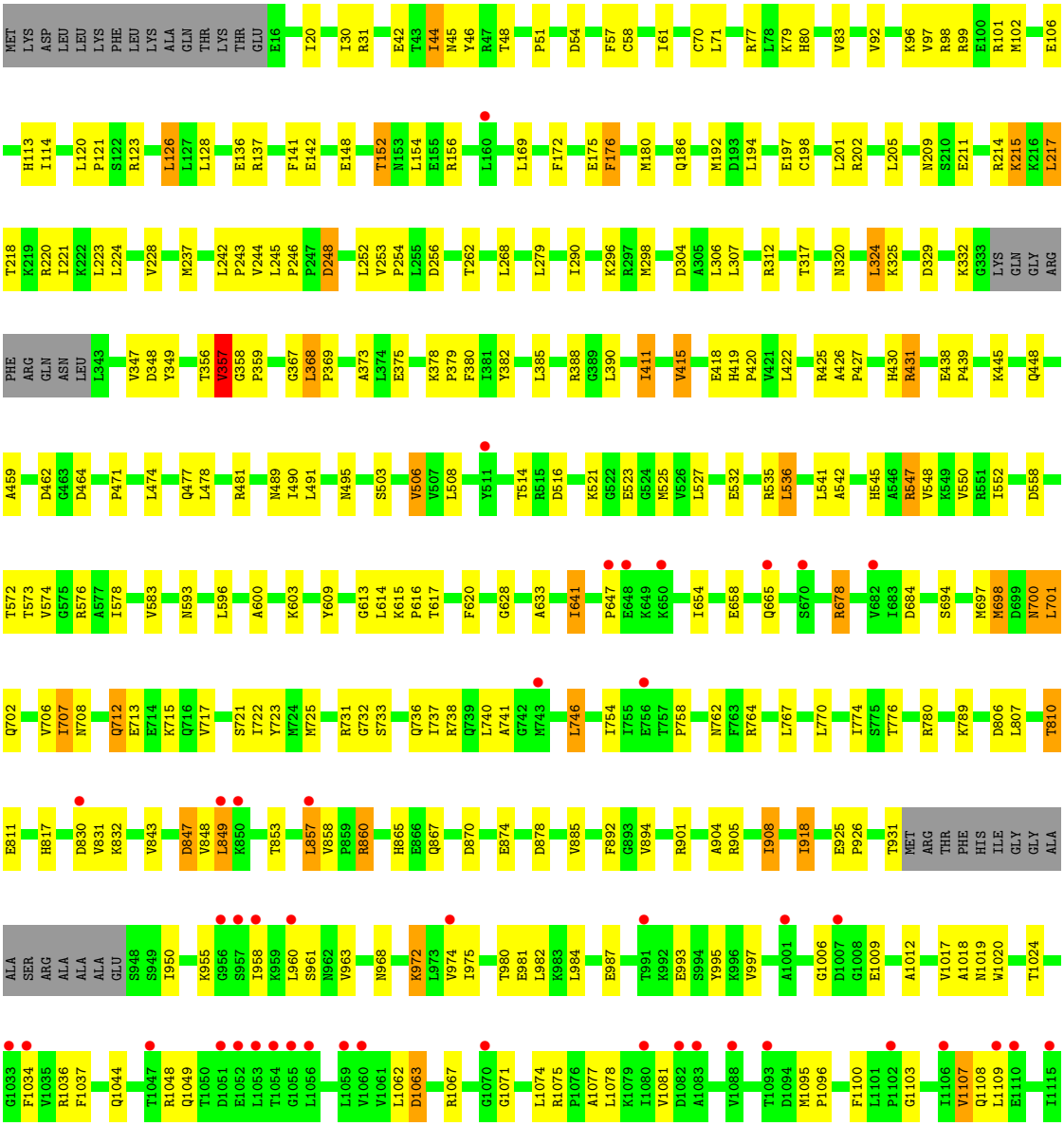
Chain D:

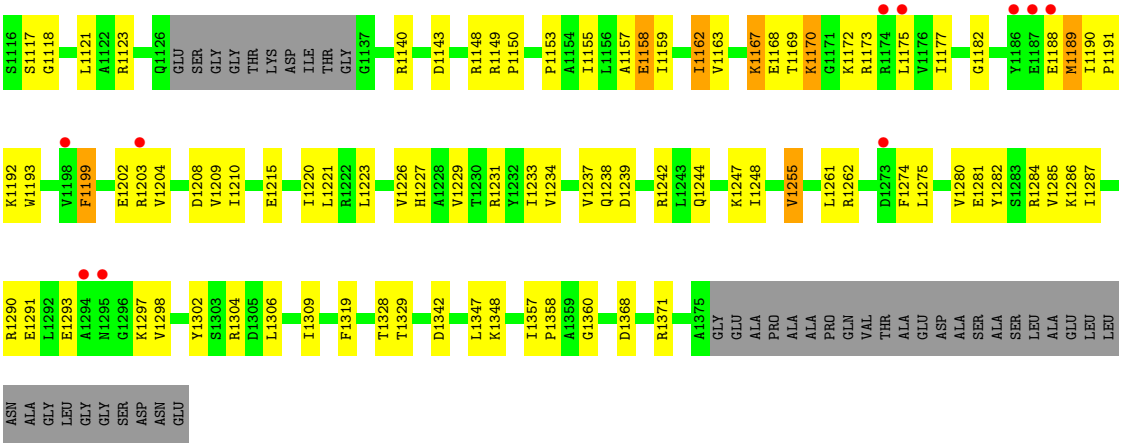




• Molecule 3: DNA-directed RNA polymerase subunit beta'

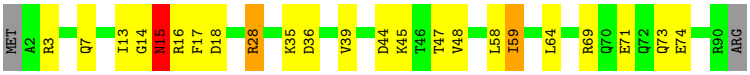
Chain J:





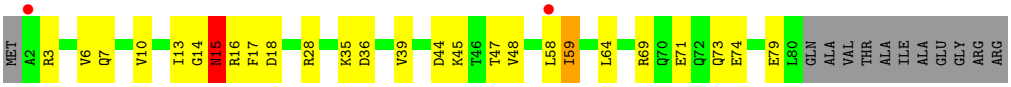
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



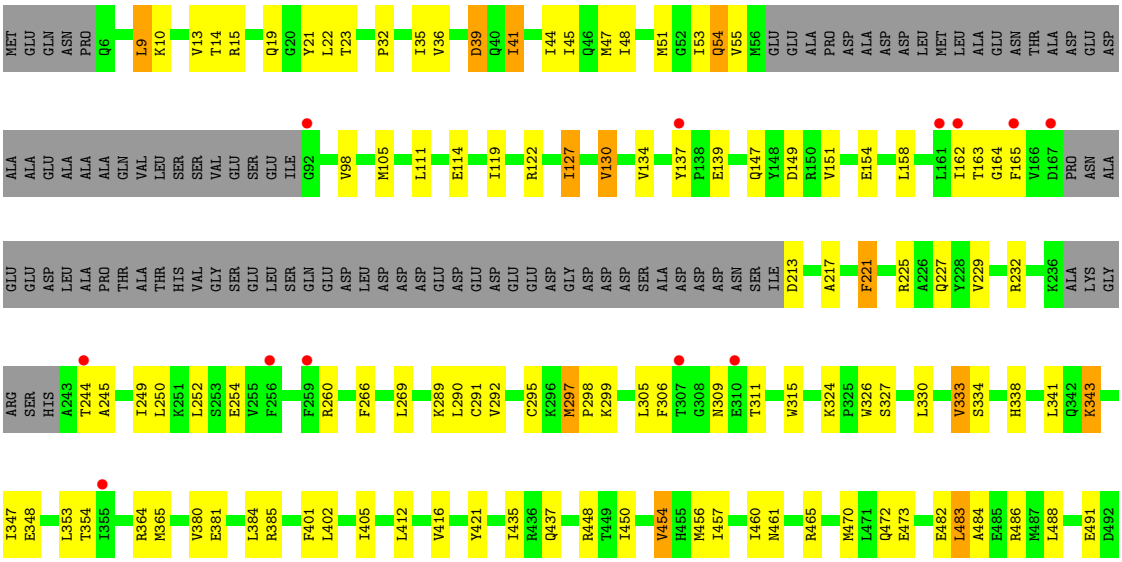
• Molecule 4: DNA-directed RNA polymerase subunit omega

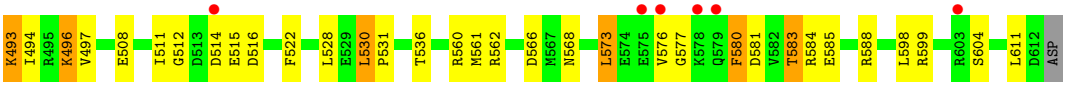
Chain K:



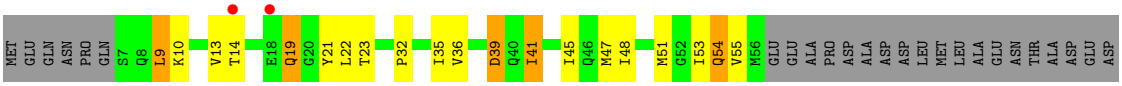
• Molecule 5: RNA polymerase sigma factor RpoD

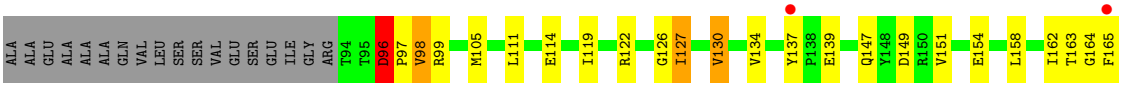
Chain F:

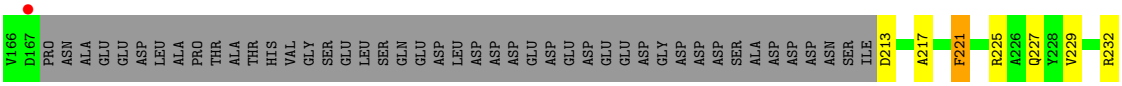


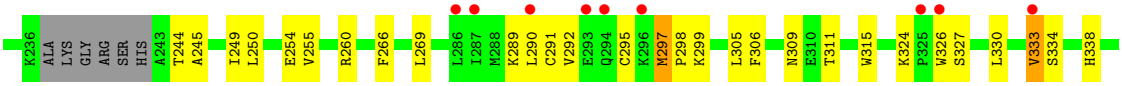


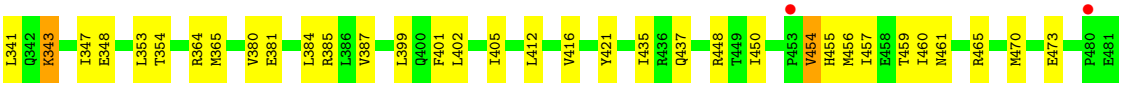
• Molecule 5: RNA polymerase sigma factor RpoD

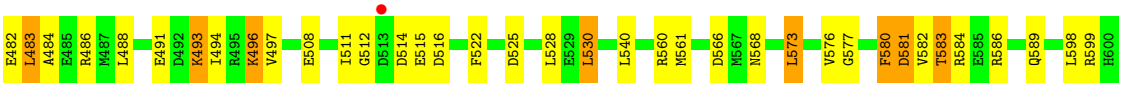


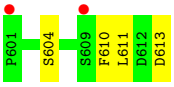




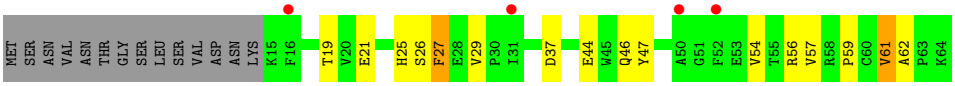




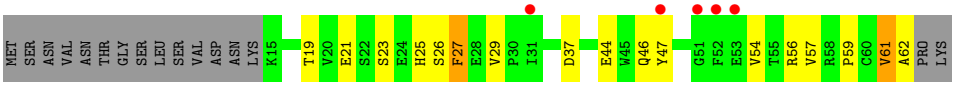




• Molecule 6: Bacterial RNA polymerase inhibitor



• Molecule 6: Bacterial RNA polymerase inhibitor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	187.51Å 205.04Å 308.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.21 – 3.79 45.21 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.21-3.79) 98.2 (45.21-3.79)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.243 , 0.282 0.243 , 0.282	Depositor DCC
R_{free} test set	5813 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	126.7	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 27.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	59147	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: MG, ZN

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	0.23	0/1751	0.49	0/2373
1	B	0.23	0/1707	0.45	0/2314
1	G	0.22	0/1771	0.49	0/2401
1	H	0.22	0/1686	0.45	0/2285
2	C	0.26	2/10739 (0.0%)	0.45	2/14489 (0.0%)
2	I	0.26	2/10735 (0.0%)	0.45	2/14484 (0.0%)
3	D	0.24	1/10603 (0.0%)	0.45	1/14316 (0.0%)
3	J	0.24	1/10450 (0.0%)	0.44	1/14112 (0.0%)
4	E	0.23	0/693	0.50	0/935
4	K	0.22	0/629	0.49	0/847
5	F	0.26	0/4214	0.49	2/5673 (0.0%)
5	L	0.27	0/4208	0.49	2/5665 (0.0%)
6	M	0.31	0/419	0.50	0/572
6	N	0.33	0/401	0.54	0/549
All	All	0.25	6/60006 (0.0%)	0.46	10/81015 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	I	0	1
4	E	0	1
4	K	0	1
5	L	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	31	GLN	CD-NE2	-8.70	1.11	1.32
2	I	31	GLN	CD-NE2	-8.41	1.11	1.32
2	I	31	GLN	CD-OE1	-7.96	1.06	1.24
2	C	31	GLN	CD-OE1	-7.79	1.06	1.24
3	D	477	GLN	CD-NE2	-6.25	1.17	1.32
3	J	477	GLN	CD-NE2	-6.08	1.17	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	19	GLN	C-N-CA	6.02	134.94	122.30
2	I	1261	GLY	N-CA-C	5.91	127.87	113.10
2	C	1261	GLY	N-CA-C	5.90	127.84	113.10
3	J	1182	GLY	N-CA-C	5.72	127.39	113.10
5	F	19	GLN	C-N-CA	5.71	134.30	122.30
3	D	1182	GLY	N-CA-C	5.62	127.14	113.10
5	F	149	ASP	CB-CG-OD2	5.22	123.00	118.30
2	C	516	ASP	CB-CG-OD2	5.20	122.98	118.30
5	L	149	ASP	CB-CG-OD2	5.20	122.98	118.30
2	I	516	ASP	CB-CG-OD2	5.11	122.89	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1261	GLY	Peptide
4	E	14	GLY	Peptide
2	I	1261	GLY	Peptide
4	K	14	GLY	Peptide
5	L	19	GLN	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	1730	0	1756	48	0
1	B	1687	0	1700	49	0
1	G	1750	0	1764	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1667	0	1689	41	0
2	C	10570	0	10582	232	0
2	I	10566	0	10576	217	0
3	D	10447	0	10671	249	0
3	J	10295	0	10510	229	0
4	E	691	0	695	15	0
4	K	627	0	634	17	0
5	F	4161	0	4171	81	0
5	L	4155	0	4168	85	0
6	M	406	0	383	10	0
6	N	389	0	363	13	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	59147	0	59662	1210	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 10.

