



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 12:09 PM EDT

PDB ID : 3NBY
Title : Crystal structure of the PKI NES-CRM1-RanGTP nuclear export complex
Authors : Guttler, T.; Madl, T.; Neumann, P.; Deichsel, D.; Corsini, L.; Monecke, T.; Ficner, R.; Sattler, M.; Gorlich, D.
Deposited on : 2010-06-04
Resolution : 3.42 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

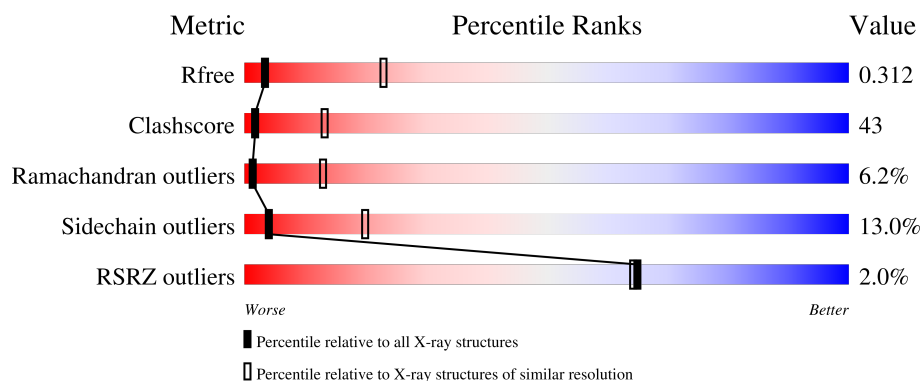
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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

Mol	Chain	Length	Quality of chain
1	B	361	<div> <div>22%</div> <div>40%</div> <div>12%</div> <div>25%</div> </div>
1	E	361	<div> <div>2%</div> <div>30%</div> <div>36%</div> <div>10%</div> <div>23%</div> </div>
2	C	176	<div> <div>35%</div> <div>52%</div> <div>9%</div> </div>
2	F	176	<div> <div>39%</div> <div>46%</div> <div>11%</div> </div>
3	A	1073	<div> <div>2%</div> <div>33%</div> <div>52%</div> <div>11%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1073	<div><div></div><div>3%</div><div>32%</div><div>53%</div><div>11%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24084 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 Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	272	Total	C	N	O	S	0	0	0
			2193	1398	376	405	14			
1	E	277	Total	C	N	O	S	0	0	0
			2221	1416	380	410	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
B	1	LEU	-	expression tag	UNP O95149
B	2	ASN	-	expression tag	UNP O95149
B	3	GLU	-	expression tag	UNP O95149
B	4	LEU	-	expression tag	UNP O95149
B	5	ALA	-	expression tag	UNP O95149
B	6	LEU	-	expression tag	UNP O95149
B	7	LYS	-	expression tag	UNP O95149
B	8	LEU	-	expression tag	UNP O95149
B	9	ALA	-	expression tag	UNP O95149
B	10	GLY	-	expression tag	UNP O95149
B	11	LEU	-	expression tag	UNP O95149
B	12	ASP	-	expression tag	UNP O95149
B	13	ILE	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149
E	1	LEU	-	expression tag	UNP O95149
E	2	ASN	-	expression tag	UNP O95149
E	3	GLU	-	expression tag	UNP O95149
E	4	LEU	-	expression tag	UNP O95149
E	5	ALA	-	expression tag	UNP O95149
E	6	LEU	-	expression tag	UNP O95149
E	7	LYS	-	expression tag	UNP O95149
E	8	LEU	-	expression tag	UNP O95149

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ALA	-	expression tag	UNP O95149
E	10	GLY	-	expression tag	UNP O95149
E	11	LEU	-	expression tag	UNP O95149
E	12	ASP	-	expression tag	UNP O95149
E	13	ILE	-	expression tag	UNP O95149

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			
2	F	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	engineered mutation	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1041	Total	C	N	O	S	0	0	0
			8413	5397	1413	1549	54			
3	D	1041	Total	C	N	O	S	0	0	0
			8413	5397	1413	1549	54			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

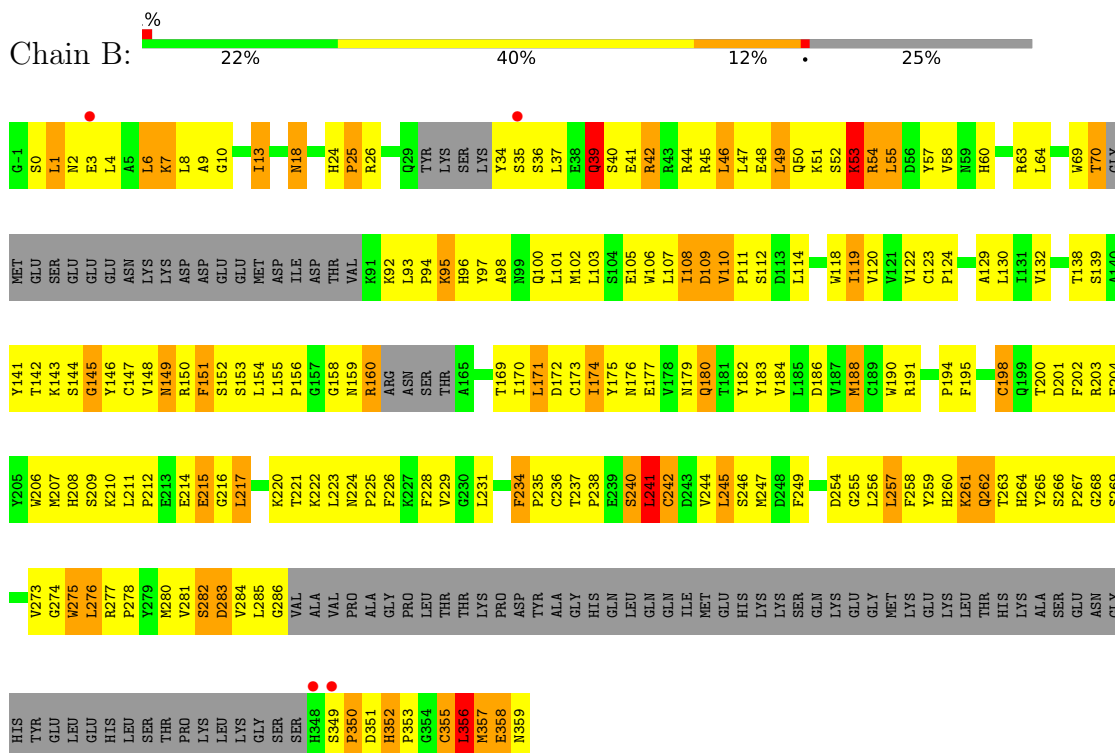
- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



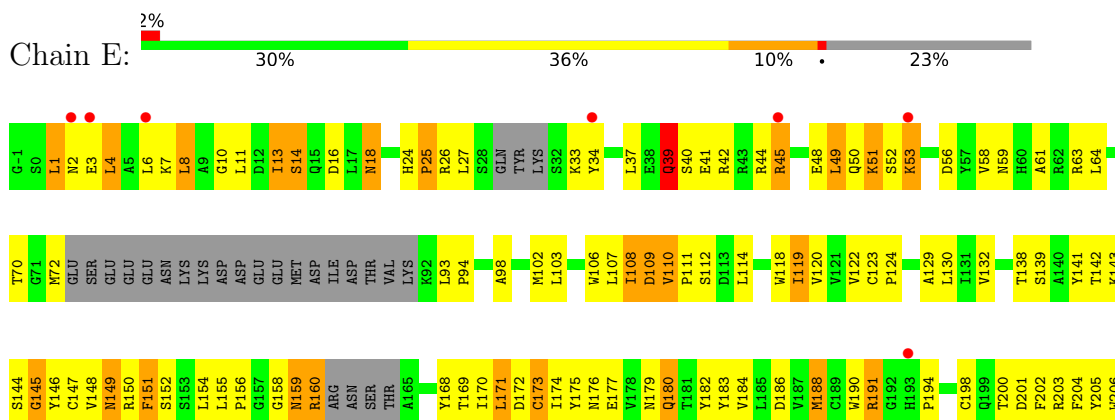
3 Residue-property plots

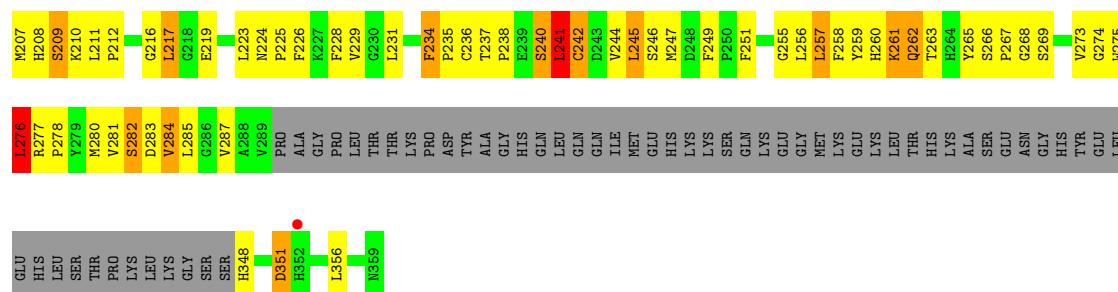
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Snurportin-1