All (1210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1173:ARG:HE	3:D:1192:LYS:HG3	1.29	0.97
3:J:1173:ARG:HE	3:J:1192:LYS:HG3	1.28	0.97
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85
3:J:1006:GLY:H	3:J:1009:GLU:HG3	1.41	0.85
3:J:418:GLU:HG3	4:K:45:LYS:H	1.41	0.83
3:D:1006:GLY:H	3:D:1009:GLU:HG3	1.42	0.83
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.44	0.83
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.44	0.82
2:C:517:GLN:HB2	2:C:523:GLU:HG2	1.63	0.80
2:I:517:GLN:HB2	2:I:523:GLU:HG2	1.63	0.79
5:F:32:PRO:HG2	5:F:35:ILE:HD12	1.63	0.79
5:L:32:PRO:HG2	5:L:35:ILE:HD12	1.64	0.79
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.65	0.78
2:C:1322:SER:HB2	3:D:340:GLN:HG2	1.65	0.77
5:L:130:VAL:HB	5:L:365:MET:HG3	1.66	0.77
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.66	0.76
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.00	0.76
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.00	0.75
5:F:130:VAL:HB	5:F:365:MET:HG3	1.68	0.75
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.68	0.74
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.70	0.73
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.22	0.73
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.71	0.72
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.72	0.72
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.71	0.72
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.72	0.72
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.72	0.71
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.72	0.71
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.72	0.71
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.72	0.71
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.72	0.71
1:A:159:ILE:HG13	1:A:162:GLU:HB2	1.73	0.70
1:G:104:LYS:HD3	1:G:110:VAL:HG22	1.73	0.69
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.74	0.69
3:J:1075:ARG:HH22	3:J:1173:ARG:NH1	1.90	0.69
5:L:324:LYS:HB2	5:L:327:SER:HB2	1.74	0.69
5:F:324:LYS:HB2	5:F:327:SER:HB2	1.74	0.69
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.74	0.69
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.74	0.69
2:I:211:ARG:NH1	2:I:357:ASN:O	2.26	0.69
1:A:104:LYS:HD3	1:A:110:VAL:HG22	1.73	0.68
2:C:490:GLN:HG2	5:F:472:GLN:HE21	1.56	0.68
1:G:159:ILE:HG13	1:G:162:GLU:HB2	1.73	0.68
1:G:58:GLU:HG2	1:G:158:ARG:HH22	1.59	0.68
2:C:211:ARG:NH1	2:C:357:ASN:O	2.26	0.68
3:D:1108:GLN:HG3	3:D:1109:LEU:HD13	1.76	0.68
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.75	0.68
3:D:358:GLY:H	3:D:359:PRO:HD3	1.59	0.68
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.76	0.68
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.59	0.68
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.76	0.68
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	1.76	0.67
3:D:885:VAL:HG21	3:D:1255:VAL:HG12	1.75	0.67
3:J:358:GLY:H	3:J:359:PRO:HD3	1.59	0.67
3:J:885:VAL:HG21	3:J:1255:VAL:HG12	1.76	0.67
3:J:1075:ARG:HH22	3:J:1173:ARG:HH12	1.43	0.67
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.76	0.67
4:E:15:ASN:OD1	4:E:18:ASP:N	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.57	0.67
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.57	0.67
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.76	0.67
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.77	0.66
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.76	0.66
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.28	0.66
4:K:15:ASN:OD1	4:K:18:ASP:N	2.26	0.66
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.60	0.66
2:I:452:ARG:NH1	2:I:584:TYR:O	2.29	0.66
2:C:115:LYS:HE3	2:C:116:ASP:H	1.62	0.65
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.78	0.65
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.78	0.65
5:L:39:ASP:OD1	5:L:39:ASP:N	2.22	0.65
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.78	0.65
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.62	0.65
3:J:209:ASN:HA	3:J:214:ARG:HE	1.62	0.65
3:J:722:ILE:HD11	3:J:737:ILE:HD12	1.78	0.65
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.79	0.65
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.78	0.65
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.62	0.65
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.80	0.64
3:D:77:ARG:HG3	3:D:79:LYS:H	1.62	0.64
2:C:452:ARG:NH1	2:C:584:TYR:O	2.31	0.64
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.78	0.64
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.78	0.64
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.78	0.64
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.78	0.64
1:G:62:ASP:OD1	1:G:141:SER:OG	2.16	0.64
3:J:77:ARG:HG3	3:J:79:LYS:H	1.62	0.64
3:J:152:THR:HG21	3:J:176:PHE:HB2	1.80	0.64
3:D:722:ILE:HD11	3:D:737:ILE:HD12	1.78	0.64
3:J:1155:ILE:HG13	3:J:1210:ILE:HB	1.80	0.64
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.78	0.64
3:D:1044:GLN:HB3	3:D:1071:GLY:HA3	1.79	0.64
3:D:209:ASN:HA	3:D:214:ARG:HE	1.62	0.64
3:D:1188:GLU:HG2	6:M:59:PRO:HD2	1.80	0.64
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.80	0.64
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.63	0.63
3:J:481:ARG:NH1	4:K:3:ARG:O	2.31	0.63
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.80	0.63
1:B:107:ILE:HG23	1:B:135:ASP:HA	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:44:GLU:HG2	6:N:54:VAL:HG21	1.81	0.63
3:D:152:THR:HG21	3:D:176:PHE:HB2	1.80	0.63
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.81	0.63
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.79	0.63
5:L:10:LYS:O	5:L:14:THR:OG1	2.10	0.63
3:D:481:ARG:NH1	4:E:3:ARG:O	2.32	0.63
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.81	0.63
2:I:528:ARG:NH2	2:I:576:SER:O	2.31	0.63
2:C:528:ARG:NH2	2:C:576:SER:O	2.31	0.63
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.81	0.63
3:D:1155:ILE:HG13	3:D:1210:ILE:HB	1.80	0.63
6:M:61:VAL:HG13	6:M:62:ALA:H	1.63	0.63
2:C:398:SER:OG	2:C:399:ALA:N	2.32	0.62
5:F:493:LYS:HA	5:F:496:LYS:HE3	1.80	0.62
6:M:44:GLU:HG2	6:M:54:VAL:HG21	1.80	0.62
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.81	0.62
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.81	0.62
5:F:483:LEU:O	5:F:486:ARG:NH1	2.32	0.62
2:I:115:LYS:HE3	2:I:116:ASP:H	1.61	0.62
2:I:702:THR:OG1	2:I:705:GLU:OE2	2.13	0.62
1:A:62:ASP:OD1	1:A:141:SER:OG	2.17	0.62
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.64	0.62
2:I:398:SER:OG	2:I:399:ALA:N	2.32	0.62
5:L:493:LYS:HA	5:L:496:LYS:HE3	1.80	0.62
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.81	0.62
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.80	0.62
5:L:483:LEU:O	5:L:486:ARG:NH1	2.32	0.61
2:C:59:ILE:HG21	2:C:472:GLU:HG3	1.82	0.61
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.81	0.61
2:I:886:LYS:HB3	2:I:917:SER:HA	1.81	0.61
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.81	0.61
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.81	0.61
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.81	0.61
2:C:886:LYS:HB3	2:C:917:SER:HA	1.81	0.61
2:I:59:ILE:HG21	2:I:472:GLU:HG3	1.82	0.61
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.66	0.61
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.32	0.61
3:J:1188:GLU:HG2	6:N:59:PRO:HD2	1.81	0.60
2:C:702:THR:OG1	2:C:705:GLU:OE2	2.13	0.60
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.84	0.60
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.66	0.60
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.84	0.60
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.32	0.60
3:D:613:GLY:O	3:D:617:THR:OG1	2.17	0.60
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.84	0.60
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.84	0.60
2:C:250:THR:HA	2:C:268:ARG:HA	1.84	0.59
1:G:166:ARG:O	1:G:168:ILE:N	2.35	0.59
3:J:356:THR:OG1	3:J:357:VAL:N	2.35	0.59
3:J:613:GLY:O	3:J:617:THR:OG1	2.18	0.59
1:A:166:ARG:O	1:A:168:ILE:N	2.35	0.59
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.85	0.59
3:D:356:THR:OG1	3:D:357:VAL:N	2.35	0.59
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.83	0.59
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.84	0.59
3:D:737:ILE:HA	3:D:740:LEU:HD12	1.85	0.59
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.85	0.59
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.32	0.59
3:D:694:SER:OG	3:D:738:ARG:NE	2.35	0.59
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.84	0.59
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.83	0.59
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.83	0.59
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.85	0.59
3:D:1262:ARG:O	3:D:1280:VAL:HG23	2.03	0.59
5:F:10:LYS:O	5:F:14:THR:OG1	2.09	0.59
2:I:14:ASP:HA	2:I:1183:ALA:HB3	1.84	0.59
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.84	0.58
2:I:250:THR:HA	2:I:268:ARG:HA	1.84	0.58
3:J:1347:LEU:HD12	3:J:1358:PRO:HG2	1.84	0.58
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.36	0.58
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.86	0.58
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.85	0.58
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.03	0.58
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.68	0.58
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.86	0.58
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.85	0.58
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.84	0.58
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.85	0.58
1:H:57:THR:HG22	1:H:58:GLU:HG2	1.85	0.58
3:D:1067:ARG:NH1	3:D:1074:LEU:O	2.36	0.58
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:694:SER:OG	3:J:738:ARG:NE	2.35	0.58
3:J:737:ILE:HA	3:J:740:LEU:HD12	1.85	0.58
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.85	0.58
1:A:12:ARG:H	1:A:30:PRO:HD2	1.69	0.58
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.68	0.58
1:G:158:ARG:HH21	1:G:172:LEU:HB3	1.69	0.58
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.69	0.58
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.85	0.58
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.86	0.58
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.86	0.58
1:B:57:THR:HG22	1:B:58:GLU:HG2	1.85	0.57
1:G:79:LEU:HD11	2:I:693:LEU:HD21	1.86	0.57
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.86	0.57
2:I:166:SER:HB3	6:N:23:SER:N	2.19	0.57
1:B:64:VAL:HG12	1:B:65:LEU:H	1.69	0.57
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.85	0.57
2:C:1261:GLY:O	2:C:1262:LYS:HB2	2.04	0.57
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.86	0.57
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.86	0.57
1:A:54:CYS:HB3	1:A:148:ARG:HG2	1.86	0.57
3:D:1173:ARG:HH21	3:D:1192:LYS:HE3	1.68	0.57
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.86	0.57
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.70	0.57
3:J:789:LYS:NZ	3:J:931:THR:O	2.34	0.57
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.87	0.57
1:G:54:CYS:HB3	1:G:148:ARG:HG2	1.86	0.57
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.86	0.57
3:D:746:LEU:HB2	3:D:754:ILE:HD11	1.86	0.57
2:I:1288:GLN:HG2	2:I:1315:MET:HE1	1.87	0.57
3:J:958:ILE:HG23	3:J:982:LEU:HD11	1.87	0.57
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.86	0.57
3:J:746:LEU:HB2	3:J:754:ILE:HD11	1.86	0.57
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.36	0.57
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.87	0.57
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.87	0.57
2:I:1261:GLY:O	2:I:1262:LYS:HB2	2.04	0.57
3:J:388:ARG:HB2	3:J:390:LEU:HD13	1.87	0.57
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.87	0.57
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.87	0.57
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.69	0.57
1:H:90:VAL:HG11	1:H:146:VAL:HG11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:44:ILE:HG13	5:L:450:ILE:HG22	1.86	0.57
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.87	0.57
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.38	0.56
2:C:840:SER:O	2:C:1047:LEU:N	2.38	0.56
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.87	0.56
3:J:1067:ARG:NH1	3:J:1074:LEU:O	2.36	0.56
3:D:701:LEU:HD12	3:D:723:TYR:HB2	1.87	0.56