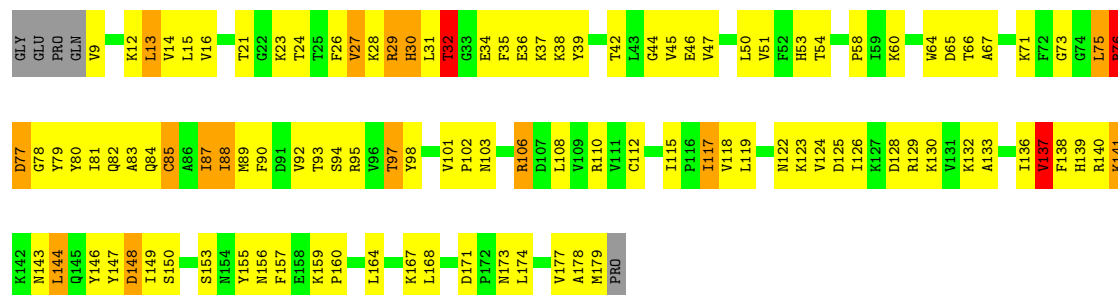
• Molecule 1: Snurportin-1





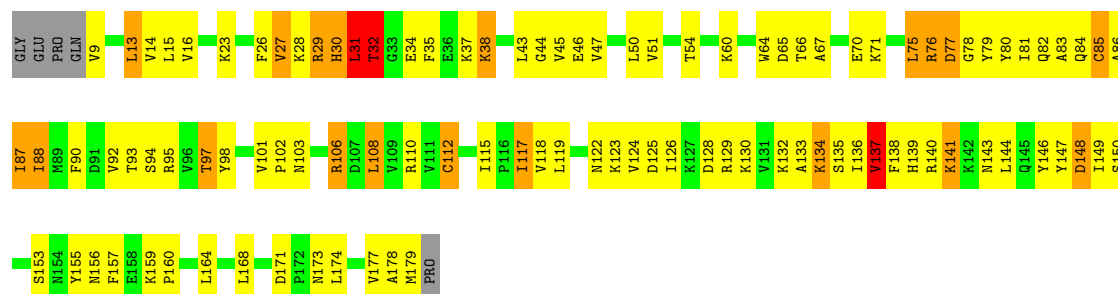
• Molecule 2: GTP-binding nuclear protein Ran

Chain C: 35% 52% 9% . .



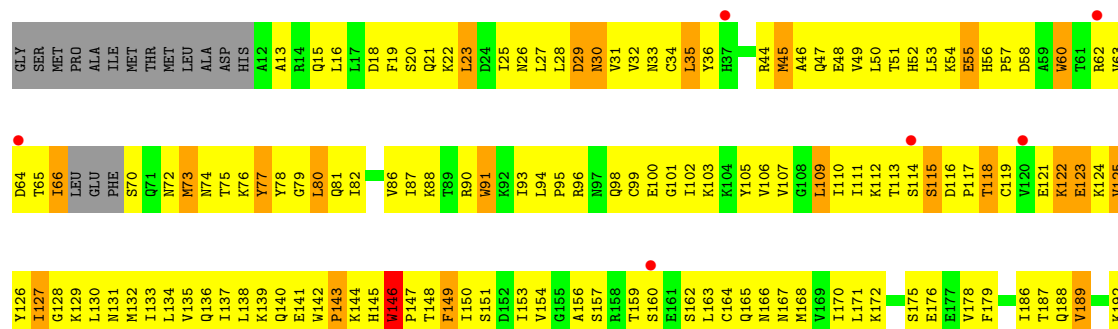
• Molecule 2: GTP-binding nuclear protein Ran

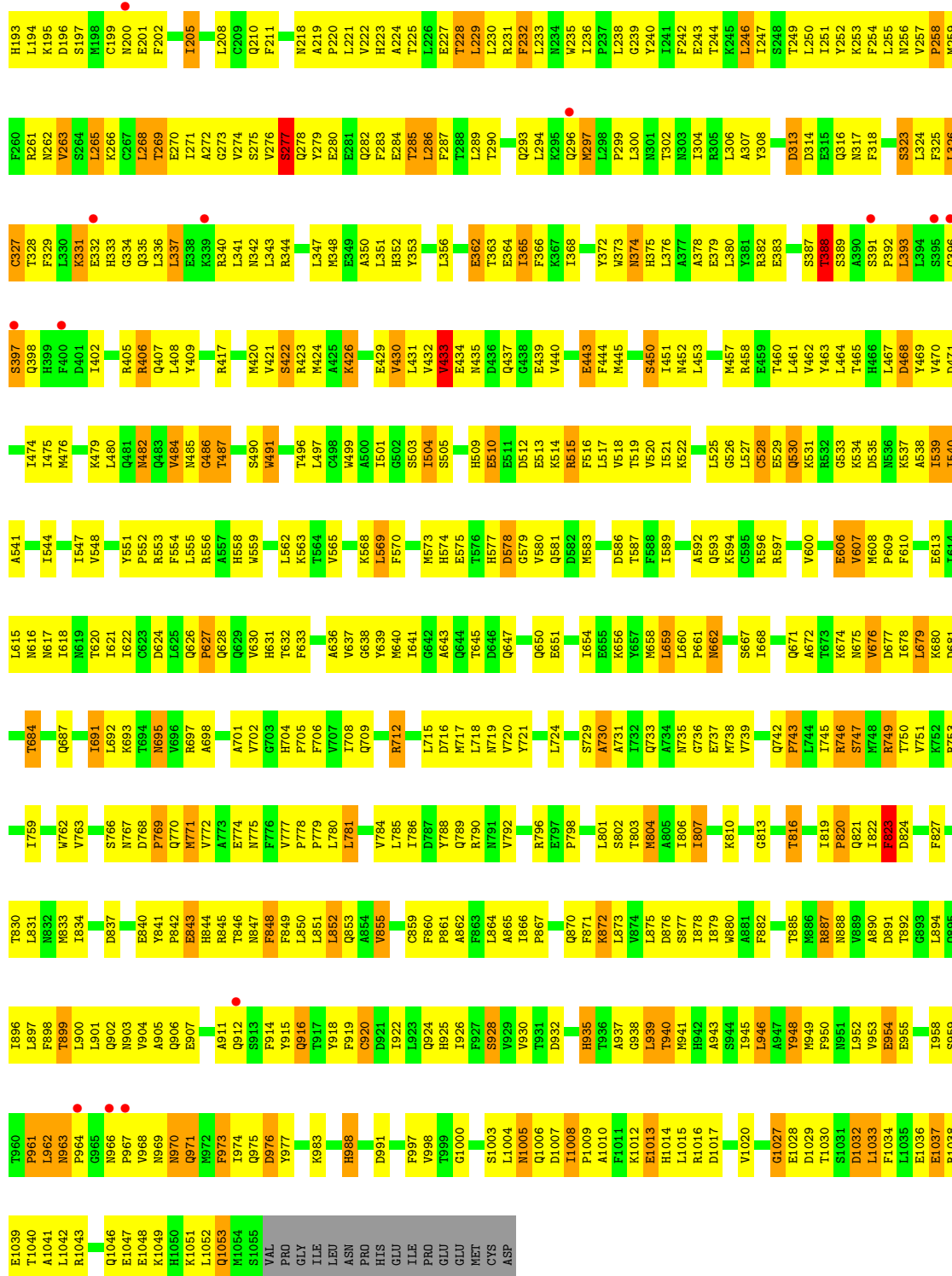
Chain F: 39% 46% 11% . .



• Molecule 3: Exportin-1

Chain A: 2% 33% 52% 11% .





• Molecule 3: Exportin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.09Å 223.73Å 163.06Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	38.63 – 3.42 38.63 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.63-3.42) 88.9 (38.63-2.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.258 , 0.315 0.257 , 0.312	Depositor DCC
R_{free} test set	5238 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 6.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	24084	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	B	0.62	0/2250	0.85	3/3046 (0.1%)
1	E	0.59	1/2278 (0.0%)	0.81	4/3084 (0.1%)
2	C	0.58	0/1423	0.74	0/1921
2	F	0.57	0/1423	0.74	1/1921 (0.1%)
3	A	0.56	2/8584 (0.0%)	0.73	1/11627 (0.0%)
3	D	0.57	0/8584	0.74	0/11627
All	All	0.58	3/24542 (0.0%)	0.76	9/33226 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	CYS	CB-SG	-5.71	1.72	1.81
3	A	491	TRP	NE1-CE2	5.53	1.44	1.37
3	A	528	CYS	CB-SG	-5.08	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	42	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	B	42	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	B	42	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	E	42	ARG	NE-CZ-NH2	10.83	125.72	120.30
2	F	31	LEU	CA-CB-CG	5.93	128.93	115.30
1	B	42	ARG	CD-NE-CZ	5.78	131.69	123.60
1	E	42	ARG	CD-NE-CZ	5.34	131.07	123.60
3	A	393	LEU	CA-CB-CG	5.28	127.44	115.30
1	E	276	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2193	0	2138	241	0
1	E	2221	0	2170	208	0
2	C	1389	0	1419	128	0
2	F	1389	0	1419	121	0
3	A	8413	0	8480	753	0
3	D	8413	0	8480	731	0
4	C	32	0	12	8	0
4	F	32	0	12	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
All	All	24084	0	24130	2091	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 43.

All (2091) 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:A:328:THR:HA	3:A:331:LYS:HD3	1.27	1.14
3:D:328:THR:HA	3:D:331:LYS:HD3	1.33	1.09
3:D:961:PRO:HG2	3:D:973:PHE:HD2	1.16	1.09
1:B:3:GLU:O	1:B:7:LYS:HB2	1.53	1.07
3:D:996:LEU:HD13	3:D:1035:LEU:HD12	1.37	1.06
1:B:159:ASN:HB2	1:B:223:LEU:HD21	1.36	1.06
3:A:528:CYS:HB2	3:A:540:ILE:HG21	1.38	1.06
3:D:528:CYS:HB2	3:D:540:ILE:HG21	1.40	1.04
3:A:962:LEU:HB3	3:A:964:PRO:HD2	1.41	1.02
1:B:255:GLY:HA2	1:B:278:PRO:HD3	1.42	1.01
1:E:4:LEU:HA	1:E:7:LYS:CB	1.89	1.01
1:E:180:GLN:HE22	3:D:684:THR:HG22	1.25	1.01
3:D:892:THR:O	3:D:896:ILE:HG13	1.61	1.01
3:A:107:VAL:O	3:A:111:ILE:HG12	1.61	1.00
3:A:482:ASN:HA	3:A:486:GLY:HA3	1.43	1.00
1:E:4:LEU:HA	1:E:7:LYS:HB2	1.01	1.00
1:B:159:ASN:OD1	1:B:160:ARG:HD2	1.63	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:961:PRO:HG2	3:D:973:PHE:CD2	1.98	0.98
1:B:1:LEU:HD13	3:A:558:HIS:HD2	1.26	0.97
3:A:892:THR:O	3:A:896:ILE:HG13	1.63	0.97
3:D:482:ASN:HA	3:D:486:GLY:HA3	1.42	0.97
1:E:40:SER:HB2	1:E:109:ASP:HB2	1.45	0.96
1:E:4:LEU:CA	1:E:7:LYS:HB2	1.94	0.96
1:E:4:LEU:O	1:E:8:LEU:N	1.97	0.96
3:D:287:PHE:CE2	3:D:337:LEU:HD11	2.00	0.96
3:A:484:VAL:HG13	3:A:530:GLN:OE1	1.66	0.95
3:D:107:VAL:O	3:D:111:ILE:HG12	1.66	0.95
3:A:900:LEU:O	3:A:904:VAL:HG23	1.66	0.95
1:E:255:GLY:HA2	1:E:278:PRO:HD3	1.47	0.95
2:C:148:ASP:HB3	2:C:155:TYR:HE2	1.31	0.94
2:C:32:THR:OG1	2:C:34:GLU:HG2	1.68	0.94
3:A:746:ARG:HG2	3:A:746:ARG:HH11	1.28	0.94
2:C:94:SER:O	2:C:97:THR:HG23	1.67	0.93
1:B:40:SER:HB2	1:B:109:ASP:HB2	1.48	0.93
3:A:287:PHE:CE2	3:A:337:LEU:HD11	2.04	0.93
3:A:887:ARG:HD3	3:A:937:ALA:HB3	1.50	0.93
3:D:484:VAL:HG13	3:D:530:GLN:OE1	1.69	0.92
2:F:94:SER:O	2:F:97:THR:HG23	1.69	0.92
3:A:337:LEU:HD13	3:A:347:LEU:HD12	1.52	0.92
2:F:148:ASP:HB3	2:F:155:TYR:HE2	1.34	0.91
3:D:900:LEU:O	3:D:904:VAL:HG23	1.69	0.91
3:D:337:LEU:HD22	3:D:347:LEU:HB2	1.52	0.91
2:F:31:LEU:HD12	2:F:32:THR:HG22	1.50	0.91
2:F:77:ASP:HA	2:F:80:TYR:CD2	2.05	0.91
1:B:41:GLU:HG3	1:B:109:ASP:HB3	1.52	0.91
3:A:337:LEU:HD22	3:A:347:LEU:HB2	1.51	0.91
3:A:672:ALA:HB2	3:A:678:ILE:HD11	1.53	0.91
1:B:4:LEU:O	1:B:8:LEU:N	2.03	0.91
1:B:124:PRO:HD3	1:B:231:LEU:HD11	1.52	0.91
3:D:672:ALA:HB2	3:D:678:ILE:HD11	1.53	0.91
3:D:746:ARG:HG2	3:D:746:ARG:HH11	1.34	0.90
2:C:93:THR:HG21	2:C:126:ILE:HD12	1.54	0.90
3:A:434:GLU:HB2	3:A:439:GLU:O	1.72	0.89
3:A:1047:GLU:O	3:A:1051:LYS:HD3	1.72	0.88
1:B:4:LEU:HD11	3:A:518:VAL:HG13	1.56	0.88
1:E:41:GLU:HG3	1:E:109:ASP:HB3	1.54	0.88
1:B:64:LEU:HD23	1:B:170:ILE:HD13	1.57	0.88
3:D:887:ARG:HD3	3:D:937:ALA:HB3	1.54	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:LEU:HD23	3:D:564:THR:HG22	1.54	0.87
3:D:650:GLN:HE22	3:D:705:PRO:HG2	1.39	0.87
1:E:124:PRO:HD3	1:E:231:LEU:HD11	1.54	0.87
3:A:650:GLN:HE22	3:A:705:PRO:HG2	1.41	0.86
1:B:55:LEU:HD12	1:B:55:LEU:H	1.38	0.86
3:A:899:THR:HG22	3:A:903:ASN:HD21	1.40	0.86
1:B:124:PRO:HD2	1:B:174:ILE:HD12	1.57	0.84
3:D:14:ARG:HH11	3:D:14:ARG:HG3	1.43	0.84
1:B:190:TRP:CD1	1:B:191:ARG:HG3	2.12	0.84
3:D:899:THR:HG22	3:D:903:ASN:HD21	1.43	0.84
1:E:209:SER:C	1:E:210:LYS:HD2	1.97	0.83
3:D:633:PHE:O	3:D:636:ALA:HB3	1.78	0.83
1:B:160:ARG:NE	1:B:160:ARG:HA	1.93	0.83
1:B:46:LEU:CD2	1:B:50:GLN:HE21	1.90	0.83
1:E:244:VAL:HG13	1:E:245:LEU:HD13	1.59	0.83
2:C:32:THR:HG1	2:C:34:GLU:HG2	1.44	0.83
1:B:160:ARG:HA	1:B:160:ARG:HE	1.42	0.83
2:C:77:ASP:HA	2:C:80:TYR:CD2	2.12	0.83
1:B:244:VAL:HG13	1:B:245:LEU:HD13	1.59	0.82
1:E:64:LEU:HD23	1:E:170:ILE:HD13	1.62	0.82
1:E:175:TYR:HB2	1:E:182:TYR:CE1	2.13	0.82
3:A:771:MET:HG2	3:A:775:ASN:HD22	1.44	0.82
3:D:225:THR:HA	3:D:228:THR:HG22	1.62	0.82
3:D:941:MET:O	3:D:945:ILE:HG13	1.79	0.82
1:B:63:ARG:HH12	1:B:70:THR:HB	1.43	0.82
3:A:736:GLY:O	3:A:739:VAL:HG23	1.80	0.82
1:E:51:LYS:NZ	1:E:263:THR:HA	1.94	0.82
2:F:93:THR:HG21	2:F:126:ILE:HD12	1.62	0.81
1:B:1:LEU:HD13	3:A:558:HIS:CD2	2.13	0.81
3:A:533:GLY:O	3:A:537:LYS:HG3	1.80	0.81
1:E:258:PHE:HD2	1:E:274:GLY:O	1.61	0.81
3:D:788:TYR:CE1	3:D:796:ARG:HB3	2.15	0.81
3:D:771:MET:HG2	3:D:775:ASN:HD22	1.44	0.81
3:A:33:ASN:HB3	3:A:44:ARG:HG3	1.63	0.81
1:B:282:SER:HA	1:B:286:GLY:HA2	1.60	0.81
1:E:129:ALA:HA	1:E:141:TYR:O	1.81	0.81
1:B:110:VAL:HG11	1:B:285:LEU:HD13	1.62	0.81
1:B:172:ASP:HB2	1:B:188:MET:HE1	1.61	0.81
1:B:258:PHE:HD2	1:B:274:GLY:O	1.64	0.81
3:A:73:MET:HB2	3:A:122:LYS:HE3	1.61	0.80
3:A:823:PHE:HZ	3:A:852:LEU:HD13	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:633:PHE:O	3:A:636:ALA:HB3	1.82	0.80
1:E:175:TYR:HE2	1:E:177:GLU:HG2	1.45	0.80
1:B:129:ALA:HA	1:B:141:TYR:O	1.82	0.79
3:A:225:THR:HA	3:A:228:THR:HG22	1.64	0.79
3:A:575:GLU:HG2	3:A:580:VAL:HG11	1.63	0.79
1:E:190:TRP:CD1	1:E:191:ARG:HG3	2.17	0.79
3:A:926:ILE:O	3:A:930:VAL:HG23	1.82	0.79
1:B:37:LEU:HB2	1:B:39:GLN:NE2	1.97	0.79
3:A:899:THR:CG2	3:A:903:ASN:HD21	1.96	0.79
1:B:102:MET:HG3	1:B:266:SER:O	1.83	0.79