2:I:166:SER:HB3	6:N:23:SER:CA	2.35	0.56
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.38	0.56
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.38	0.56
3:J:51:PRO:HB2	3:J:58:CYS:HA	1.86	0.56
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.87	0.56
3:J:1173:ARG:HH21	3:J:1192:LYS:HE3	1.70	0.56
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.86	0.56
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.87	0.56
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.87	0.56
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.87	0.56
3:J:701:LEU:HD12	3:J:723:TYR:HB2	1.87	0.56
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.87	0.56
2:C:975:ILE:HG12	2:C:1014:LEU:HD13	1.88	0.56
3:D:218:THR:HA	3:D:221:ILE:HG22	1.88	0.56
2:C:829:THR:HG23	2:C:1059:ARG:HA	1.88	0.56
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.33	0.56
2:I:930:ASP:OD2	2:I:931:VAL:N	2.39	0.56
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.70	0.56
3:D:388:ARG:HB2	3:D:390:LEU:HD13	1.87	0.56
3:D:51:PRO:HB2	3:D:58:CYS:HA	1.86	0.56
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.87	0.56
3:J:218:THR:HA	3:J:221:ILE:HG22	1.88	0.56
3:J:1173:ARG:NE	3:J:1192:LYS:HG3	2.11	0.56
1:B:11:PRO:HG3	1:B:31:LEU:HD13	1.88	0.56
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.69	0.56
1:G:12:ARG:H	1:G:30:PRO:HD2	1.69	0.55
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.87	0.55
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.87	0.55
1:H:11:PRO:HG3	1:H:31:LEU:HD13	1.87	0.55
2:I:373:GLY:O	5:L:99:ARG:NH1	2.39	0.55
1:B:74:VAL:HG11	1:B:81:ILE:HD11	1.88	0.55
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.39	0.55
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.86	0.55
5:F:573:LEU:H	5:F:573:LEU:HD23	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ARG:HE	1:H:38:THR:HB	1.71	0.55
2:I:840:SER:O	2:I:1047:LEU:N	2.39	0.55
5:F:560:ARG:NH1	5:F:566:ASP:OD1	2.40	0.55
5:L:560:ARG:NH1	5:L:566:ASP:OD1	2.39	0.55
5:F:39:ASP:OD1	5:F:39:ASP:N	2.22	0.55
1:G:96:ASP:HA	1:G:148:ARG:HD3	1.89	0.55
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.86	0.55
5:F:583:THR:HG22	5:F:584:ARG:H	1.72	0.55
3:J:1143:ASP:OD1	3:J:1148:ARG:NH1	2.39	0.55
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.87	0.55
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.72	0.55
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.70	0.55
3:D:958:ILE:HG23	3:D:982:LEU:HD11	1.87	0.55
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.89	0.55
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.89	0.55
5:L:9:LEU:HD22	6:N:46:GLN:O	2.07	0.55
5:L:573:LEU:HD23	5:L:573:LEU:H	1.71	0.55
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.21	0.54
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.87	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.89	0.54
2:C:930:ASP:OD2	2:C:931:VAL:N	2.39	0.54
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.54
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.90	0.54
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.88	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.89	0.54
5:L:583:THR:HG22	5:L:584:ARG:H	1.72	0.54
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.22	0.54
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.42	0.54
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.89	0.54
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.72	0.54
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.89	0.54
3:D:1036:ARG:HG2	3:D:1037:PHE:H	1.73	0.54
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.90	0.54
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.43	0.54
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.42	0.54
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.89	0.54
5:F:21:TYR:HB3	5:F:54:GLN:HG3	1.90	0.54
5:L:21:TYR:HB3	5:L:54:GLN:HG3	1.88	0.54
1:H:64:VAL:HG12	1:H:65:LEU:H	1.73	0.54
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.90	0.54
1:H:61:ILE:HG22	1:H:63:GLY:H	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.73	0.54
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.90	0.53
3:D:394:ILE:HG21	5:F:536:THR:HA	1.90	0.53
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.89	0.53
1:A:96:ASP:HA	1:A:148:ARG:HD3	1.89	0.53
3:D:44:ILE:HG13	5:F:450:ILE:HG22	1.91	0.53
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.23	0.53
5:F:330:LEU:O	5:F:334:SER:OG	2.21	0.53
5:F:530:LEU:HD23	5:F:530:LEU:H	1.74	0.53
1:G:117:HIS:NE2	1:G:121:VAL:O	2.41	0.53
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.90	0.53
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.23	0.53
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.74	0.53
5:L:330:LEU:O	5:L:334:SER:OG	2.21	0.53
1:A:14:VAL:HG22	1:A:15:ASP:H	1.74	0.53
2:C:1160:ASP:O	2:C:1161:LEU:HB2	2.08	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.74	0.53
1:G:14:VAL:HG22	1:G:15:ASP:H	1.74	0.53
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.88	0.53
3:J:712:GLN:HG2	3:J:713:GLU:H	1.73	0.53
2:I:905:ILE:O	5:L:599:ARG:NH1	2.41	0.53
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.42	0.53
5:L:229:VAL:HG12	5:L:232:ARG:HH12	1.73	0.53
2:C:905:ILE:O	5:F:599:ARG:NH1	2.42	0.53
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.91	0.53
1:G:80:GLU:O	1:G:84:ASN:ND2	2.42	0.53
2:I:1296:ASP:HB3	2:I:1320:PRO:HB3	1.91	0.53
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.91	0.53
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.90	0.53
1:B:61:ILE:HG22	1:B:63:GLY:H	1.73	0.53
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.91	0.53
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.90	0.53
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.33	0.53
3:J:1199:PHE:CD2	3:J:1202:GLU:HB3	2.44	0.53
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.74	0.53
2:C:520:PRO:HG3	2:C:714:VAL:HG11	1.90	0.53
2:C:1296:ASP:HB3	2:C:1320:PRO:HB3	1.89	0.53
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.42	0.53
2:I:1160:ASP:O	2:I:1161:LEU:HB2	2.08	0.53
5:L:530:LEU:H	5:L:530:LEU:HD23	1.73	0.53
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.44	0.52
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.91	0.52
1:A:13:LEU:HD23	1:A:13:LEU:H	1.74	0.52
1:A:117:HIS:NE2	1:A:121:VAL:O	2.42	0.52
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.92	0.52
3:D:712:GLN:HG2	3:D:713:GLU:H	1.73	0.52
2:I:886:LYS:H	2:I:917:SER:HB3	1.74	0.52
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.74	0.52
1:G:13:LEU:H	1:G:13:LEU:HD23	1.74	0.52
1:A:80:GLU:O	1:A:84:ASN:ND2	2.42	0.52
3:D:1199:PHE:CD2	3:D:1202:GLU:HB3	2.44	0.52
5:F:229:VAL:HG12	5:F:232:ARG:HH12	1.73	0.52
5:F:511:ILE:HG12	5:F:512:GLY:H	1.73	0.52
1:G:23:HIS:HB2	1:G:206:GLU:HA	1.91	0.52
2:I:30:ILE:HD12	2:I:30:ILE:H	1.75	0.52
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.92	0.52
5:L:511:ILE:HG12	5:L:512:GLY:H	1.73	0.52
2:C:558:VAL:HG11	2:C:573:ASN:HB3	1.92	0.52
5:F:9:LEU:HD22	6:M:46:GLN:O	2.10	0.52
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.91	0.52
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.92	0.51
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.92	0.51
3:J:136:GLU:OE2	3:J:312:ARG:NH1	2.42	0.51
2:C:886:LYS:H	2:C:917:SER:HB3	1.74	0.51
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.42	0.51
3:D:847:ASP:OD1	3:D:847:ASP:N	2.42	0.51
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.75	0.51
2:C:1086:PRO:HB2	2:C:1212:LEU:HD23	1.92	0.51
2:C:232:ILE:HG13	2:C:331:LYS:O	2.10	0.51
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.91	0.51
3:D:961:SER:HB2	3:D:981:GLU:HB3	1.93	0.51
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.46	0.51
3:J:961:SER:HB2	3:J:981:GLU:HB3	1.93	0.51
5:F:10:LYS:HA	5:F:13:VAL:HG12	1.93	0.51
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.51
1:H:13:LEU:HD23	1:H:13:LEU:H	1.76	0.51
2:I:558:VAL:HG11	2:I:573:ASN:HB3	1.92	0.51
1:A:23:HIS:HB2	1:A:206:GLU:HA	1.91	0.51
3:D:1173:ARG:NE	3:D:1192:LYS:HG3	2.12	0.51
2:I:1086:PRO:HB2	2:I:1212:LEU:HD23	1.92	0.51
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.93	0.51
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.91	0.51
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.92	0.51
5:L:491:GLU:HG3	5:L:491:GLU:O	2.11	0.51
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.93	0.51
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.92	0.51
3:D:1280:VAL:CG2	3:D:1304:ARG:HE	2.24	0.51
3:J:425:ARG:HG2	3:J:426:ALA:H	1.76	0.51
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.93	0.51
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.24	0.50
3:D:1167:LYS:HB2	3:D:1167:LYS:NZ	2.26	0.50
2:I:255:ILE:HB	2:I:263:VAL:HB	1.93	0.50
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.93	0.50
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.93	0.50
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.92	0.50
3:D:425:ARG:HG2	3:D:426:ALA:H	1.75	0.50
3:D:978:ARG:HB2	3:D:1199:PHE:CZ	2.46	0.50
5:F:491:GLU:O	5:F:491:GLU:HG3	2.11	0.50
3:J:1150:PRO:O	6:N:26:SER:OG	2.29	0.50
5:L:127:ILE:O	5:L:130:VAL:HG22	2.11	0.50
5:F:98:VAL:HG22	5:F:402:LEU:HD11	1.93	0.50
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.93	0.50
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.93	0.50
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.45	0.50
5:L:10:LYS:HA	5:L:13:VAL:HG12	1.92	0.50
5:L:98:VAL:HG22	5:L:402:LEU:HD11	1.93	0.50
2:C:255:ILE:HB	2:C:263:VAL:HB	1.93	0.50
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.45	0.50
1:H:59:VAL:O	1:H:171:LEU:N	2.45	0.50
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.93	0.50
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.50
3:J:1280:VAL:CG2	3:J:1304:ARG:HE	2.24	0.50
3:D:665:GLN:OE1	3:D:678:ARG:NH2	2.44	0.50
3:D:1077:ALA:HB2	3:D:1100:PHE:CD1	2.46	0.50
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.75	0.50
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.47	0.50
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.93	0.50
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.94	0.50
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.76	0.50
5:F:53:ILE:O	5:F:54:GLN:NE2	2.36	0.50
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.94	0.50
2:I:1024:GLU:HA	2:I:1027:LYS:HG2	1.93	0.50
1:A:228:LEU:HD21	1:B:224:LEU:HD23	1.93	0.50
3:D:1293:GLU:HG3	3:J:1227:HIS:HB2	1.93	0.50
1:G:208:ASN:OD1	1:G:208:ASN:N	2.44	0.50
3:J:665:GLN:OE1	3:J:678:ARG:NH2	2.44	0.50
6:M:19:THR:HB	6:M:56:ARG:HB3	1.93	0.50
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.42	0.50
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.94	0.50
1:B:13:LEU:H	1:B:13:LEU:HD23	1.76	0.49
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.93	0.49
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.12	0.49
3:D:847:ASP:HB3	3:D:860:ARG:H	1.77	0.49
6:N:19:THR:HB	6:N:56:ARG:HB3	1.93	0.49
1:H:34:GLY:N	1:H:199:ASP:OD2	2.46	0.49
2:I:232:ILE:HG13	2:I:331:LYS:O	2.10	0.49
3:D:54:ASP:HA	3:D:61:ILE:HD11	1.95	0.49
1:G:211:ILE:HD12	1:G:215:GLU:HG2	1.94	0.49
2:I:808:ASN:H	3:J:633:ALA:HB2	1.76	0.49
3:J:733:SER:O	3:J:737:ILE:HG12	2.12	0.49
5:L:165:PHE:CZ	5:L:217:ALA:HA	2.47	0.49
3:D:963:VAL:HB	3:D:980:THR:HG23	1.94	0.49
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.45	0.49
1:G:23:HIS:HB2	1:G:205:MET:O	2.13	0.49
1:H:86:LYS:HE2	1:H:174:ASP:HB2	1.94	0.49
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.78	0.49
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.30	0.49
2:C:808:ASN:H	3:D:633:ALA:HB2	1.76	0.49
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.47	0.49
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.93	0.49
3:J:847:ASP:HB3	3:J:860:ARG:H	1.78	0.49
5:L:126:GLY:O	5:L:130:VAL:HG13	2.11	0.49
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.94	0.49
3:D:349:TYR:CE2	3:D:379:PRO:HG2	2.48	0.49
1:H:32:GLU:HA	1:H:198:LEU:HD12	1.95	0.49
3:D:290:ILE:HD12	3:D:290:ILE:H	1.77	0.49
3:D:576:ARG:NH1	3:D:593:ASN:O	2.46	0.49
5:F:515:GLU:HG2	5:F:516:ASP:H	1.78	0.49
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.94	0.49
2:I:1254:VAL:HG22	2:I:1255:THR:HG23	1.94	0.49
3:J:198:CYS:O	3:J:202:ARG:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:963:VAL:HB	3:J:980:THR:HG23	1.94	0.49
5:F:165:PHE:CZ	5:F:217:ALA:HA	2.47	0.49