1:B:13:ILE:HG21	3:A:575:GLU:CD	2.02	0.78
3:A:586:ASP:O	3:A:589:ILE:HG22	1.83	0.78
3:D:476:MET:HE3	3:D:501:ILE:HG12	1.64	0.78
3:D:996:LEU:CD1	3:D:1035:LEU:HD12	2.12	0.78
3:A:569:LEU:HD21	3:A:587:THR:HG22	1.63	0.78
3:A:899:THR:HG22	3:A:903:ASN:ND2	1.99	0.78
2:C:28:LYS:O	2:C:32:THR:HG23	1.82	0.78
3:A:485:ASN:O	3:A:487:THR:N	2.16	0.78
3:A:834:ILE:HG22	3:A:845:ARG:HG2	1.65	0.78
3:D:225:THR:HA	3:D:228:THR:CG2	2.13	0.78
3:D:337:LEU:HD13	3:D:347:LEU:HD12	1.65	0.78
3:D:990:GLN:HB3	3:D:1028:GLU:HG2	1.64	0.78
3:A:219:ALA:HB3	3:A:220:PRO:HD3	1.65	0.78
3:D:219:ALA:HB3	3:D:220:PRO:HD3	1.66	0.78
3:D:569:LEU:HD21	3:D:587:THR:HG22	1.64	0.77
3:D:823:PHE:HZ	3:D:852:LEU:HD13	1.48	0.77
1:E:37:LEU:HB2	1:E:39:GLN:NE2	1.99	0.77
3:D:899:THR:HG22	3:D:903:ASN:ND2	2.00	0.77
1:E:160:ARG:CG	1:E:160:ARG:HH11	1.97	0.77
3:D:586:ASP:O	3:D:589:ILE:HG22	1.84	0.77
3:D:819:ILE:O	3:D:823:PHE:HB2	1.84	0.77
3:D:899:THR:CG2	3:D:903:ASN:HD21	1.98	0.77
3:D:926:ILE:O	3:D:930:VAL:HG23	1.84	0.77
1:B:144:SER:O	1:B:146:TYR:N	2.18	0.77
3:A:476:MET:HE3	3:A:501:ILE:HG12	1.67	0.77
3:D:433:VAL:HG12	3:D:441:VAL:HG23	1.65	0.77
1:B:209:SER:C	1:B:210:LYS:HD2	2.06	0.76
1:E:119:ILE:HD11	1:E:259:TYR:HB2	1.68	0.76
3:A:819:ILE:O	3:A:823:PHE:HB2	1.85	0.76
3:D:340:ARG:HB3	3:D:342:ASN:OD1	1.85	0.76
3:A:340:ARG:HB3	3:A:342:ASN:OD1	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:575:GLU:HG2	3:D:580:VAL:HG11	1.67	0.75
3:A:866:ILE:HB	3:A:867:PRO:HD2	1.68	0.75
3:D:632:THR:HA	3:D:697:ARG:HH22	1.51	0.75
3:D:706:PHE:CZ	3:D:709:GLN:HG2	2.21	0.75
1:B:119:ILE:HD11	1:B:259:TYR:HB2	1.68	0.75
3:D:123:GLU:O	3:D:127:ILE:HD13	1.85	0.75
3:A:337:LEU:CD2	3:A:347:LEU:HB2	2.17	0.75
3:A:274:VAL:HG12	3:A:275:SER:H	1.51	0.75
1:B:4:LEU:HA	1:B:7:LYS:HB2	1.68	0.75
1:B:175:TYR:HB2	1:B:182:TYR:CE1	2.21	0.74
3:A:518:VAL:O	3:A:522:LYS:HB2	1.86	0.74
1:E:56:ASP:OD1	1:E:59:ASN:HB2	1.85	0.74
2:C:122:ASN:O	2:C:123:LYS:HB2	1.87	0.74
2:F:177:VAL:HG22	2:F:178:ALA:H	1.52	0.74
3:D:238:LEU:HD22	3:D:242:PHE:HE2	1.52	0.74
1:B:55:LEU:HD13	1:B:57:TYR:CE2	2.22	0.74
1:B:175:TYR:HE2	1:B:177:GLU:HG2	1.51	0.74
1:E:102:MET:HG3	1:E:266:SER:O	1.87	0.74
3:A:225:THR:HA	3:A:228:THR:CG2	2.18	0.74
3:A:479:LYS:HE2	3:A:479:LYS:HA	1.69	0.74
3:D:555:LEU:HB3	3:D:562:LEU:HD13	1.68	0.74
3:A:941:MET:O	3:A:945:ILE:HG13	1.87	0.74
3:A:970:ASN:HD22	3:A:970:ASN:N	1.84	0.74
3:D:479:LYS:HA	3:D:479:LYS:HE2	1.68	0.74
3:D:996:LEU:HD13	3:D:1035:LEU:CD1	2.17	0.73
3:A:238:LEU:HD22	3:A:242:PHE:HE2	1.52	0.73
3:A:681:ASP:HB3	3:A:684:THR:HG23	1.69	0.73
3:D:518:VAL:O	3:D:522:LYS:HB2	1.88	0.73
3:D:570:PHE:O	3:D:573:MET:HB2	1.87	0.73
1:B:119:ILE:HD13	1:B:259:TYR:O	1.87	0.73
3:A:424:MET:HA	3:A:457:MET:HE2	1.71	0.73
2:F:110:ARG:NH2	3:D:176:GLU:OE1	2.20	0.73
2:F:126:ILE:HG22	2:F:128:ASP:H	1.54	0.73
1:E:175:TYR:CE2	1:E:177:GLU:HG2	2.24	0.72
3:D:763:VAL:O	3:D:810:LYS:HG2	1.88	0.72
1:B:4:LEU:CD1	3:A:518:VAL:HG13	2.19	0.72
3:A:471:ASP:O	3:A:475:ILE:HG13	1.89	0.72
3:A:706:PHE:CZ	3:A:709:GLN:HG2	2.24	0.72
1:B:13:ILE:HD11	3:A:538:ALA:HA	1.71	0.72
2:F:90:PHE:HB2	2:F:97:THR:OG1	1.88	0.72
2:C:90:PHE:HB2	2:C:97:THR:OG1	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:834:ILE:O	3:D:845:ARG:NH2	2.23	0.72
3:D:970:ASN:HD22	3:D:970:ASN:N	1.86	0.72
1:B:46:LEU:HD22	1:B:50:GLN:HE21	1.53	0.72
1:E:124:PRO:HD2	1:E:174:ILE:HD12	1.71	0.72
3:A:106:VAL:O	3:A:110:ILE:HG13	1.90	0.72
3:A:541:ALA:HA	3:A:544:ILE:HD12	1.71	0.72
3:D:23:LEU:HD11	3:D:26:ASN:HB2	1.72	0.72
3:D:274:VAL:HG12	3:D:275:SER:H	1.54	0.72
3:A:25:ILE:H	3:A:25:ILE:HD12	1.54	0.71
3:D:121:GLU:C	3:D:123:GLU:H	1.91	0.71
1:B:63:ARG:HH11	1:B:95:LYS:HZ2	1.36	0.71
2:C:14:VAL:HG21	2:C:80:TYR:CD1	2.25	0.71
3:D:105:TYR:O	3:D:109:LEU:HD12	1.91	0.71
3:D:698:ALA:O	3:D:702:VAL:HG23	1.90	0.71
1:B:24:HIS:HE1	1:B:108:ILE:HG23	1.56	0.71
3:A:327:CYS:O	3:A:331:LYS:HB3	1.90	0.71
3:A:788:TYR:CE1	3:A:796:ARG:HB3	2.26	0.71
3:D:224:ALA:O	3:D:228:THR:HG22	1.90	0.71
1:E:172:ASP:HB2	1:E:188:MET:HE1	1.72	0.71
3:D:533:GLY:O	3:D:537:LYS:HG3	1.91	0.71
2:C:44:GLY:HA3	3:A:45:MET:HE3	1.72	0.71
2:C:54:THR:HB	2:C:174:LEU:HD11	1.72	0.71
3:D:293:GLN:O	3:D:297:MET:HG3	1.90	0.71
1:B:357:MET:HG3	3:A:719:ASN:ND2	2.05	0.71
3:A:575:GLU:CG	3:A:580:VAL:HG11	2.20	0.71
1:E:8:LEU:CD2	3:D:564:THR:HG22	2.20	0.71
1:E:211:LEU:HB2	1:E:212:PRO:HD3	1.73	0.71
2:F:44:GLY:HA3	3:D:45:MET:CE	2.20	0.71
2:C:126:ILE:HG22	2:C:128:ASP:H	1.56	0.71
1:B:107:LEU:HB2	1:B:274:GLY:HA3	1.73	0.71
1:E:144:SER:O	1:E:146:TYR:N	2.24	0.71
1:B:13:ILE:HG21	3:A:575:GLU:OE1	1.90	0.70
1:B:241:LEU:O	1:B:244:VAL:HG12	1.91	0.70
2:F:54:THR:HB	2:F:174:LEU:HD11	1.72	0.70
3:D:106:VAL:O	3:D:110:ILE:HG13	1.91	0.70
3:D:497:LEU:O	3:D:501:ILE:HG13	1.91	0.70
3:D:681:ASP:HB3	3:D:684:THR:HG23	1.72	0.70
3:A:50:LEU:O	3:A:53:LEU:HG	1.92	0.70
1:E:119:ILE:HD13	1:E:259:TYR:O	1.91	0.70
3:A:698:ALA:O	3:A:702:VAL:HG23	1.91	0.70