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.94	0.49
2:C:516:ASP:OD1	2:C:516:ASP:O	2.31	0.49
2:C:1105:SER:HA	3:D:736:GLN:NE2	2.28	0.49
2:C:1301:ARG:HG3	2:C:1302:THR:H	1.78	0.49
3:D:198:CYS:O	3:D:202:ARG:HG3	2.13	0.49
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.77	0.49
5:L:297:MET:HB2	5:L:326:TRP:HB2	1.95	0.49
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.95	0.48
3:D:700:ASN:ND2	3:D:700:ASN:O	2.46	0.48
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	1.95	0.48
5:F:164:GLY:O	5:F:260:ARG:HB2	2.13	0.48
2:I:117:ILE:HG21	2:I:488:MET:HG2	1.95	0.48
2:I:232:ILE:HA	2:I:237:LEU:HA	1.94	0.48
3:J:700:ASN:O	3:J:700:ASN:ND2	2.46	0.48
1:A:23:HIS:HB2	1:A:205:MET:O	2.13	0.48
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.94	0.48
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.94	0.48
2:I:349:GLU:O	2:I:353:VAL:HG23	2.13	0.48
2:I:516:ASP:OD1	2:I:516:ASP:O	2.30	0.48
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.13	0.48
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.48	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.12	0.48
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.48	0.48
5:F:266:PHE:HA	5:F:269:LEU:HD12	1.95	0.48
3:J:732:GLY:HA2	3:J:736:GLN:NE2	2.29	0.48
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.48	0.48
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.95	0.48
2:C:60:GLN:HA	2:C:67:GLU:HA	1.95	0.48
3:D:1297:LYS:HB3	3:J:1302:TYR:O	2.13	0.48
3:J:54:ASP:HA	3:J:61:ILE:HD11	1.94	0.48
1:A:211:ILE:HD12	1:A:215:GLU:HG2	1.94	0.48
2:C:117:ILE:HG21	2:C:488:MET:HG2	1.95	0.48
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.36	0.48
5:F:291:CYS:HA	5:F:295:CYS:HB2	1.95	0.48
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.94	0.48
3:D:490:ILE:HG13	3:D:491:LEU:HG	1.96	0.48
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.31	0.48
3:J:478:LEU:HG	4:K:47:THR:HG23	1.96	0.48
3:D:732:GLY:HA2	3:D:736:GLN:NE2	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.48	0.48
2:I:144:VAL:HB	2:I:526:HIS:CE1	2.49	0.48
3:J:576:ARG:NH1	3:J:593:ASN:O	2.46	0.48
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	1.95	0.48
5:F:297:MET:HB2	5:F:326:TRP:HB2	1.96	0.48
2:I:166:SER:HB3	6:N:23:SER:HA	1.95	0.48
2:C:138:ILE:HD13	2:C:143:ARG:HG3	1.96	0.48
2:C:509:SER:HB3	2:C:512:SER:HB3	1.94	0.48
2:C:1254:VAL:HG22	2:C:1255:THR:HG23	1.94	0.48
5:F:225:ARG:O	5:F:229:VAL:HG13	2.14	0.48
2:I:60:GLN:HA	2:I:67:GLU:HA	1.95	0.48
2:I:402:ARG:HG2	2:I:416:GLY:H	1.79	0.48
2:I:523:GLU:HB3	2:I:527:LYS:HE3	1.95	0.48
2:I:1105:SER:HA	3:J:736:GLN:NE2	2.28	0.48
3:J:1077:ALA:HA	3:J:1100:PHE:HA	1.96	0.48
5:L:164:GLY:O	5:L:260:ARG:HB2	2.13	0.48
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.95	0.48
1:B:34:GLY:N	1:B:199:ASP:OD2	2.45	0.47
2:C:1247:SER:HB3	3:D:375:GLU:O	2.14	0.47
3:D:523:GLU:OE2	3:D:547:ARG:NH1	2.44	0.47
3:D:1077:ALA:HA	3:D:1100:PHE:HA	1.96	0.47
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.96	0.47
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.95	0.47
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.97	0.47
3:J:523:GLU:OE2	3:J:547:ARG:NH1	2.44	0.47
3:J:1034:PHE:HB2	3:J:1081:VAL:HG23	1.95	0.47
2:C:523:GLU:HB3	2:C:527:LYS:HE3	1.95	0.47
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.13	0.47
3:D:1063:ASP:HB3	3:D:1103:GLY:HA3	1.97	0.47
5:F:309:ASN:C	5:F:311:THR:H	2.18	0.47
2:I:494:ASN:OD1	2:I:495:ALA:N	2.37	0.47
2:I:1301:ARG:HG3	2:I:1302:THR:H	1.78	0.47
5:L:47:MET:HB2	6:N:27:PHE:CZ	2.49	0.47
5:L:266:PHE:HA	5:L:269:LEU:HD12	1.95	0.47
5:F:162:ILE:HD13	5:F:221:PHE:HE2	1.77	0.47
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.95	0.47
5:F:576:VAL:O	5:F:580:PHE:HB2	2.14	0.47
3:J:332:LYS:HG2	3:J:1328:THR:HB	1.97	0.47
3:J:490:ILE:HG13	3:J:491:LEU:HG	1.96	0.47
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.14	0.47
5:L:515:GLU:HG2	5:L:516:ASP:H	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.97	0.47
2:C:488:MET:O	2:C:490:GLN:N	2.41	0.47
2:C:1240:ASP:HA	3:D:445:LYS:HD3	1.96	0.47
3:D:332:LYS:HG2	3:D:1328:THR:HB	1.97	0.47
5:L:291:CYS:HA	5:L:295:CYS:HB2	1.95	0.47
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.96	0.47
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.97	0.47
4:K:44:ASP:HB3	4:K:48:VAL:HB	1.97	0.47
1:B:102:LEU:O	1:B:141:SER:HA	2.15	0.47
2:C:30:ILE:HD12	2:C:30:ILE:H	1.79	0.47
2:C:349:GLU:O	2:C:353:VAL:HG23	2.14	0.47
2:C:1146:GLN:NE2	2:C:1160:ASP:O	2.47	0.47
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	1.97	0.47
3:D:968:ASN:OD1	3:D:972:LYS:N	2.48	0.47
3:D:1063:ASP:O	3:D:1067:ARG:HG3	2.14	0.47
1:G:103:ASN:OD1	1:G:141:SER:HB3	2.14	0.47
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.96	0.47
2:I:1146:GLN:NE2	2:I:1160:ASP:O	2.47	0.47
2:I:1247:SER:HB3	3:J:375:GLU:O	2.14	0.47
5:L:225:ARG:O	5:L:229:VAL:HG13	2.15	0.47
5:L:309:ASN:C	5:L:311:THR:H	2.18	0.47
1:B:191:ARG:NH2	3:D:409:TRP:HB3	2.29	0.47
2:C:232:ILE:HA	2:C:237:LEU:HA	1.94	0.47
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.97	0.47
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.97	0.47
5:F:484:ALA:H	5:F:494:ILE:HD11	1.80	0.47
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.97	0.47
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.97	0.47
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.97	0.47
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.50	0.47
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.80	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.48	0.47
2:I:1083:GLU:H	2:I:1083:GLU:HG3	1.45	0.47
2:C:56:VAL:O	2:C:59:ILE:HG23	2.15	0.47
2:C:1105:SER:HA	3:D:736:GLN:HE22	1.80	0.47
3:D:478:LEU:HG	4:E:47:THR:HG23	1.97	0.47
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	1.95	0.47
3:D:1100:PHE:HB2	3:D:1200:GLU:OE1	2.15	0.47
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.50	0.47
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.97	0.47
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1105:SER:HA	3:J:736:GLN:HE22	1.80	0.47
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.97	0.47
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.50	0.47
3:J:358:GLY:N	3:J:359:PRO:HD3	2.28	0.47
5:L:540:LEU:HD23	5:L:610:PHE:CD2	2.50	0.47
5:L:576:VAL:O	5:L:580:PHE:HB2	2.14	0.47
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.97	0.46
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.97	0.46
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	1.96	0.46
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.18	0.46
5:F:47:MET:HB2	6:M:27:PHE:CZ	2.50	0.46
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.29	0.46
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.78	0.46
3:J:968:ASN:OD1	3:J:972:LYS:N	2.48	0.46
2:C:541:GLU:N	2:C:541:GLU:OE1	2.47	0.46
3:D:335:GLN:HB2	5:F:516:ASP:OD1	2.16	0.46
2:I:402:ARG:CG	2:I:416:GLY:H	2.29	0.46
2:I:809:GLY:O	2:I:812:PHE:HB2	2.15	0.46
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.81	0.46
5:L:96:ASP:HA	5:L:97:PRO:HD2	1.86	0.46
2:C:13:LYS:HD3	2:C:1149:TYR:HA	1.98	0.46
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.50	0.46
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.97	0.46
3:D:984:LEU:HD22	3:D:993:GLU:HG3	1.98	0.46
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.50	0.46
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.95	0.46
3:J:1360:GLY:HA2	4:K:17:PHE:CE2	2.51	0.46
1:B:178:SER:HA	1:B:179:PRO:HD3	1.67	0.46
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.97	0.46
2:I:91:THR:HG21	2:I:503:LYS:HE2	1.97	0.46
5:L:461:ASN:O	5:L:465:ARG:HG3	2.16	0.46
2:C:402:ARG:HG2	2:C:416:GLY:H	1.79	0.46
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.97	0.46
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.97	0.46
2:I:56:VAL:O	2:I:59:ILE:HG23	2.15	0.46
2:I:1108:ASN:O	2:I:1110:GLY:N	2.49	0.46
2:I:1240:ASP:HA	3:J:445:LYS:HD3	1.97	0.46
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.97	0.46
3:J:349:TYR:CE2	3:J:379:PRO:HG2	2.48	0.46
3:J:1063:ASP:HB3	3:J:1103:GLY:HA3	1.97	0.46
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:HB3	1:B:80:GLU:HG2	1.98	0.46
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.97	0.46
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.80	0.46
3:J:1024:THR:HG21	3:J:1123:ARG:HD2	1.97	0.46
3:J:1167:LYS:HB2	3:J:1167:LYS:NZ	2.30	0.46
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.45	0.46
3:D:860:ARG:HB3	3:D:861:ASN:H	1.52	0.46
3:D:974:VAL:HG21	3:D:1118:GLY:HA2	1.98	0.46
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.51	0.46
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.97	0.46
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.98	0.46
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.30	0.46
3:D:70:CYS:SG	3:D:71:LEU:N	2.89	0.46
5:F:461:ASN:O	5:F:465:ARG:HG3	2.16	0.46
2:I:1085:MET:HA	2:I:1086:PRO:HD3	1.85	0.46
6:N:21:GLU:HG2	6:N:26:SER:HB2	1.98	0.46
1:A:49:SER:OG	1:A:50:SER:N	2.48	0.46
1:A:58:GLU:HG2	1:A:158:ARG:NH2	2.29	0.46
2:C:402:ARG:CG	2:C:416:GLY:H	2.29	0.46
3:D:1215:GLU:HB3	3:D:1220:ILE:HD11	1.98	0.46
5:F:511:ILE:HG21	5:F:522:PHE:HE2	1.81	0.46
1:H:102:LEU:O	1:H:141:SER:HA	2.15	0.46
2:I:13:LYS:HD3	2:I:1149:TYR:HA	1.97	0.46
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.98	0.46
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.97	0.46
5:L:380:VAL:HG22	5:L:416:VAL:HG21	1.98	0.46
1:A:45:ARG:HE	1:B:38:THR:HB	1.80	0.46
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.79	0.46
2:C:692:THR:OG1	2:C:693:LEU:N	2.48	0.46
3:D:550:VAL:HG23	3:D:552:ILE:HG23	1.98	0.46
3:D:1024:THR:HG21	3:D:1123:ARG:HD2	1.97	0.46
3:J:1006:GLY:N	3:J:1009:GLU:HG3	2.22	0.46
5:L:245:ALA:O	5:L:249:ILE:HG13	2.16	0.46
2:C:138:ILE:HB	2:C:143:ARG:HG3	1.97	0.45
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.96	0.45
2:C:1108:ASN:O	2:C:1110:GLY:N	2.49	0.45
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.99	0.45
3:D:1189:MET:HB2	6:M:57:VAL:HB	1.98	0.45
2:I:488:MET:O	2:I:490:GLN:N	2.41	0.45
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.98	0.45
3:J:984:LEU:HD22	3:J:993:GLU:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1107:VAL:HG12	3:J:1108:GLN:H	1.81	0.45
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.96	0.45
3:D:342:LEU:HD23	3:D:342:LEU:HA	1.71	0.45
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.98	0.45
1:H:76:GLU:HB3	1:H:80:GLU:HG2	1.97	0.45
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.32	0.45
2:I:541:GLU:OE1	2:I:541:GLU:N	2.47	0.45
2:I:809:GLY:O	3:J:357:VAL:HG11	2.16	0.45
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.18	0.45
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.99	0.45
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.97	0.45
2:C:809:GLY:O	2:C:812:PHE:HB2	2.15	0.45
5:F:245:ALA:O	5:F:249:ILE:HG13	2.16	0.45
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.98	0.45
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.80	0.45
3:J:514:THR:HG22	3:J:576:ARG:HG2	1.99	0.45
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.98	0.45
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.97	0.45
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.99	0.45
3:J:1215:GLU:HB3	3:J:1220:ILE:HD11	1.98	0.45
1:A:103:ASN:OD1	1:A:141:SER:HB3	2.16	0.45
3:D:1168:GLU:O	3:D:1168:GLU:HG3	2.16	0.45
3:D:1173:ARG:HH21	3:D:1192:LYS:CE	2.30	0.45
5:L:297:MET:HA	5:L:298:PRO:HD3	1.79	0.45
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.99	0.45
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.81	0.45
3:D:832:LYS:HD3	3:D:1242:ARG:HH12	1.81	0.45
3:D:1107:VAL:HG12	3:D:1108:GLN:H	1.81	0.45
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.98	0.45
1:G:49:SER:OG	1:G:50:SER:N	2.49	0.45
2:I:88:ARG:HG2	2:I:90:VAL:HG23	1.99	0.45
3:J:385:LEU:HD23	3:J:411:ILE:HG13	1.98	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.98	0.45
4:K:35:LYS:HB3	4:K:35:LYS:HE2	1.84	0.45
5:L:53:ILE:O	5:L:54:GLN:NE2	2.36	0.45
2:C:494:ASN:OD1	2:C:495:ALA:N	2.38	0.45
2:C:548:ARG:O	3:D:780:ARG:NH1	2.50	0.45
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.98	0.45
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.82	0.45
2:I:548:ARG:O	3:J:780:ARG:NH1	2.50	0.45
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:511:ILE:HG21	5:L:522:PHE:HE2	1.81	0.45