3:A:141:GLU:HB2	3:A:145:HIS:HB2	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:VAL:HG21	2:F:80:TYR:CD1	2.27	0.70
3:A:632:THR:HA	3:A:697:ARG:HH22	1.57	0.69
3:A:770:GLN:O	3:A:774:GLU:HG3	1.92	0.69
2:C:93:THR:HG21	2:C:126:ILE:CD1	2.21	0.69
3:A:23:LEU:HD11	3:A:26:ASN:HB2	1.74	0.69
3:D:846:THR:HG23	3:D:888:ASN:HD22	1.58	0.69
1:E:241:LEU:O	1:E:244:VAL:HG12	1.91	0.69
2:F:122:ASN:O	2:F:123:LYS:HB2	1.92	0.69
3:D:116:ASP:C	3:D:118:THR:H	1.96	0.69
3:D:179:PHE:CE1	3:D:195:LYS:HG3	2.26	0.69
3:A:763:VAL:O	3:A:810:LYS:HG2	1.92	0.69
3:A:804:MET:SD	3:A:807:ILE:HD11	2.33	0.69
3:A:497:LEU:O	3:A:501:ILE:HG13	1.91	0.69
1:E:282:SER:HB3	1:E:287:VAL:HA	1.74	0.69
1:B:151:PHE:N	1:B:151:PHE:HD1	1.91	0.69
3:A:823:PHE:CZ	3:A:852:LEU:HD13	2.27	0.69
3:D:50:LEU:O	3:D:53:LEU:HG	1.93	0.69
3:D:25:ILE:H	3:D:25:ILE:HD12	1.57	0.69
3:D:373:TRP:HA	3:D:373:TRP:CE3	2.28	0.69
1:B:24:HIS:O	1:B:26:ARG:N	2.26	0.68
3:A:224:ALA:O	3:A:228:THR:HG22	1.93	0.68
2:F:31:LEU:HB3	2:F:50:LEU:HD21	1.74	0.68
3:D:17:LEU:HD23	3:D:22:LYS:NZ	2.08	0.68
3:D:866:ILE:HB	3:D:867:PRO:HD2	1.73	0.68
3:A:45:MET:O	3:A:49:VAL:HG23	1.93	0.68
1:E:63:ARG:NH1	1:E:72:MET:HB2	2.07	0.68
1:E:160:ARG:HH11	1:E:160:ARG:HG2	1.55	0.68
2:F:103:ASN:O	2:F:106:ARG:HB3	1.94	0.68
3:A:658:MET:O	3:A:662:ASN:HB2	1.93	0.68
3:D:471:ASP:O	3:D:475:ILE:HG13	1.93	0.68
3:D:766:SER:H	3:D:810:LYS:NZ	1.91	0.68
3:A:109:LEU:O	3:A:113:THR:HG23	1.94	0.68
3:D:424:MET:HA	3:D:457:MET:HE2	1.76	0.68
3:A:834:ILE:O	3:A:845:ARG:NH2	2.27	0.68
1:E:24:HIS:HE1	1:E:108:ILE:HG23	1.59	0.68
3:D:916:GLN:HE22	3:D:959:SER:HB2	1.58	0.68
3:D:14:ARG:HH11	3:D:14:ARG:CG	2.06	0.68
3:D:337:LEU:CD2	3:D:347:LEU:HB2	2.21	0.68
1:B:260:HIS:CE1	1:B:262:GLN:HG3	2.28	0.68
3:A:555:LEU:HB3	3:A:562:LEU:HD13	1.75	0.68
2:F:139:HIS:HB2	2:F:144:LEU:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:627:PRO:O	3:D:630:VAL:HG12	1.93	0.68
3:D:759:ILE:HD13	3:D:780:LEU:HD21	1.75	0.68
3:A:179:PHE:CE1	3:A:195:LYS:HG3	2.27	0.67
3:A:678:ILE:HD12	3:A:679:LEU:N	2.10	0.67
2:F:77:ASP:HB2	3:D:77:TYR:OH	1.94	0.67
1:E:107:LEU:HB2	1:E:274:GLY:HA3	1.76	0.67
1:B:175:TYR:CE2	1:B:177:GLU:HG2	2.30	0.67
1:E:1:LEU:HG	1:E:2:ASN:N	2.10	0.67
3:D:834:ILE:HG22	3:D:845:ARG:HG2	1.76	0.67
1:E:24:HIS:ND1	1:E:25:PRO:HD2	2.09	0.67
3:D:631:HIS:CE1	3:D:693:LYS:HB2	2.29	0.67
3:D:823:PHE:CZ	3:D:852:LEU:HD13	2.29	0.67
3:A:164:CYS:SG	3:A:221:LEU:HD11	2.35	0.67
3:A:284:GLU:HG3	3:A:343:LEU:HD21	1.77	0.67
3:A:179:PHE:HE1	3:A:195:LYS:HG3	1.59	0.67
3:A:973:PHE:CD1	3:A:973:PHE:C	2.66	0.67
1:E:217:LEU:HG	1:E:228:PHE:HB2	1.76	0.67
3:A:105:TYR:O	3:A:109:LEU:HD12	1.95	0.67
3:D:45:MET:O	3:D:49:VAL:HG23	1.94	0.67
3:D:770:GLN:O	3:D:774:GLU:HG3	1.95	0.67
2:C:14:VAL:HG21	2:C:80:TYR:HD1	1.60	0.67
3:A:528:CYS:HB2	3:A:540:ILE:CG2	2.21	0.67
3:A:615:LEU:HD23	3:A:618:ILE:HD11	1.77	0.67
1:E:160:ARG:HG2	1:E:160:ARG:NH1	2.06	0.67
1:B:42:ARG:O	1:B:45:ARG:HB2	1.93	0.67
1:E:151:PHE:N	1:E:151:PHE:HD1	1.93	0.67
3:A:293:GLN:O	3:A:297:MET:HG3	1.94	0.66
3:A:704:HIS:CD2	3:A:767:ASN:H	2.13	0.66
3:D:593:GLN:HG3	3:D:639:TYR:CD2	2.29	0.66
2:C:75:LEU:HD12	2:C:75:LEU:N	2.10	0.66
3:A:570:PHE:O	3:A:573:MET:HB2	1.95	0.66
3:D:131:ASN:HD21	3:D:166:ASN:HD21	1.42	0.66
3:A:819:ILE:HD12	3:A:855:VAL:CG2	2.25	0.66
3:A:902:GLN:O	3:A:906:GLN:NE2	2.28	0.66
3:A:916:GLN:HE22	3:A:959:SER:HB2	1.60	0.66
3:A:1040:THR:HA	3:A:1043:ARG:HG2	1.76	0.66
3:D:179:PHE:HE1	3:D:195:LYS:HG3	1.59	0.66
3:D:678:ILE:HD12	3:D:679:LEU:N	2.11	0.66
1:B:211:LEU:HB2	1:B:212:PRO:HD3	1.78	0.66
3:A:150:ILE:HG23	3:A:151:SER:H	1.60	0.66
1:E:51:LYS:HZ3	1:E:263:THR:HA	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:LEU:HD22	3:D:558:HIS:HD2	1.60	0.66
1:E:260:HIS:CE1	1:E:262:GLN:HG3	2.30	0.66
2:F:15:LEU:HD22	2:F:23:LYS:HB3	1.77	0.66
3:D:902:GLN:O	3:D:906:GLN:NE2	2.29	0.66
3:D:997:PHE:HD1	3:D:1014:HIS:CE1	2.14	0.66
1:B:154:LEU:HG	1:B:224:ASN:HB2	1.76	0.66
3:D:769:PRO:HG2	3:D:770:GLN:H	1.61	0.66
3:A:286:LEU:HD12	3:A:286:LEU:O	1.95	0.66
3:A:509:HIS:O	3:A:512:ASP:HB2	1.96	0.66
2:C:44:GLY:HA3	3:A:45:MET:CE	2.24	0.66
3:A:759:ILE:HD13	3:A:780:LEU:HD21	1.77	0.66
1:E:277:ARG:NH2	3:D:620:THR:HG21	2.11	0.66
2:F:14:VAL:HG21	2:F:80:TYR:HD1	1.60	0.66
3:D:819:ILE:HD12	3:D:855:VAL:CG2	2.25	0.66
3:A:78:TYR:O	3:A:81:GLN:HB2	1.96	0.65
3:D:509:HIS:O	3:D:512:ASP:HB2	1.96	0.65
3:A:131:ASN:HD21	3:A:166:ASN:HD21	1.44	0.65
3:D:373:TRP:HA	3:D:373:TRP:HE3	1.61	0.65
2:C:139:HIS:HB2	2:C:144:LEU:O	1.97	0.65
3:A:762:TRP:HH2	3:A:772:VAL:HG22	1.61	0.65
1:E:147:CYS:SG	1:E:150:ARG:NH2	2.69	0.65
3:D:76:LYS:O	3:D:80:LEU:HD22	1.96	0.65
3:D:327:CYS:O	3:D:331:LYS:HB3	1.96	0.65
3:D:736:GLY:O	3:D:739:VAL:HG22	1.96	0.65
1:B:24:HIS:ND1	1:B:25:PRO:HD2	2.11	0.65
3:A:373:TRP:HA	3:A:373:TRP:CE3	2.32	0.65
1:E:24:HIS:O	1:E:26:ARG:N	2.27	0.65
3:D:905:ALA:HB3	3:D:906:GLN:NE2	2.11	0.65
3:A:900:LEU:HA	3:A:903:ASN:HD22	1.61	0.65
3:D:541:ALA:HA	3:D:544:ILE:HD12	1.79	0.65
1:B:175:TYR:CE2	1:B:177:GLU:HA	2.32	0.65
2:C:103:ASN:O	2:C:106:ARG:HB3	1.97	0.65
1:E:1:LEU:O	1:E:4:LEU:HD12	1.97	0.65
3:D:266:LYS:O	3:D:270:GLU:HG2	1.96	0.65
3:D:658:MET:O	3:D:662:ASN:HB2	1.96	0.65
2:F:124:VAL:HG22	2:F:150:SER:HB2	1.77	0.65
3:D:150:ILE:HG23	3:D:151:SER:H	1.62	0.65
3:D:788:TYR:O	3:D:796:ARG:HG2	1.97	0.65
1:B:138:THR:HG22	1:B:151:PHE:CE1	2.32	0.65
2:F:44:GLY:HA3	3:D:45:MET:HE3	1.78	0.65
2:C:148:ASP:HB3	2:C:155:TYR:CE2	2.23	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:THR:HG21	2:F:126:ILE:CD1	2.26	0.65
1:B:63:ARG:NH1	1:B:95:LYS:NZ	2.45	0.64
3:A:30:ASN:HB3	3:A:47:GLN:NE2	2.12	0.64
3:A:766:SER:H	3:A:810:LYS:NZ	1.94	0.64
2:F:64:TRP:CE3	2:F:79:TYR:HB3	2.33	0.64
3:D:1035:LEU:O	3:D:1036:GLU:C	2.35	0.64
1:B:281:VAL:HG13	1:B:282:SER:H	1.63	0.64
1:E:175:TYR:CE2	1:E:177:GLU:HA	2.33	0.64
1:E:186:ASP:OD1	1:E:203:ARG:HD2	1.96	0.64
3:D:30:ASN:HB3	3:D:47:GLN:NE2	2.13	0.64
3:D:528:CYS:HB2	3:D:540:ILE:CG2	2.23	0.64
1:B:159:ASN:HB2	1:B:223:LEU:CD2	2.21	0.64
3:D:434:GLU:HG3	3:D:439:GLU:O	1.96	0.64
1:B:351:ASP:HB2	1:B:352:HIS:ND1	2.12	0.64
2:F:178:ALA:O	2:F:179:MET:HB2	1.97	0.64
1:B:3:GLU:O	1:B:7:LYS:CB	2.39	0.64
3:A:823:PHE:O	3:A:827:PHE:CB	2.45	0.64
3:A:1038:ARG:HA	3:A:1041:ALA:HB3	1.79	0.64
1:B:186:ASP:OD1	1:B:203:ARG:HD2	1.97	0.64
1:B:349:SER:HB3	1:B:350:PRO:HD2	1.80	0.64
3:A:56:HIS:N	3:A:57:PRO:HD3	2.13	0.64
2:F:92:VAL:HG13	2:F:122:ASN:O	1.98	0.64
3:D:336:LEU:HD12	3:D:336:LEU:O	1.96	0.64
3:D:804:MET:SD	3:D:807:ILE:HD11	2.38	0.64
1:B:4:LEU:HD11	3:A:518:VAL:HA	1.80	0.64
1:B:151:PHE:N	1:B:151:PHE:CD1	2.63	0.64
2:C:87:ILE:HA	2:C:118:VAL:O	1.97	0.64
3:A:336:LEU:HD12	3:A:336:LEU:O	1.96	0.64
3:D:463:TYR:O	3:D:467:LEU:HG	1.98	0.64
3:A:299:PRO:HD2	3:A:302:THR:HG21	1.77	0.64
3:A:949:MET:O	3:A:953:VAL:HG23	1.97	0.64
2:F:101:VAL:HB	2:F:102:PRO:HD3	1.80	0.64
1:B:217:LEU:HG	1:B:228:PHE:HB2	1.79	0.64
3:A:860:PHE:N	3:A:861:PRO:HD2	2.13	0.64
3:D:485:ASN:O	3:D:487:THR:N	2.30	0.64
3:D:622:ILE:HG21	3:D:633:PHE:CD2	2.33	0.64
1:B:63:ARG:HH11	1:B:95:LYS:NZ	1.96	0.64
1:B:111:PRO:HD2	1:B:114:LEU:HD13	1.79	0.63
2:C:77:ASP:HB2	3:A:77:TYR:OH	1.97	0.63
2:C:115:ILE:O	2:C:115:ILE:HG13	1.98	0.63
3:A:56:HIS:C	3:A:58:ASP:H	2.02	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:290:THR:O	3:A:293:GLN:HB2	1.98	0.63
3:D:434:GLU:HA	3:D:439:GLU:O	1.98	0.63
3:D:798:PRO:HG3	3:D:844:HIS:CE1	2.32	0.63
3:A:82:ILE:O	3:A:86:VAL:HG23	1.98	0.63
3:D:78:TYR:O	3:D:81:GLN:HB2	1.99	0.63
3:D:575:GLU:CG	3:D:580:VAL:HG11	2.27	0.63
3:D:261:ARG:HD2	3:D:318:PHE:CG	2.33	0.63
3:D:650:GLN:NE2	3:D:705:PRO:HG2	2.12	0.63
3:D:960:THR:HG22	3:D:963:ASN:H	1.62	0.63
3:D:628:GLN:NE2	3:D:628:GLN:H	1.96	0.63
3:D:1008:ILE:HD12	3:D:1008:ILE:O	1.98	0.63
1:B:6:LEU:O	1:B:9:ALA:HB3	1.98	0.63
3:D:949:MET:O	3:D:953:VAL:HG23	1.98	0.63
1:B:120:VAL:HA	1:B:257:LEU:O	1.99	0.63
3:A:127:ILE:HG22	3:A:131:ASN:ND2	2.12	0.63
3:A:841:TYR:O	3:A:845:ARG:HG3	1.99	0.63
3:D:528:CYS:CB	3:D:540:ILE:HG21	2.24	0.63
3:D:1048:GLU:O	3:D:1052:LEU:HG	1.99	0.63
3:D:860:PHE:N	3:D:861:PRO:HD2	2.14	0.63
3:D:900:LEU:HA	3:D:903:ASN:HD22	1.64	0.63
3:A:132:MET:HE3	3:A:135:VAL:HB	1.80	0.62
3:A:762:TRP:CH2	3:A:772:VAL:HG22	2.34	0.62
3:A:1043:ARG:NH1	3:A:1043:ARG:HA	2.13	0.62
3:D:476:MET:CE	3:D:501:ILE:HG12	2.28	0.62
1:B:154:LEU:HD13	1:B:215:GLU:HG2	1.81	0.62
3:A:516:PHE:CE1	3:A:520:VAL:HG21	2.34	0.62
3:A:568:LYS:HE2	3:A:568:LYS:HA	1.79	0.62
3:A:997:PHE:HD1	3:A:1014:HIS:CE1	2.18	0.62
1:E:151:PHE:N	1:E:151:PHE:CD1	2.64	0.62
3:A:769:PRO:HG2	3:A:770:GLN:H	1.63	0.62
2:F:87:ILE:HA	2:F:118:VAL:O	1.99	0.62
3:D:299:PRO:HD2	3:D:302:THR:HG21	1.79	0.62
3:A:115:SER:HB3	3:A:162:SER:CB	2.28	0.62
3:A:627:PRO:O	3:A:630:VAL:HG12	1.99	0.62
1:E:154:LEU:HG	1:E:224:ASN:HB2	1.79	0.62
2:C:92:VAL:HG13	2:C:122:ASN:O	2.00	0.62
2:F:32:THR:OG1	2:F:34:GLU:HG2	2.00	0.62
3:D:56:HIS:N	3:D:57:PRO:HD3	2.15	0.62
3:D:860:PHE:HE1	3:D:900:LEU:HG	1.64	0.62
1:B:4:LEU:HD22	3:A:521:ILE:HD11	1.81	0.62
1:B:260:HIS:O	1:B:263:THR:HG22	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ARG:NH2	3:A:620:THR:HG21	2.15	0.62
3:A:153:ILE:HA	3:A:156:ALA:HB3	1.81	0.62
3:A:804:MET:HB3	3:A:851:LEU:HD13	1.82	0.62
3:D:513:GLU:HA	3:D:516:PHE:HB3	1.80	0.62
3:D:637:VAL:O	3:D:641:ILE:HD12	1.99	0.62
3:A:607:VAL:HG22	3:A:608:MET:SD	2.40	0.62
3:D:141:GLU:HB2	3:D:145:HIS:HB2	1.82	0.62
3:D:286:LEU:HD12	3:D:286:LEU:O	1.99	0.62
3:D:516:PHE:CE1	3:D:520:VAL:HG21	2.35	0.62
1:B:204:PHE:O	1:B:207:MET:HB2	2.00	0.62
2:C:64:TRP:CE3	2:C:79:TYR:HB3	2.35	0.62
3:A:337:LEU:HD22	3:A:347:LEU:CB	2.26	0.62
3:A:627:PRO:O	3:A:631:HIS:CD2	2.53	0.62
2:F:148:ASP:HB3	2:F:155:TYR:CE2	2.26	0.62
3:D:30:ASN:N	3:D:30:ASN:ND2	2.48	0.62
3:D:421:VAL:HG11	3:D:476:MET:HG2	1.81	0.62
3:A:266:LYS:O	3:A:270:GLU:HG2	1.98	0.62
3:A:513:GLU:HA	3:A:516:PHE:HB3	1.81	0.62