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.98	0.45
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.98	0.45
2:C:736:VAL:HG23	2:C:748:ILE:HA	1.99	0.45
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.98	0.45
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.71	0.45
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.87	0.45
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.98	0.45
1:H:106:GLY:H	1:H:133:LEU:HD23	1.81	0.45
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.99	0.45
2:C:143:ARG:HD2	2:C:514:PHE:HA	1.99	0.45
1:G:42:ALA:O	1:G:46:ILE:HG12	2.17	0.45
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.52	0.45
3:J:1221:LEU:HD23	3:J:1229:VAL:HG11	1.99	0.45
3:D:514:THR:HG22	3:D:576:ARG:HG2	1.99	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.45
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.17	0.45
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.99	0.45
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.82	0.45
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.81	0.45
3:J:993:GLU:OE1	3:J:995:TYR:OH	2.30	0.45
3:J:1168:GLU:O	3:J:1168:GLU:HG3	2.17	0.45
3:D:1150:PRO:O	6:M:26:SER:OG	2.34	0.44
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.99	0.44
2:I:143:ARG:HD2	2:I:514:PHE:HA	1.99	0.44
3:J:572:THR:OG1	3:J:573:THR:N	2.50	0.44
3:J:1078:LEU:HD12	3:J:1121:LEU:HB3	1.99	0.44
4:K:69:ARG:O	4:K:73:GLN:HG2	2.17	0.44
2:C:148:GLN:HG2	2:C:149:LEU:H	1.83	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.86	0.44
2:I:11:ILE:HD13	2:I:11:ILE:HA	1.83	0.44
3:J:770:LEU:HD22	3:J:770:LEU:H	1.82	0.44
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.98	0.44
1:A:42:ALA:O	1:A:46:ILE:HG12	2.17	0.44
1:B:106:GLY:H	1:B:133:LEU:HD23	1.81	0.44
3:D:741:ALA:O	3:D:762:ASN:ND2	2.51	0.44
2:I:765:ILE:HG13	2:I:787:PRO:HG3	1.99	0.44
3:J:1169:THR:HG22	3:J:1170:LYS:HB2	1.99	0.44
5:L:158:LEU:HD22	5:L:162:ILE:HD11	1.99	0.44
5:L:470:MET:HA	5:L:473:GLU:HB3	2.00	0.44
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1078:LEU:HD12	3:D:1121:LEU:HB3	1.99	0.44
3:D:1282:TYR:HE1	3:D:1286:LYS:HE2	1.83	0.44
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.99	0.44
5:L:290:LEU:HD22	5:L:333:VAL:HG21	2.00	0.44
2:C:15:PHE:HE1	2:C:1194:GLU:HB3	1.83	0.44
2:C:243:PRO:HA	2:C:246:LEU:HD12	1.99	0.44
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.82	0.44
3:D:99:ARG:HG3	3:D:248:ASP:HB3	2.00	0.44
3:D:789:LYS:NZ	3:D:931:THR:O	2.34	0.44
1:H:35:PHE:HA	1:H:38:THR:HG22	1.99	0.44
3:J:1173:ARG:HH21	3:J:1192:LYS:CE	2.30	0.44
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.00	0.44
4:K:64:LEU:HA	4:K:64:LEU:HD23	1.86	0.44
6:M:21:GLU:HG2	6:M:26:SER:HB2	2.00	0.44
2:C:809:GLY:O	3:D:357:VAL:HG11	2.17	0.44
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.83	0.44
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.99	0.44
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.99	0.44
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.17	0.44
3:J:70:CYS:SG	3:J:71:LEU:N	2.90	0.44
3:J:298:MET:SD	5:L:402:LEU:HB3	2.57	0.44
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.83	0.44
3:J:550:VAL:HG23	3:J:552:ILE:HG23	1.98	0.44
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.48	0.44
3:D:224:LEU:O	3:D:228:VAL:HG23	2.17	0.44
3:D:298:MET:SD	5:F:402:LEU:HB3	2.57	0.44
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	2.00	0.44
5:F:147:GLN:O	5:F:151:VAL:HG23	2.17	0.44
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.82	0.44
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.00	0.44
5:L:9:LEU:HD22	6:N:47:TYR:HA	2.00	0.44
2:C:88:ARG:HG2	2:C:90:VAL:HG23	1.99	0.44
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.99	0.44
2:C:820:GLU:HA	2:C:1079:ILE:HD11	2.00	0.44
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.91	0.44
3:D:870:ASP:O	3:D:874:GLU:HG2	2.17	0.44
4:E:69:ARG:O	4:E:73:GLN:HG2	2.17	0.44
5:F:290:LEU:HD22	5:F:333:VAL:HG21	2.00	0.44
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.99	0.44
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.85	0.44
3:J:654:ILE:O	3:J:658:GLU:N	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:484:ALA:H	5:L:494:ILE:HD11	1.82	0.44
2:C:558:VAL:CG1	2:C:573:ASN:HB3	2.48	0.44
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.99	0.44
3:D:901:ARG:HA	3:D:908:ILE:HA	2.00	0.44
5:F:348:GLU:HA	5:F:353:LEU:O	2.18	0.44
2:I:243:PRO:HA	2:I:246:LEU:HD12	1.99	0.44
2:I:870:ILE:HG21	2:I:931:VAL:HG11	2.00	0.44
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.81	0.44
2:I:1333:LEU:HB2	2:I:1335:ILE:HG12	2.00	0.44
3:J:870:ASP:O	3:J:874:GLU:HG2	2.17	0.44
6:N:61:VAL:HG22	6:N:62:ALA:H	1.82	0.44
1:B:35:PHE:HA	1:B:38:THR:HG22	1.99	0.43
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.99	0.43
2:C:28:LEU:HD21	2:C:524:ILE:HG13	2.00	0.43
2:C:56:VAL:HG11	2:C:468:LEU:HB3	2.00	0.43
2:C:1151:LEU:HD23	2:C:1151:LEU:HA	1.87	0.43
3:D:385:LEU:HD23	3:D:411:ILE:HG13	1.99	0.43
2:I:1253:LEU:HD23	5:L:525:ASP:OD1	2.18	0.43
3:J:1149:ARG:NH2	3:J:1153:PRO:HG2	2.33	0.43
2:I:206:ALA:O	2:I:209:ILE:HG22	2.18	0.43
2:I:387:ASN:HA	2:I:391:SER:HB2	2.00	0.43
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.83	0.43
2:C:170:VAL:HG23	2:C:171:LEU:N	2.33	0.43
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.54	0.43
2:C:520:PRO:HB3	2:C:714:VAL:HG21	2.00	0.43
2:C:617:ALA:HA	2:C:636:CYS:SG	2.59	0.43
3:D:807:LEU:HD11	3:D:894:VAL:HG23	1.99	0.43
3:D:1169:THR:HG22	3:D:1170:LYS:HB2	1.99	0.43
3:D:1286:LYS:HD2	3:D:1290:ARG:HH22	1.83	0.43
5:F:381:GLU:HA	5:F:384:LEU:HG	2.01	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.00	0.43
2:I:389:PHE:HB3	2:I:420:LEU:HD12	2.00	0.43
3:J:99:ARG:HG3	3:J:248:ASP:HB3	2.00	0.43
3:J:609:TYR:HB2	3:J:617:THR:HG21	2.00	0.43
3:J:741:ALA:O	3:J:762:ASN:ND2	2.51	0.43
5:L:348:GLU:HA	5:L:353:LEU:O	2.18	0.43
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.85	0.43
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.99	0.43
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.45	0.43
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.82	0.43
2:I:23:ASP:OD1	2:I:23:ASP:N	2.42	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:253:PHE:CZ	2:I:287:VAL:HG12	2.54	0.43
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.52	0.43
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	2.00	0.43
3:J:224:LEU:O	3:J:228:VAL:HG23	2.17	0.43
5:L:448:ARG:HH21	5:L:450:ILE:HG13	1.82	0.43
3:D:1231:ARG:HA	3:D:1234:VAL:HG22	2.00	0.43
2:I:98:VAL:HG21	2:I:124:MET:HE3	2.00	0.43
2:I:666:SER:HB2	2:I:704:MET:HG3	2.00	0.43
1:B:48:LEU:HD12	1:B:183:ILE:HD11	2.01	0.43
1:B:198:LEU:HD13	1:B:198:LEU:HA	1.76	0.43
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.19	0.43
4:E:71:GLU:HA	4:E:74:GLU:HG2	2.01	0.43
5:F:448:ARG:HH21	5:F:450:ILE:HG13	1.83	0.43
5:F:470:MET:HA	5:F:473:GLU:HB3	2.00	0.43
2:I:1116:HIS:O	2:I:1119:MET:HB3	2.19	0.43
5:L:147:GLN:O	5:L:151:VAL:HG23	2.17	0.43
2:C:339:ASN:HB3	2:C:343:HIS:H	1.84	0.43
2:C:389:PHE:HB3	2:C:420:LEU:HD12	2.00	0.43
3:D:470:VAL:HA	3:D:471:PRO:HD3	1.79	0.43
2:I:778:GLU:O	2:I:781:ASP:HB2	2.18	0.43
3:J:697:MET:O	3:J:701:LEU:HB2	2.19	0.43
1:B:33:ARG:NH1	2:C:1081:PRO:HG3	2.32	0.43
1:B:98:VAL:HG11	1:B:121:VAL:HG22	2.01	0.43
2:C:739:ASP:OD1	2:C:739:ASP:N	2.42	0.43
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.00	0.43
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.54	0.43
3:D:367:GLY:HA3	3:D:448:GLN:HB2	2.01	0.43
3:D:770:LEU:O	3:D:774:ILE:HG13	2.19	0.43
3:D:968:ASN:HB3	3:D:1118:GLY:HA3	2.00	0.43
5:F:41:ILE:O	5:F:45:ILE:HG13	2.18	0.43
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.99	0.43
3:J:857:LEU:HD13	3:J:858:VAL:HG12	2.01	0.43
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.87	0.43
2:C:778:GLU:O	2:C:781:ASP:HB2	2.18	0.43
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.29	0.43
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.54	0.43
3:D:211:GLU:O	3:D:215:LYS:HB2	2.19	0.43
3:D:495:ASN:ND2	3:D:1247:LYS:O	2.52	0.43
5:F:158:LEU:HD22	5:F:162:ILE:HD11	1.99	0.43
2:I:27:LEU:HB3	2:I:528:ARG:HD2	2.01	0.43
2:I:46:GLN:OE1	2:I:47:TYR:N	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:558:VAL:CG1	2:I:573:ASN:HB3	2.48	0.43
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.89	0.43
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.99	0.43
2:C:206:ALA:O	2:C:209:ILE:HG22	2.18	0.43
2:C:666:SER:HB2	2:C:704:MET:HG3	2.01	0.43
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.43
3:D:609:TYR:HB2	3:D:617:THR:HG21	2.01	0.43
3:D:697:MET:O	3:D:701:LEU:HB2	2.19	0.43
2:I:148:GLN:HG2	2:I:149:LEU:H	1.83	0.43
2:I:975:ILE:HG12	2:I:1014:LEU:HD13	2.01	0.43
2:I:1073:LYS:HD3	3:J:462:ASP:HB2	2.01	0.43
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.70	0.43
3:J:211:GLU:O	3:J:215:LYS:HB2	2.19	0.43
3:J:367:GLY:HA3	3:J:448:GLN:HB2	2.01	0.43
3:J:968:ASN:HB3	3:J:1118:GLY:HA3	2.01	0.43
3:J:1282:TYR:HE1	3:J:1286:LYS:HE2	1.83	0.43
1:B:29:GLU:HB2	1:B:30:PRO:HA	2.01	0.42
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.83	0.42
3:D:30:ILE:HG23	3:D:243:PRO:HG3	2.00	0.42
3:D:572:THR:OG1	3:D:573:THR:N	2.50	0.42
3:D:960:LEU:HB3	3:D:963:VAL:HG11	2.01	0.42
1:H:67:GLU:HG2	1:H:82:LEU:HD11	2.01	0.42
1:H:115:ILE:HD11	1:H:130:ILE:HD11	2.01	0.42
2:I:170:VAL:HG23	2:I:171:LEU:N	2.34	0.42
2:I:347:ILE:HD11	2:I:433:ILE:HD11	2.01	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.84	0.42
3:J:495:ASN:ND2	3:J:1247:LYS:O	2.52	0.42
3:J:521:LYS:HD3	3:J:541:LEU:O	2.19	0.42
3:J:901:ARG:HA	3:J:908:ILE:HA	2.00	0.42
3:J:960:LEU:HB3	3:J:963:VAL:HG11	2.01	0.42
3:J:1231:ARG:HA	3:J:1234:VAL:HG22	2.00	0.42
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.18	0.42
4:K:71:GLU:HA	4:K:74:GLU:HG2	2.01	0.42
5:L:381:GLU:HA	5:L:384:LEU:HG	2.00	0.42
3:D:128:LEU:HA	3:D:192:MET:HE1	2.02	0.42
3:D:857:LEU:HD13	3:D:858:VAL:HG12	2.01	0.42
1:H:48:LEU:HD12	1:H:183:ILE:HD11	2.01	0.42
3:J:368:LEU:HD23	3:J:369:PRO:HD2	2.01	0.42
1:B:67:GLU:HG2	1:B:82:LEU:HD11	2.01	0.42
2:C:870:ILE:HG21	2:C:931:VAL:HG11	2.00	0.42
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:97:VAL:HG12	3:D:101:ARG:HG3	2.00	0.42
3:D:600:ALA:O	3:D:603:LYS:HG2	2.19	0.42
5:F:250:LEU:O	5:F:254:GLU:HG2	2.19	0.42
1:G:14:VAL:CG1	1:G:27:THR:HB	2.50	0.42
2:I:545:PHE:O	2:I:548:ARG:N	2.52	0.42
2:I:1080:ASN:HA	2:I:1081:PRO:HD3	1.92	0.42
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.85	0.42
3:J:77:ARG:HB3	3:J:80:HIS:CE1	2.54	0.42
3:J:368:LEU:HD22	3:J:373:ALA:HB2	2.01	0.42
3:J:574:VAL:O	3:J:578:ILE:HG13	2.19	0.42
3:J:807:LEU:HD11	3:J:894:VAL:HG23	2.00	0.42
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.00	0.42
2:C:387:ASN:HA	2:C:391:SER:HB2	2.00	0.42
2:C:888:THR:HG23	2:C:916:SER:OG	2.20	0.42
2:C:1236:ASN:OD1	2:C:1236:ASN:N	2.51	0.42
3:D:574:VAL:O	3:D:578:ILE:HG13	2.19	0.42
1:G:58:GLU:HG2	1:G:158:ARG:NH2	2.29	0.42
2:I:28:LEU:HD21	2:I:524:ILE:HG13	2.00	0.42
3:J:1191:PRO:HB2	3:J:1193:TRP:CD1	2.54	0.42
5:L:41:ILE:O	5:L:45:ILE:HG13	2.19	0.42
5:L:456:MET:O	5:L:460:ILE:HG13	2.19	0.42
1:A:14:VAL:CG1	1:A:27:THR:HB	2.50	0.42
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.60	0.42
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.45	0.42
2:C:1326:LEU:HD21	3:D:339:ARG:HD2	2.01	0.42
1:G:57:THR:O	1:G:59:VAL:HG23	2.19	0.42
2:I:28:LEU:HD22	2:I:527:LYS:HD2	2.02	0.42
2:I:617:ALA:HA	2:I:636:CYS:SG	2.59	0.42
3:J:137:ARG:HG3	3:J:142:GLU:HB2	2.02	0.42
3:J:201:LEU:HD11	3:J:220:ARG:NH1	2.35	0.42
3:J:422:LEU:HD13	3:J:471:PRO:HG3	2.02	0.42
3:J:698:MET:O	3:J:702:GLN:HG2	2.19	0.42
3:J:1286:LYS:HD2	3:J:1290:ARG:HH22	1.83	0.42
5:L:250:LEU:O	5:L:254:GLU:HG2	2.20	0.42
2:C:207:THR:HG21	2:C:351:LEU:HG	2.02	0.42
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.92	0.42
2:C:538:LEU:H	2:C:538:LEU:HG	1.64	0.42
2:C:998:LEU:H	2:C:998:LEU:HD12	1.84	0.42
3:D:380:PHE:HB3	3:D:415:VAL:HG11	2.01	0.42
3:D:521:LYS:HD3	3:D:541:LEU:O	2.19	0.42
2:I:888:THR:HG23	2:I:916:SER:OG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.00	0.42
3:J:525:MET:O	3:J:548:VAL:HG13	2.19	0.42
1:A:155:ALA:HA	1:A:158:ARG:HG3	2.02	0.42
2:C:490:GLN:HG2	5:F:472:GLN:NE2	2.29	0.42
2:C:615:VAL:HA	2:C:638:SER:HA	2.02	0.42
3:D:525:MET:O	3:D:548:VAL:HG13	2.19	0.42
2:I:302:ILE:HG22	2:I:309:LEU:HA	2.01	0.42
5:L:292:VAL:HG11	5:L:299:LYS:HE3	2.02	0.42
5:L:581:ASP:HB3	5:L:582:VAL:H	1.70	0.42