3:D:940:THR:OG1	3:D:1012:LYS:HE3	2.00	0.62
1:B:258:PHE:CD2	1:B:274:GLY:O	2.51	0.62
1:E:7:LYS:HB3	3:D:525:LEU:HD23	1.82	0.62
3:D:82:ILE:O	3:D:86:VAL:HG23	2.00	0.62
3:D:399:HIS:HB3	3:D:401:ASP:H	1.64	0.62
1:B:147:CYS:SG	1:B:150:ARG:NH2	2.72	0.61
3:A:30:ASN:N	3:A:30:ASN:ND2	2.48	0.61
3:A:74:ASN:O	3:A:77:TYR:HB3	2.00	0.61
3:A:193:HIS:O	3:A:197:SER:HB2	2.00	0.61
3:A:484:VAL:HG22	3:A:527:LEU:HB2	1.81	0.61
3:A:846:THR:HG23	3:A:888:ASN:HD22	1.65	0.61
1:E:111:PRO:HD2	1:E:114:LEU:HD13	1.82	0.61
1:E:180:GLN:NE2	3:D:684:THR:HG22	2.06	0.61
3:D:54:LYS:O	3:D:55:GLU:HB2	2.00	0.61
3:D:484:VAL:HG22	3:D:527:LEU:HB2	1.81	0.61
1:B:51:LYS:HZ2	1:B:264:HIS:HB2	1.65	0.61
3:A:192:LYS:HA	3:A:192:LYS:HE3	1.82	0.61
1:E:98:ALA:HB2	1:E:145:GLY:N	2.15	0.61
1:E:260:HIS:O	1:E:263:THR:HG22	2.00	0.61
1:B:40:SER:O	1:B:44:ARG:HG3	2.00	0.61
1:B:110:VAL:HG11	1:B:285:LEU:CD1	2.30	0.61
1:E:258:PHE:CD2	1:E:274:GLY:O	2.49	0.61
3:D:615:LEU:HD23	3:D:618:ILE:HD11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:NH1	1:B:70:THR:H	1.98	0.61
3:A:650:GLN:NE2	3:A:705:PRO:HG2	2.14	0.61
3:A:788:TYR:O	3:A:796:ARG:HG2	2.00	0.61
1:E:190:TRP:O	1:E:191:ARG:C	2.39	0.61
3:D:192:LYS:HA	3:D:192:LYS:HE3	1.83	0.61
3:D:996:LEU:HD22	3:D:1033:LEU:HD11	1.82	0.61
2:C:153:SER:O	3:A:433:VAL:HG21	2.00	0.61
3:A:388:THR:OG1	3:A:402:ILE:HD13	2.00	0.61
1:B:46:LEU:HD23	1:B:50:GLN:HG3	1.82	0.61
1:B:98:ALA:HB2	1:B:145:GLY:N	2.16	0.61
1:B:225:PRO:HB2	1:B:226:PHE:CD2	2.36	0.61
3:D:153:ILE:HA	3:D:156:ALA:HB3	1.82	0.61
1:B:349:SER:HB3	1:B:350:PRO:CD	2.31	0.61
3:A:628:GLN:HA	3:A:631:HIS:HD2	1.66	0.61
3:A:628:GLN:NE2	3:A:628:GLN:H	1.99	0.61
3:A:877:SER:O	3:A:880:TRP:HB3	2.01	0.61
2:F:13:LEU:HD12	2:F:13:LEU:C	2.21	0.61
3:A:127:ILE:O	3:A:130:LEU:N	2.32	0.60
1:E:40:SER:O	1:E:44:ARG:HG3	2.01	0.60
2:F:115:ILE:HG13	2:F:115:ILE:O	2.01	0.60
3:D:846:THR:HG23	3:D:888:ASN:ND2	2.16	0.60
3:D:1044:GLN:HG3	3:D:1044:GLN:O	2.00	0.60
3:A:966:ASN:N	3:A:967:PRO:HD2	2.15	0.60
3:D:337:LEU:HD23	3:D:343:LEU:HB3	1.83	0.60
1:B:130:LEU:HG	1:B:132:VAL:HG23	1.83	0.60
3:A:373:TRP:HA	3:A:373:TRP:HE3	1.66	0.60
3:D:43:GLN:HA	3:D:46:ALA:HB3	1.83	0.60
3:D:132:MET:HE3	3:D:135:VAL:HB	1.82	0.60
3:D:945:ILE:O	3:D:949:MET:HG3	2.02	0.60
3:A:33:ASN:CB	3:A:44:ARG:HG3	2.31	0.60
3:A:99:CYS:HA	3:A:102:ILE:HD12	1.83	0.60
3:D:96:ARG:HH22	3:D:145:HIS:HB3	1.65	0.60
3:D:164:CYS:SG	3:D:221:LEU:HD11	2.42	0.60
3:D:704:HIS:HD2	3:D:766:SER:CB	2.13	0.60
1:B:1:LEU:CD1	3:A:558:HIS:HD2	2.08	0.60
3:A:116:ASP:HB2	3:A:119:CYS:HB2	1.83	0.60
3:A:178:VAL:HG11	3:A:194:LEU:HB3	1.84	0.60
3:A:344:ARG:O	3:A:348:MET:HG2	2.01	0.60
3:A:1014:HIS:O	3:A:1017:ASP:HB3	2.02	0.60
1:E:146:TYR:CD1	1:E:148:VAL:HG22	2.36	0.60
3:D:1008:ILE:HD12	3:D:1008:ILE:C	2.22	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:823:PHE:O	3:A:827:PHE:HB2	2.01	0.60
3:A:961:PRO:HD3	3:A:970:ASN:OD1	2.02	0.60
1:E:284:VAL:HG12	1:E:285:LEU:CD1	2.31	0.60
3:D:362:GLU:O	3:D:364:GLU:N	2.32	0.60
1:B:103:LEU:HD13	1:B:268:GLY:HA2	1.84	0.60
1:B:358:GLU:O	1:B:359:ASN:O	2.19	0.60
3:A:274:VAL:HG12	3:A:275:SER:N	2.17	0.60
3:D:568:LYS:HA	3:D:568:LYS:HE2	1.84	0.60
3:A:25:ILE:HD12	3:A:25:ILE:N	2.17	0.60
3:A:265:LEU:O	3:A:268:LEU:N	2.35	0.60
3:A:746:ARG:HG2	3:A:746:ARG:NH1	2.09	0.60
3:A:1008:ILE:HD12	3:A:1008:ILE:O	2.02	0.60
3:D:290:THR:O	3:D:293:GLN:HB2	2.02	0.60
1:B:146:TYR:CD1	1:B:148:VAL:HG22	2.37	0.60
2:C:124:VAL:HG22	2:C:150:SER:HB2	1.83	0.60
3:A:218:ASN:C	3:A:218:ASN:OD1	2.40	0.60
3:A:938:GLY:O	3:A:941:MET:N	2.35	0.59
1:E:138:THR:HG22	1:E:151:PHE:CE1	2.37	0.59
3:D:74:ASN:O	3:D:77:TYR:HB3	2.02	0.59
3:D:116:ASP:HB2	3:D:119:CYS:HB2	1.84	0.59
3:D:833:MET:HB3	3:D:841:TYR:CD1	2.37	0.59
3:D:1000:GLY:HA2	3:D:1042:LEU:HD13	1.84	0.59
1:E:51:LYS:HZ1	1:E:263:THR:HA	1.64	0.59
1:E:159:ASN:O	1:E:160:ARG:HG2	2.02	0.59
3:D:484:VAL:HA	3:D:527:LEU:HD13	1.84	0.59
3:D:733:GLN:HB2	3:D:792:VAL:HG11	1.85	0.59
3:A:639:TYR:N	3:A:701:ALA:HB1	2.17	0.59
1:E:120:VAL:HA	1:E:257:LEU:O	2.03	0.59
3:A:285:THR:O	3:A:289:LEU:HB2	2.03	0.59
3:A:925:HIS:O	3:A:928:SER:HB3	2.02	0.59
1:E:4:LEU:HD22	3:D:521:ILE:HD11	1.84	0.59
1:E:255:GLY:C	1:E:256:LEU:HD23	2.23	0.59
1:E:280:MET:O	1:E:284:VAL:HG23	2.02	0.59
2:F:159:LYS:HB2	2:F:160:PRO:HD3	1.83	0.59
3:D:150:ILE:HG21	3:D:201:GLU:CD	2.23	0.59
3:D:515:ARG:HH11	3:D:515:ARG:HG3	1.68	0.59
3:A:529:GLU:O	3:A:530:GLN:C	2.39	0.59
3:A:1048:GLU:O	3:A:1052:LEU:HG	2.02	0.59
2:F:81:ILE:HD11	3:D:77:TYR:CD1	2.38	0.59
3:D:420:MET:HB2	3:D:461:LEU:HD13	1.83	0.59
3:D:678:ILE:HD12	3:D:679:LEU:HG	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:MET:HB3	3:D:851:LEU:HD13	1.84	0.59
3:A:632:THR:CA	3:A:697:ARG:HH22	2.16	0.59
3:D:208:LEU:C	3:D:208:LEU:HD23	2.23	0.59
3:D:337:LEU:HD22	3:D:347:LEU:CB	2.30	0.59
3:D:638:GLY:HA3	3:D:701:ALA:HB3	1.85	0.59
1:B:210:LYS:HD2	1:B:210:LYS:N	2.18	0.59
1:B:282:SER:HA	1:B:286:GLY:CA	2.30	0.59