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.72	0.42
1:A:197:ASP:N	1:A:197:ASP:OD1	2.53	0.42
2:C:11:ILE:HD13	2:C:11:ILE:HA	1.83	0.42
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.91	0.42
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.42
3:D:950:ILE:HG13	3:D:1020:TRP:CH2	2.55	0.42
3:D:955:LYS:HG2	3:D:1012:ALA:HA	2.02	0.42
1:G:155:ALA:HA	1:G:158:ARG:HG3	2.01	0.42
2:I:15:PHE:HE1	2:I:1194:GLU:HB3	1.83	0.42
2:I:47:TYR:HD2	2:I:47:TYR:HA	1.76	0.42
2:I:207:THR:HG21	2:I:351:LEU:HG	2.01	0.42
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.35	0.42
3:J:847:ASP:OD1	3:J:847:ASP:N	2.42	0.42
3:J:1291:GLU:HG2	3:J:1297:LYS:HD3	2.02	0.42
2:C:28:LEU:HD22	2:C:527:LYS:HD2	2.01	0.42
2:C:242:VAL:HB	2:C:245:ARG:HH11	1.85	0.42
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.84	0.42
2:C:1333:LEU:HB2	2:C:1335:ILE:HG12	2.00	0.42
3:D:368:LEU:HD22	3:D:373:ALA:HB2	2.01	0.42
3:D:368:LEU:HD23	3:D:369:PRO:HD2	2.02	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
3:D:698:MET:O	3:D:702:GLN:HG2	2.19	0.42
3:D:1124:ILE:HA	3:D:1125:PRO:HD3	1.93	0.42
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.50	0.42
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.34	0.42
5:F:297:MET:HA	5:F:298:PRO:HD3	1.79	0.42
2:I:253:PHE:HZ	2:I:287:VAL:HG12	1.85	0.42
3:J:380:PHE:HB3	3:J:415:VAL:HG11	2.01	0.42
3:J:849:LEU:HG	3:J:853:THR:HG22	2.02	0.42
3:J:955:LYS:HG2	3:J:1012:ALA:HA	2.02	0.42
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.86	0.42
1:A:224:LEU:HD22	1:B:228:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ILE:HD11	1:B:130:ILE:HD11	2.01	0.42
2:C:302:ILE:HG22	2:C:309:LEU:HA	2.01	0.42
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.02	0.42
5:F:343:LYS:O	5:F:347:ILE:HG13	2.20	0.42
5:F:348:GLU:HG2	5:F:354:THR:HA	2.02	0.42
5:F:456:MET:O	5:F:460:ILE:HG13	2.19	0.42
1:H:98:VAL:HG11	1:H:121:VAL:HG22	2.01	0.42
2:I:10:ARG:CZ	2:I:697:LYS:HD3	2.49	0.42
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.86	0.42
2:C:10:ARG:CZ	2:C:697:LYS:HD3	2.49	0.41
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	2.01	0.41
3:D:341:ASN:ND2	3:D:341:ASN:H	2.18	0.41
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.52	0.41
5:F:292:VAL:HG11	5:F:299:LYS:HE3	2.01	0.41
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.71	0.41
1:G:56:VAL:HG13	1:G:173:VAL:HG21	2.02	0.41
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.60	0.41
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.41
1:B:48:LEU:HD21	3:D:535:ARG:HG3	2.02	0.41
2:C:724:VAL:HA	2:C:734:ILE:HD13	2.02	0.41
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.55	0.41
3:D:45:ASN:HB3	3:D:48:THR:O	2.21	0.41
3:D:268:LEU:HG	3:D:324:LEU:HD22	2.02	0.41
3:D:806:ASP:HA	3:D:1347:LEU:HD13	2.02	0.41
5:F:598:LEU:O	5:F:604:SER:HB3	2.20	0.41
2:C:46:GLN:OE1	2:C:47:TYR:N	2.47	0.41
2:C:253:PHE:HZ	2:C:287:VAL:HG12	1.85	0.41
2:C:1116:HIS:CD2	3:D:641:ILE:HB	2.55	0.41
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.35	0.41
3:D:1159:ILE:HG23	3:D:1177:ILE:HG21	2.02	0.41
1:G:197:ASP:OD1	1:G:197:ASP:N	2.53	0.41
1:H:62:ASP:HB3	1:H:141:SER:O	2.21	0.41
2:I:367:TYR:CE1	2:I:380:ALA:HB1	2.56	0.41
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.35	0.41
1:B:98:VAL:HG12	1:B:146:VAL:HG22	2.02	0.41
3:D:378:LYS:HE2	3:D:382:TYR:OH	2.20	0.41
1:G:11:PRO:HD2	1:H:227:GLN:HA	2.02	0.41
2:I:40:GLU:O	2:I:73:TYR:OH	2.38	0.41
2:I:615:VAL:HA	2:I:638:SER:HA	2.02	0.41
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.92	0.41
3:J:600:ALA:O	3:J:603:LYS:HG2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:806:ASP:HA	3:J:1347:LEU:HD13	2.02	0.41
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.20	0.41
1:A:19:VAL:HG11	1:A:23:HIS:CE1	2.55	0.41
2:C:27:LEU:HB3	2:C:528:ARG:HD2	2.01	0.41
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.01	0.41
2:C:367:TYR:CE1	2:C:380:ALA:HB1	2.55	0.41
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.02	0.41
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.82	0.41
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.55	0.41
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.84	0.41
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.20	0.41
1:G:179:PRO:HB3	1:G:211:ILE:HB	2.02	0.41
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.03	0.41
3:J:770:LEU:O	3:J:774:ILE:HG13	2.19	0.41
5:L:343:LYS:O	5:L:347:ILE:HG13	2.20	0.41
5:L:348:GLU:HG2	5:L:354:THR:HA	2.02	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.93	0.41
1:A:228:LEU:HD12	1:B:221:ALA:HB1	2.02	0.41
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.86	0.41
3:D:418:GLU:H	4:E:45:LYS:NZ	2.19	0.41
5:F:562:ARG:HA	5:F:562:ARG:HD2	1.94	0.41
5:F:585:GLU:HA	5:F:588:ARG:HD3	2.03	0.41
2:I:242:VAL:HB	2:I:245:ARG:HH11	1.86	0.41
2:I:550:VAL:HG11	3:J:776:THR:HG22	2.03	0.41
2:I:980:VAL:O	2:I:984:VAL:HB	2.20	0.41
2:I:1061:GLN:NE2	2:I:1240:ASP:OD2	2.54	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.86	0.41
1:A:52:PRO:HG2	1:A:219:ARG:NH1	2.36	0.41
1:A:179:PRO:HB3	1:A:211:ILE:HB	2.02	0.41
1:B:219:ARG:O	1:B:223:ILE:HG13	2.21	0.41
2:C:153:PRO:O	2:C:401:GLY:HA2	2.21	0.41
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.54	0.41
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.86	0.41
5:F:32:PRO:CG	5:F:35:ILE:HD12	2.42	0.41
2:I:697:LYS:HA	2:I:698:PRO:HD3	1.91	0.41
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.02	0.41
3:J:268:LEU:HG	3:J:324:LEU:HD22	2.02	0.41
3:J:347:VAL:HG12	3:J:348:ASP:O	2.21	0.41
1:B:62:ASP:HB3	1:B:141:SER:O	2.21	0.41
2:C:310:ILE:HD13	2:C:325:LEU:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:519:ASN:HA	2:C:520:PRO:HD3	1.94	0.41
2:C:765:ILE:HG13	2:C:787:PRO:HG3	2.03	0.41
2:C:1312:ASN:OD1	2:C:1314:GLN:HG3	2.21	0.41
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.87	0.41
3:D:1100:PHE:HB2	3:D:1200:GLU:CD	2.41	0.41
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.21	0.41
4:E:59:ILE:HD11	4:E:64:LEU:HG	2.03	0.41
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.55	0.41
2:I:890:LYS:NZ	2:I:891:GLY:O	2.52	0.41
3:J:30:ILE:HG23	3:J:243:PRO:HG3	2.01	0.41
3:J:148:GLU:H	3:J:156:ARG:HG3	1.85	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.73	0.41
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.55	0.41
2:C:40:GLU:O	2:C:73:TYR:OH	2.38	0.41
2:C:684:ASN:OD1	2:C:687:ARG:NH1	2.54	0.41
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.56	0.41
3:D:34:SER:HG	3:D:104:HIS:CG	2.33	0.41
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.56	0.41
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.35	0.41
3:D:245:LEU:HD12	3:D:246:PRO:HD2	2.03	0.41
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.03	0.41
3:D:347:VAL:HG12	3:D:348:ASP:O	2.20	0.41
3:D:1149:ARG:HB3	3:D:1149:ARG:NH1	2.36	0.41
5:F:9:LEU:HD22	6:M:47:TYR:HA	2.02	0.41
5:F:165:PHE:HZ	5:F:217:ALA:HA	1.85	0.41
1:G:19:VAL:HG11	1:G:23:HIS:CE1	2.56	0.41
1:G:61:ILE:HG22	1:G:62:ASP:H	1.86	0.41
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	2.03	0.41
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.79	0.41
2:I:163:LYS:HB3	2:I:163:LYS:HE3	1.78	0.41
2:I:402:ARG:NE	2:I:417:SER:O	2.49	0.41
2:I:710:VAL:HA	2:I:715:THR:HG21	2.03	0.41
3:J:325:LYS:HG3	3:J:329:ASP:HB2	2.03	0.41
3:J:583:VAL:HG22	3:J:620:PHE:CZ	2.56	0.41
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.55	0.41
3:J:1347:LEU:HG	3:J:1357:ILE:HG23	2.03	0.41
4:K:6:VAL:O	4:K:10:VAL:HG23	2.21	0.41
5:L:32:PRO:CG	5:L:35:ILE:HD12	2.43	0.41
5:L:455:HIS:O	5:L:459:THR:OG1	2.35	0.41
1:A:57:THR:O	1:A:59:VAL:HG23	2.19	0.41
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.03	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.86	0.41
3:D:1191:PRO:HB2	3:D:1193:TRP:CD1	2.55	0.41
2:I:124:MET:HB2	2:I:498:ILE:HD13	2.03	0.41
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.86	0.41
3:J:245:LEU:HD12	3:J:246:PRO:HD2	2.03	0.41
3:J:378:LYS:HE2	3:J:382:TYR:OH	2.20	0.41
3:J:514:THR:HG21	3:J:596:LEU:HD12	2.03	0.41
3:J:810:THR:HG23	3:J:811:GLU:H	1.86	0.41
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.56	0.41
1:A:56:VAL:HG13	1:A:173:VAL:HG21	2.02	0.40
1:A:61:ILE:HG22	1:A:62:ASP:H	1.86	0.40
1:B:44:ARG:CZ	3:D:538:ARG:HH21	2.34	0.40
2:C:10:ARG:HD2	2:C:1181:PRO:HG2	2.03	0.40
2:C:75:LEU:HD13	2:C:75:LEU:HA	1.93	0.40
2:C:122:VAL:HG21	2:C:493:ILE:HG23	2.03	0.40
2:C:545:PHE:O	2:C:548:ARG:N	2.52	0.40
3:D:721:SER:O	3:D:725:MET:HG3	2.22	0.40
1:G:175:ALA:HB1	1:G:177:TYR:CZ	2.56	0.40
1:H:108:GLY:O	1:H:133:LEU:HB2	2.21	0.40
1:H:219:ARG:O	1:H:223:ILE:HG13	2.21	0.40
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.86	0.40
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.52	0.40
2:C:22:LEU:HG	2:C:603:ILE:HG21	2.03	0.40
3:D:111:THR:O	3:D:239:LEU:N	2.51	0.40
3:D:137:ARG:HG3	3:D:142:GLU:HB2	2.02	0.40
3:D:810:THR:HG23	3:D:811:GLU:H	1.86	0.40
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	2.02	0.40
5:F:15:ARG:HA	5:F:15:ARG:HD2	1.92	0.40
1:G:67:GLU:H	1:G:67:GLU:HG2	1.70	0.40
2:I:152:SER:HA	2:I:153:PRO:HD3	1.98	0.40
2:I:153:PRO:O	2:I:401:GLY:HA2	2.21	0.40
2:I:724:VAL:HA	2:I:734:ILE:HD13	2.02	0.40
2:I:1116:HIS:CD2	3:J:641:ILE:HB	2.55	0.40
3:J:45:ASN:HB3	3:J:48:THR:O	2.21	0.40
3:J:128:LEU:HA	3:J:192:MET:HE1	2.02	0.40
3:J:418:GLU:H	4:K:45:LYS:NZ	2.18	0.40
3:J:1149:ARG:HB3	3:J:1149:ARG:NH1	2.36	0.40
5:L:456:MET:HE2	5:L:497:VAL:HG13	2.02	0.40
5:L:586:ARG:O	5:L:589:GLN:HB2	2.21	0.40
2:C:325:LEU:O	2:C:330:HIS:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	2.03	0.40
2:C:994:ARG:HA	2:C:997:TRP:CD1	2.56	0.40
3:D:452:LEU:HD13	3:D:500:ILE:HG22	2.03	0.40
5:F:127:ILE:O	5:F:130:VAL:N	2.53	0.40
3:J:242:LEU:HA	3:J:243:PRO:HD3	1.94	0.40
3:J:721:SER:O	3:J:725:MET:HG3	2.21	0.40
4:K:59:ILE:HD11	4:K:64:LEU:HG	2.02	0.40
5:L:165:PHE:HZ	5:L:217:ALA:HA	1.85	0.40
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.03	0.40
5:L:598:LEU:O	5:L:604:SER:HB3	2.21	0.40
1:A:113:ALA:HB2	1:A:126:PRO:HB3	2.03	0.40
1:B:41:ASN:O	1:B:45:ARG:HG3	2.21	0.40
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.86	0.40
2:C:1128:ILE:O	2:C:1132:LEU:HB2	2.22	0.40
3:D:707:ILE:HG22	3:D:708:ASN:H	1.87	0.40
3:D:863:LEU:HD11	3:D:901:ARG:HB3	2.04	0.40
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.94	0.40
5:F:227:GLN:HG3	5:F:252:LEU:HA	2.04	0.40
1:G:52:PRO:HG2	1:G:219:ARG:NH1	2.36	0.40
1:H:41:ASN:O	1:H:45:ARG:HG3	2.21	0.40
1:H:198:LEU:HD13	1:H:198:LEU:HA	1.76	0.40
2:I:325:LEU:O	2:I:330:HIS:HB2	2.21	0.40
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.03	0.40
3:J:516:ASP:HB3	3:J:573:THR:HG21	2.04	0.40
3:J:707:ILE:HG22	3:J:708:ASN:H	1.86	0.40
3:J:968:ASN:HA	3:J:1117:SER:HB2	2.04	0.40
3:J:1309:ILE:H	3:J:1309:ILE:HG13	1.69	0.40
1:B:6:THR:O	1:B:6:THR:OG1	2.39	0.40
2:C:653:MET:HG2	2:C:654:ASP:N	2.37	0.40
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.35	0.40
2:C:737:ASN:HB3	2:C:739:ASP:OD1	2.22	0.40
2:C:887:VAL:HB	2:C:913:VAL:HG21	2.02	0.40
3:D:73:GLY:O	3:D:76:LYS:HE3	2.21	0.40
3:D:325:LYS:HE2	3:D:330:MET:SD	2.62	0.40
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.04	0.40
3:D:583:VAL:HG22	3:D:620:PHE:CZ	2.57	0.40
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.54	0.40
5:F:456:MET:HE2	5:F:497:VAL:HG13	2.03	0.40
1:G:172:LEU:HD12	1:G:172:LEU:H	1.86	0.40
2:I:653:MET:HG2	2:I:654:ASP:N	2.37	0.40
3:J:1159:ILE:HG23	3:J:1177:ILE:HG21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1175:LEU:HD22	3:J:1190:ILE:HD11	2.02	0.40
3:J:1189:MET:HB2	6:N:57:VAL:HB	2.02	0.40
5:L:227:GLN:HB3	5:L:255:VAL:HG21	2.03	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	222/239 (93%)	194 (87%)	26 (12%)	2 (1%)	17 54
1	B	216/239 (90%)	187 (87%)	29 (13%)	0	100 100
1	G	226/239 (95%)	197 (87%)	26 (12%)	3 (1%)	12 48
1	H	213/239 (89%)	187 (88%)	26 (12%)	0	100 100
2	C	1338/1342 (100%)	1213 (91%)	121 (9%)	4 (0%)	41 74
2	I	1338/1342 (100%)	1210 (90%)	124 (9%)	4 (0%)	41 74
3	D	1339/1407 (95%)	1229 (92%)	108 (8%)	2 (0%)	51 83
3	J	1317/1407 (94%)	1217 (92%)	98 (7%)	2 (0%)	47 79
4	E	87/91 (96%)	74 (85%)	12 (14%)	1 (1%)	14 51
4	K	77/91 (85%)	68 (88%)	8 (10%)	1 (1%)	12 48
5	F	513/613 (84%)	471 (92%)	42 (8%)	0	100 100
5	L	511/613 (83%)	469 (92%)	41 (8%)	1 (0%)	47 79
6	M	48/64 (75%)	43 (90%)	4 (8%)	1 (2%)	7 40
6	N	46/64 (72%)	42 (91%)	3 (6%)	1 (2%)	6 39
All	All	7491/7990 (94%)	6801 (91%)	668 (9%)	22 (0%)	41 74

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	61	VAL
2	C	170	VAL
2	C	1262	LYS
2	I	170	VAL
2	I	1262	LYS
3	D	357	VAL
3	J	357	VAL
1	A	14	VAL
4	E	15	ASN
1	G	14	VAL
4	K	15	ASN
2	C	163	LYS
1	G	232	VAL
2	I	163	LYS
2	C	1186	VAL
2	I	1186	VAL
6	M	61	VAL
3	D	831	VAL
3	J	831	VAL
1	A	167	PRO
1	G	167	PRO
5	L	96	ASP

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	191/206 (93%)	175 (92%)	16 (8%)	11 40
1	B	184/206 (89%)	166 (90%)	18 (10%)	8 33
1	G	191/206 (93%)	175 (92%)	16 (8%)	11 40
1	H	183/206 (89%)	168 (92%)	15 (8%)	11 40
2	C	1155/1157 (100%)	1059 (92%)	96 (8%)	11 40
2	I	1154/1157 (100%)	1061 (92%)	93 (8%)	11 41
3	D	1125/1168 (96%)	1030 (92%)	95 (8%)	11 40
3	J	1110/1168 (95%)	1017 (92%)	93 (8%)	11 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	72/75 (96%)	65 (90%)	7 (10%)	8 33
4	K	67/75 (89%)	59 (88%)	8 (12%)	5 26
5	F	444/540 (82%)	400 (90%)	44 (10%)	8 32
5	L	445/540 (82%)	400 (90%)	45 (10%)	7 32
6	M	43/56 (77%)	39 (91%)	4 (9%)	9 35
6	N	41/56 (73%)	37 (90%)	4 (10%)	8 33
All	All	6405/6816 (94%)	5851 (91%)	554 (9%)	10 40

All (554) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	17	GLU
1	A	19	VAL
1	A	27	THR
1	A	35	PHE
1	A	54	CYS
1	A	57	THR
1	A	58	GLU
1	A	71	LYS
1	A	172	LEU
1	A	207	THR
1	A	212	ASP
1	A	215	GLU
1	A	228	LEU
1	A	231	PHE
1	B	6	THR
1	B	8	PHE
1	B	13	LEU
1	B	16	ILE
1	B	28	LEU
1	B	31	LEU
1	B	50	SER
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	80	GLU
1	B	105	SER
1	B	124	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	140	ILE
1	B	142	MET
1	B	158	ARG
1	B	183	ILE
1	B	194	GLN
2	C	10	ARG
2	C	11	ILE
2	C	39	ILE
2	C	47	TYR
2	C	60	GLN
2	C	70	TYR
2	C	91	THR
2	C	115	LYS
2	C	117	ILE
2	C	131	THR
2	C	132	ASP
2	C	202	ARG
2	C	235	ASN
2	C	237	LEU
2	C	238	GLN
2	C	285	ILE
2	C	306	THR
2	C	321	LEU
2	C	327	GLN
2	C	331	LYS
2	C	361	SER
2	C	369	MET
2	C	413	GLU
2	C	419	ILE
2	C	423	ASP
2	C	443	ASP
2	C	487	LEU
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	600	THR
2	C	604	HIS
2	C	615	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	637	ARG
2	C	648	ASP
2	C	649	GLN
2	C	657	THR
2	C	663	VAL
2	C	672	GLU
2	C	690	VAL
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	714	VAL
2	C	717	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	807	TRP
2	C	817	LEU
2	C	828	PHE
2	C	853	ASP
2	C	857	VAL
2	C	859	GLU
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	979	LEU
2	C	992	LEU
2	C	995	ASP
2	C	1006	GLU
2	C	1019	ASP
2	C	1040	ASP
2	C	1080	ASN
2	C	1082	ILE
2	C	1083	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1108	ASN
2	C	1119	MET
2	C	1132	LEU
2	C	1156	ARG
2	C	1176	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1210	ILE
2	C	1233	LEU
2	C	1237	HIS
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1254	VAL
2	C	1339	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	20	ILE
3	D	42	GLU
3	D	44	ILE
3	D	46	TYR
3	D	83	VAL
3	D	92	VAL
3	D	96	LYS
3	D	102	MET
3	D	126	LEU
3	D	152	THR
3	D	154	LEU
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	186	GLN
3	D	197	GLU
3	D	215	LYS
3	D	217	LEU
3	D	237	MET
3	D	244	VAL
3	D	248	ASP
3	D	252	LEU
3	D	256	ASP
3	D	262	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	324	LEU
3	D	340	GLN
3	D	341	ASN
3	D	357	VAL
3	D	368	LEU
3	D	411	ILE
3	D	415	VAL
3	D	430	HIS
3	D	431	ARG
3	D	506	VAL
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	558	ASP
3	D	641	ILE
3	D	678	ARG
3	D	684	ASP
3	D	698	MET
3	D	700	ASN
3	D	701	LEU
3	D	707	ILE
3	D	712	GLN
3	D	717	VAL
3	D	746	LEU
3	D	764	ARG
3	D	767	LEU
3	D	810	THR
3	D	830	ASP
3	D	843	VAL
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	857	LEU
3	D	860	ARG
3	D	878	ASP
3	D	908	ILE
3	D	918	ILE
3	D	972	LYS
3	D	987	GLU
3	D	997	VAL
3	D	1017	VAL
3	D	1019	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1048	ARG
3	D	1049	GLN
3	D	1062	LEU
3	D	1063	ASP
3	D	1107	VAL
3	D	1140	ARG
3	D	1158	GLU
3	D	1162	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1170	LYS
3	D	1172	LYS
3	D	1189	MET
3	D	1199	PHE
3	D	1204	VAL
3	D	1208	ASP
3	D	1209	VAL
3	D	1244	GLN
3	D	1255	VAL
3	D	1261	LEU
3	D	1274	PHE
3	D	1275	LEU
3	D	1284	ARG
3	D	1285	VAL
3	D	1293	GLU
3	D	1306	LEU
3	D	1329	THR
3	D	1348	LYS
4	E	13	ILE
4	E	15	ASN
4	E	28	ARG
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU
4	E	59	ILE
5	F	9	LEU
5	F	22	LEU
5	F	23	THR
5	F	36	VAL
5	F	39	ASP
5	F	41	ILE
5	F	44	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	48	ILE
5	F	51	MET
5	F	54	GLN
5	F	55	VAL
5	F	114	GLU
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	163	THR
5	F	213	ASP
5	F	221	PHE
5	F	244	THR
5	F	297	MET
5	F	306	PHE
5	F	333	VAL
5	F	338	HIS
5	F	341	LEU
5	F	343	LYS
5	F	364	ARG
5	F	401	PHE
5	F	421	TYR
5	F	437	GLN
5	F	454	VAL
5	F	482	GLU
5	F	483	LEU
5	F	488	LEU
5	F	493	LYS
5	F	496	LYS
5	F	514	ASP
5	F	528	LEU
5	F	530	LEU
5	F	568	ASN
5	F	573	LEU
5	F	580	PHE
5	F	581	ASP
5	F	583	THR
5	F	611	LEU
1	G	9	LEU
1	G	13	LEU
1	G	17	GLU
1	G	19	VAL
1	G	27	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	35	PHE
1	G	54	CYS
1	G	57	THR
1	G	58	GLU
1	G	71	LYS
1	G	172	LEU
1	G	207	THR
1	G	212	ASP
1	G	215	GLU
1	G	228	LEU
1	G	231	PHE
1	H	13	LEU
1	H	16	ILE
1	H	28	LEU
1	H	50	SER
1	H	60	GLU
1	H	65	LEU
1	H	75	GLN
1	H	80	GLU
1	H	105	SER
1	H	124	VAL
1	H	140	ILE
1	H	142	MET
1	H	158	ARG
1	H	183	ILE
1	H	194	GLN
2	I	10	ARG
2	I	11	ILE
2	I	39	ILE
2	I	47	TYR
2	I	60	GLN
2	I	70	TYR
2	I	91	THR
2	I	115	LYS
2	I	117	ILE
2	I	131	THR
2	I	132	ASP
2	I	202	ARG
2	I	235	ASN
2	I	237	LEU
2	I	238	GLN
2	I	285	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	306	THR
2	I	321	LEU
2	I	327	GLN
2	I	331	LYS
2	I	361	SER
2	I	369	MET
2	I	413	GLU
2	I	419	ILE
2	I	423	ASP
2	I	443	ASP
2	I	487	LEU
2	I	493	ILE
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	600	THR
2	I	604	HIS
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	637	ARG
2	I	648	ASP
2	I	649	GLN
2	I	657	THR
2	I	663	VAL
2	I	672	GLU
2	I	690	VAL
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	705	GLU
2	I	717	VAL
2	I	748	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	807	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	817	LEU
2	I	828	PHE
2	I	853	ASP
2	I	857	VAL
2	I	859	GLU
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU
2	I	992	LEU
2	I	1006	GLU
2	I	1040	ASP
2	I	1080	ASN
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1119	MET
2	I	1132	LEU
2	I	1156	ARG
2	I	1176	LEU
2	I	1180	MET
2	I	1198	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1237	HIS
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1254	VAL
2	I	1339	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	42	GLU
3	J	44	ILE
3	J	46	TYR
3	J	83	VAL
3	J	92	VAL
3	J	96	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	102	MET
3	J	126	LEU
3	J	152	THR
3	J	154	LEU
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	186	GLN
3	J	197	GLU
3	J	215	LYS
3	J	217	LEU
3	J	237	MET
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	256	ASP
3	J	262	THR
3	J	324	LEU
3	J	357	VAL
3	J	368	LEU
3	J	411	ILE
3	J	415	VAL
3	J	430	HIS
3	J	431	ARG
3	J	506	VAL
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	558	ASP
3	J	641	ILE
3	J	678	ARG
3	J	684	ASP
3	J	698	MET
3	J	700	ASN
3	J	701	LEU
3	J	707	ILE
3	J	712	GLN
3	J	717	VAL
3	J	746	LEU
3	J	764	ARG
3	J	767	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	810	THR
3	J	830	ASP
3	J	843	VAL
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	857	LEU
3	J	860	ARG
3	J	878	ASP
3	J	908	ILE
3	J	918	ILE
3	J	972	LYS
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1019	ASN
3	J	1048	ARG
3	J	1049	GLN
3	J	1062	LEU
3	J	1063	ASP
3	J	1107	VAL
3	J	1140	ARG
3	J	1158	GLU
3	J	1162	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1170	LYS
3	J	1172	LYS
3	J	1189	MET
3	J	1199	PHE
3	J	1204	VAL
3	J	1208	ASP
3	J	1209	VAL
3	J	1244	GLN
3	J	1255	VAL
3	J	1261	LEU
3	J	1274	PHE
3	J	1275	LEU
3	J	1284	ARG
3	J	1285	VAL
3	J	1293	GLU
3	J	1306	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	1329	THR
3	J	1348	LYS
4	K	13	ILE
4	K	15	ASN
4	K	28	ARG
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
4	K	59	ILE
4	K	79	GLU
5	L	9	LEU
5	L	22	LEU
5	L	23	THR
5	L	36	VAL
5	L	39	ASP
5	L	41	ILE
5	L	48	ILE
5	L	51	MET
5	L	54	GLN
5	L	55	VAL
5	L	96	ASP
5	L	98	VAL
5	L	114	GLU
5	L	127	ILE
5	L	130	VAL
5	L	154	GLU
5	L	163	THR
5	L	213	ASP
5	L	221	PHE
5	L	244	THR
5	L	297	MET
5	L	306	PHE
5	L	333	VAL
5	L	338	HIS
5	L	341	LEU
5	L	343	LYS
5	L	364	ARG
5	L	401	PHE
5	L	421	TYR
5	L	437	GLN
5	L	454	VAL
5	L	482	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	483	LEU
5	L	488	LEU
5	L	493	LYS
5	L	496	LYS
5	L	514	ASP
5	L	528	LEU
5	L	530	LEU
5	L	568	ASN
5	L	573	LEU
5	L	580	PHE
5	L	581	ASP
5	L	583	THR
5	L	611	LEU
6	M	25	HIS
6	M	27	PHE
6	M	29	VAL
6	M	37	ASP
6	N	25	HIS
6	N	27	PHE
6	N	29	VAL
6	N	37	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	37	HIS
3	D	680	ASN
3	D	712	GLN
3	D	736	GLN
2	I	31	GLN
2	I	1061	GLN
3	J	477	GLN
3	J	680	ASN
3	J	712	GLN
3	J	736	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	224/239 (93%)	0.06	1 (0%) 92 89	45, 79, 110, 138	0
1	B	220/239 (92%)	0.23	17 (7%) 13 11	54, 96, 118, 134	0
1	G	228/239 (95%)	-0.05	2 (0%) 84 79	49, 82, 112, 136	0
1	H	217/239 (90%)	0.13	8 (3%) 41 34	58, 98, 119, 135	0
2	C	1340/1342 (99%)	-0.00	22 (1%) 72 64	24, 72, 107, 132	0
2	I	1340/1342 (99%)	0.04	43 (3%) 47 38	29, 76, 113, 139	0
3	D	1345/1407 (95%)	0.10	44 (3%) 46 38	26, 67, 119, 138	0
3	J	1325/1407 (94%)	0.10	54 (4%) 37 31	27, 68, 114, 137	0
4	E	89/91 (97%)	-0.19	0 100 100	30, 69, 97, 111	0
4	K	79/91 (86%)	-0.11	2 (2%) 57 49	32, 71, 107, 119	0
5	F	521/613 (84%)	0.11	18 (3%) 44 36	35, 93, 119, 135	0
5	L	519/613 (84%)	0.12	19 (3%) 41 34	39, 92, 119, 138	0
6	M	50/64 (78%)	0.36	4 (8%) 12 10	71, 92, 116, 127	0
6	N	48/64 (75%)	0.54	5 (10%) 6 5	75, 96, 117, 125	0
All	All	7545/7990 (94%)	0.07	239 (3%) 47 38	24, 77, 116, 139	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	252	SER	8.6
3	J	1054	THR	8.0
3	J	1053	LEU	7.0
5	F	167	ASP	6.9
2	C	257	ALA	6.1
5	L	18	GLU	5.9
3	J	1052	GLU	5.6
5	F	579	GLN	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	106	GLY	5.4
2	C	251	ALA	5.4
3	D	957	SER	5.4
5	L	167	ASP	5.3
5	L	480	PRO	5.2
2	C	258	ASN	5.1
2	C	265	LYS	5.1
3	D	984	LEU	4.9
2	I	165	HIS	4.9
5	F	244	THR	4.9
2	C	253	PHE	4.9
3	J	1055	GLY	4.8
2	I	998	LEU	4.8
3	D	1053	LEU	4.7
2	I	167	SER	4.6
3	J	1056	LEU	4.6
2	I	999	GLU	4.5
3	D	1054	THR	4.4
5	F	575	GLU	4.4
3	D	958	ILE	4.4
1	B	146	VAL	4.3
1	B	66	HIS	4.3
3	D	983	LYS	4.2
3	J	1051	ASP	4.1
3	D	1044	GLN	4.1
5	F	259	PHE	4.1
2	I	252	SER	4.0
3	D	993	GLU	4.0
3	J	743	MET	4.0
3	D	931	THR	3.9
2	C	282	VAL	3.9
5	F	92	GLY	3.9
1	B	172	LEU	3.9
3	D	1052	GLU	3.8
1	B	158	ARG	3.8
2	I	264	GLU	3.8
2	I	987	GLU	3.8
2	I	232	ILE	3.8
1	B	69	SER	3.6
5	F	165	PHE	3.6
2	I	168	GLY	3.6
3	D	1109	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	L	290	LEU	3.5
3	D	1103	GLY	3.5
1	B	90	VAL	3.5
3	J	1001	ALA	3.5
5	F	307	THR	3.5
3	J	1080	ILE	3.4
3	J	1294	ALA	3.4
3	J	648	GLU	3.4
3	D	1051	ASP	3.4
3	J	1295	ASN	3.4
1	B	107	ILE	3.4
3	D	1083	ALA	3.4
3	J	1102	PRO	3.3
3	D	1045	THR	3.3
3	D	1039	ASP	3.3
5	L	325	PRO	3.3
3	D	743	MET	3.3
3	D	1042	ASP	3.3
2	C	226	GLU	3.3
2	I	230	PHE	3.3
3	J	1187	GLU	3.2
3	D	754	ILE	3.2
5	L	137	TYR	3.2
6	M	50	ALA	3.2
3	J	1059	LEU	3.1
2	C	1000	LEU	3.1
5	L	165	PHE	3.1
3	J	1186	TYR	3.1
2	I	251	ALA	3.1
3	D	985	ILE	3.1
6	N	52	PHE	3.1
2	C	165	HIS	3.1
2	C	266	GLY	3.1
2	I	333	ILE	3.0
1	B	135	ASP	3.0
3	J	830	ASP	3.0
2	I	1004	ASP	3.0
6	N	53	GLU	3.0
3	D	952	VAL	3.0
2	I	236	LYS	3.0
3	J	974	VAL	2.9
2	C	316	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	L	296	LYS	2.9
5	F	514	ASP	2.9
2	C	255	ILE	2.9
2	C	230	PHE	2.9
3	D	319	SER	2.9
3	J	1188	GLU	2.8
1	B	55	ALA	2.8
5	F	603	ARG	2.8
5	F	256	PHE	2.8
5	L	287	ILE	2.8
2	I	124	MET	2.8
3	J	1109	LEU	2.8
3	D	1057	SER	2.8
2	I	972	PHE	2.8
6	M	31	ILE	2.8
5	L	601	PRO	2.8
3	J	665	GLN	2.8
5	F	137	TYR	2.7
2	C	241	LEU	2.7
3	D	1043	GLY	2.7
2	C	277	LEU	2.7
2	I	978	VAL	2.7
3	J	957	SER	2.7
5	L	294	GLN	2.7
5	F	576	VAL	2.7
3	D	1063	ASP	2.7
5	L	513	ASP	2.7
3	J	1088	VAL	2.7
1	B	144	ILE	2.7
3	J	1110	GLU	2.6
2	I	75	LEU	2.6
2	I	237	LEU	2.6
3	D	857	LEU	2.6
1	B	59	VAL	2.6
2	I	979	LEU	2.6
1	B	67	GLU	2.6
2	I	1167	GLU	2.6
5	F	310	GLU	2.6
2	C	696	ASP	2.6
3	D	991	THR	2.6
3	D	1056	LEU	2.6
6	M	52	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	1021	LEU	2.6
3	D	1055	GLY	2.6
2	C	292	ILE	2.5
1	H	204	GLU	2.5
1	B	173	VAL	2.5
2	I	997	TRP	2.5
3	D	1012	ALA	2.5
3	J	960	LEU	2.5
5	F	578	LYS	2.5
3	D	1189	MET	2.5
1	B	56	VAL	2.5
3	D	959	LYS	2.5
5	L	333	VAL	2.5
3	J	1047	THR	2.5
2	I	989	LEU	2.5
2	C	254	ASP	2.5
3	J	1007	ASP	2.5
3	J	849	LEU	2.4
3	J	1203	ARG	2.4
2	I	169	LYS	2.4
4	K	58	LEU	2.4
3	J	1198	VAL	2.4
2	I	986	ALA	2.4
1	H	172	LEU	2.4
3	J	1033	GLY	2.4
3	D	965	SER	2.4
3	J	1273	ASP	2.4
1	B	147	GLN	2.4
3	D	1058	SER	2.4
5	L	293	GLU	2.4
3	J	160	LEU	2.4
3	J	1060	VAL	2.4
3	J	850	LYS	2.4
3	J	1174	ARG	2.4
5	L	326	TRP	2.4
3	J	1082	ASP	2.3
3	J	1115	ILE	2.3
2	I	312	ALA	2.3
3	D	1035	VAL	2.3
3	J	1034	PHE	2.3
3	J	682	VAL	2.3
5	L	286	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	253	PHE	2.3
5	L	609	SER	2.3
2	I	166	SER	2.3
3	J	1106	ILE	2.3
2	C	317	LEU	2.3
3	D	209	ASN	2.3
3	J	1093	THR	2.3
2	C	262	TYR	2.3
2	I	235	ASN	2.3
6	M	16	PHE	2.3
2	I	990	ASP	2.3
3	J	650	LYS	2.3
1	G	90	VAL	2.3
2	I	1018	TYR	2.2
5	L	14	THR	2.2
3	J	1175	LEU	2.2
2	I	740	GLU	2.2
3	D	956	GLY	2.2
3	J	1070	GLY	2.2
3	J	857	LEU	2.2
3	J	756	GLU	2.2
6	N	47	TYR	2.2
3	D	318	GLY	2.2
2	I	867	GLU	2.2
3	D	756	GLU	2.2
3	J	991	THR	2.2
5	F	355	ILE	2.2
2	I	976	ARG	2.2
1	G	193	GLU	2.2
3	J	647	PRO	2.2
1	H	158	ARG	2.2
2	I	164	THR	2.1
1	A	35	PHE	2.1
3	D	1041	ILE	2.1
2	I	334	GLU	2.1
2	I	100	LEU	2.1
2	I	996	ARG	2.1
3	D	1059	LEU	2.1
3	D	1104	LYS	2.1
1	B	99	ILE	2.1
1	H	107	ILE	2.1
2	I	248	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	J	956	GLY	2.1
5	F	162	ILE	2.1
4	K	2	ALA	2.1
2	I	120	GLN	2.1
1	B	121	VAL	2.1
2	I	995	ASP	2.1
3	D	1065	ALA	2.1
2	I	1334	GLY	2.1
3	J	958	ILE	2.0
2	C	243	PRO	2.0
5	L	453	PRO	2.0
3	D	1080	ILE	2.0
3	J	511	TYR	2.0
3	J	670	SER	2.0
6	N	51	GLY	2.0
1	H	123	ILE	2.0
3	J	1083	ALA	2.0
1	H	74	VAL	2.0
5	F	161	LEU	2.0
1	H	96	ASP	2.0
6	N	31	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
7	MG	D	1501	1/1	0.84	0.61	51,51,51,51	0
7	MG	J	1501	1/1	0.90	0.70	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	ZN	D	1503	1/1	0.96	0.42	278,278,278,278	0
8	ZN	J	1502	1/1	0.97	0.15	168,168,168,168	0
8	ZN	D	1502	1/1	0.98	0.12	103,103,103,103	0
8	ZN	J	1503	1/1	0.99	0.19	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.