2:C:13:LEU:C	2:C:13:LEU:HD12	2.22	0.59
3:A:833:MET:HB3	3:A:841:TYR:CD1	2.38	0.59
1:E:225:PRO:HB2	1:E:226:PHE:CD2	2.38	0.59
3:D:704:HIS:CD2	3:D:767:ASN:H	2.21	0.59
3:A:631:HIS:CE1	3:A:693:LYS:HB2	2.37	0.59
3:D:95:PRO:HG2	3:D:98:GLN:HE21	1.68	0.59
1:B:4:LEU:HA	1:B:7:LYS:CB	2.32	0.59
1:E:11:LEU:HG	3:D:572:PHE:HZ	1.68	0.59
2:F:84:GLN:O	2:F:85:CYS:HB3	2.03	0.59
2:F:139:HIS:O	2:F:143:ASN:N	2.35	0.59
3:A:973:PHE:HD1	3:A:974:ILE:N	2.01	0.58
3:A:988:HIS:H	3:A:988:HIS:CD2	2.20	0.58
1:E:50:GLN:O	1:E:52:SER:N	2.31	0.58
3:D:56:HIS:C	3:D:58:ASP:H	2.06	0.58
3:D:621:ILE:HG22	3:D:622:ILE:HG23	1.85	0.58
3:D:762:TRP:CH2	3:D:772:VAL:HG22	2.38	0.58
1:B:206:TRP:O	1:B:210:LYS:HB2	2.03	0.58
2:F:75:LEU:HD12	2:F:75:LEU:N	2.18	0.58
3:D:168:MET:HE2	3:D:171:LEU:HD12	1.84	0.58
3:D:823:PHE:O	3:D:827:PHE:CB	2.51	0.58
3:A:208:LEU:HD23	3:A:208:LEU:C	2.24	0.58
1:E:107:LEU:HD23	1:E:276:LEU:HD22	1.85	0.58
3:D:193:HIS:O	3:D:197:SER:HB2	2.03	0.58
3:D:961:PRO:HD3	3:D:970:ASN:OD1	2.03	0.58
1:B:58:VAL:HA	1:B:194:PRO:HG2	1.84	0.58
3:D:252:TYR:O	3:D:256:ASN:ND2	2.36	0.58
3:D:639:TYR:N	3:D:701:ALA:HB1	2.18	0.58
3:A:769:PRO:CG	3:A:770:GLN:H	2.16	0.58
3:D:803:THR:O	3:D:807:ILE:HG12	2.02	0.58
3:A:121:GLU:O	3:A:123:GLU:N	2.36	0.58
1:E:130:LEU:HG	1:E:132:VAL:HG23	1.85	0.58
1:B:146:TYR:CE2	3:A:626:GLN:NE2	2.71	0.58
3:A:115:SER:HB3	3:A:162:SER:HB3	1.84	0.58
3:A:569:LEU:HD11	3:A:587:THR:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:529:GLU:O	3:D:530:GLN:C	2.41	0.58
2:C:137:VAL:HG12	2:C:140:ARG:NH1	2.19	0.58
3:A:202:PHE:O	3:A:205:ILE:HG23	2.04	0.58
3:D:528:CYS:HA	3:D:540:ILE:HD13	1.84	0.58
3:D:534:LYS:HE2	3:D:577:HIS:HB2	1.86	0.58
3:D:963:ASN:N	3:D:964:PRO:HD3	2.19	0.58
3:D:996:LEU:CD2	3:D:1033:LEU:HD11	2.33	0.58
3:A:93:ILE:CG2	3:A:1027:GLY:HA3	2.33	0.58
3:A:897:LEU:O	3:A:901:LEU:HG	2.03	0.58
1:B:190:TRP:O	1:B:191:ARG:C	2.42	0.57
2:C:39:TYR:HE1	4:C:217:GTP:O2B	1.86	0.57
3:A:256:ASN:OD1	3:A:257:VAL:HG23	2.04	0.57
1:E:356:LEU:O	3:D:719:ASN:ND2	2.37	0.57
2:F:88:ILE:HD11	2:F:117:ILE:CD1	2.34	0.57
3:D:344:ARG:O	3:D:348:MET:HG2	2.04	0.57
3:D:1003:SER:C	3:D:1005:ASN:H	2.06	0.57
1:B:146:TYR:HD1	1:B:148:VAL:HG22	1.67	0.57
3:A:252:TYR:O	3:A:256:ASN:ND2	2.37	0.57
3:A:515:ARG:HH11	3:A:515:ARG:HG3	1.69	0.57
2:F:138:PHE:HA	2:F:141:LYS:NZ	2.19	0.57
2:F:177:VAL:HG22	2:F:178:ALA:N	2.19	0.57
3:A:54:LYS:O	3:A:55:GLU:HB2	2.04	0.57
3:A:261:ARG:HD2	3:A:318:PHE:CG	2.39	0.57
3:D:769:PRO:CG	3:D:770:GLN:H	2.16	0.57
2:C:159:LYS:HB2	2:C:160:PRO:HD3	1.85	0.57
3:A:123:GLU:C	3:A:125:VAL:H	2.06	0.57
3:A:521:ILE:CG2	3:A:547:ILE:HG21	2.34	0.57
2:F:134:LYS:HE3	2:F:135:SER:OG	2.04	0.57
3:D:964:PRO:HG2	3:D:968:VAL:HB	1.86	0.57
1:B:258:PHE:O	1:B:273:VAL:HA	2.03	0.57
3:A:150:ILE:HG21	3:A:201:GLU:CD	2.25	0.57
3:A:304:ILE:CG1	3:A:356:LEU:HB3	2.35	0.57
3:A:678:ILE:HD12	3:A:679:LEU:HG	1.86	0.57
3:A:746:ARG:HH11	3:A:746:ARG:CG	2.09	0.57
3:D:131:ASN:ND2	3:D:166:ASN:HD21	2.02	0.57
3:A:195:LYS:C	3:A:197:SER:H	2.07	0.57
3:A:463:TYR:O	3:A:467:LEU:HG	2.04	0.57
3:A:1030:THR:HG23	3:A:1032:ASP:OD1	2.05	0.57
3:D:25:ILE:HD12	3:D:25:ILE:N	2.20	0.57
3:D:274:VAL:HG12	3:D:275:SER:N	2.20	0.57
3:D:877:SER:O	3:D:880:TRP:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:LEU:O	2:C:78:GLY:N	2.35	0.57
2:C:149:ILE:HG22	2:C:156:ASN:O	2.03	0.57
3:A:846:THR:HG23	3:A:888:ASN:ND2	2.19	0.57
1:E:103:LEU:HD13	1:E:268:GLY:HA2	1.87	0.57
1:E:206:TRP:O	1:E:210:LYS:HB2	2.05	0.57
1:E:260:HIS:O	1:E:261:LYS:C	2.41	0.57
3:D:943:ALA:HB2	3:D:1015:LEU:HD12	1.85	0.57
2:C:31:LEU:C	2:C:32:THR:HG22	2.25	0.57
3:A:134:LEU:O	3:A:138:LEU:HG	2.05	0.57
3:A:637:VAL:O	3:A:641:ILE:HD12	2.05	0.57
2:F:88:ILE:HD11	2:F:117:ILE:HD11	1.87	0.57
3:D:265:LEU:O	3:D:268:LEU:N	2.38	0.57
3:D:823:PHE:O	3:D:827:PHE:HB2	2.04	0.57
3:D:871:PHE:CZ	3:D:875:LEU:HD11	2.40	0.57
1:B:49:LEU:HG	1:B:49:LEU:O	2.05	0.57
3:A:113:THR:HG21	3:A:126:TYR:HE2	1.69	0.57
3:A:434:GLU:CB	3:A:439:GLU:O	2.51	0.57
3:A:574:HIS:HD2	3:A:624:ASP:HB2	1.69	0.57
3:A:875:LEU:O	3:A:878:ILE:N	2.37	0.57
3:D:304:ILE:CG1	3:D:356:LEU:HB3	2.35	0.57
3:D:202:PHE:O	3:D:205:ILE:HG23	2.05	0.57
1:B:98:ALA:HA	1:B:145:GLY:H	1.69	0.56
3:A:866:ILE:HB	3:A:867:PRO:CD	2.35	0.56
3:A:1008:ILE:HD12	3:A:1008:ILE:C	2.25	0.56
1:E:10:GLY:HA3	1:E:34:TYR:CZ	2.40	0.56
1:E:244:VAL:CG1	1:E:245:LEU:HD13	2.33	0.56
3:A:484:VAL:HA	3:A:527:LEU:HD13	1.86	0.56
3:A:593:GLN:HG3	3:A:639:TYR:CD2	2.39	0.56
3:A:875:LEU:HD21	3:A:914:PHE:CE1	2.40	0.56
3:A:1000:GLY:HA2	3:A:1042:LEU:HD13	1.87	0.56
1:E:284:VAL:HG12	1:E:285:LEU:HD13	1.87	0.56
2:F:44:GLY:HA3	3:D:45:MET:HE1	1.86	0.56
3:D:62:ARG:NH2	3:D:79:GLY:HA2	2.19	0.56
1:B:107:LEU:HD23	1:B:276:LEU:HD22	1.87	0.56
3:A:74:ASN:O	3:A:77:TYR:CB	2.54	0.56
3:A:76:LYS:O	3:A:80:LEU:HD22	2.05	0.56
3:A:420:MET:HB2	3:A:461:LEU:HD13	1.88	0.56
3:A:476:MET:CE	3:A:501:ILE:HG12	2.35	0.56
3:A:480:LEU:HB2	3:A:497:LEU:HD21	1.87	0.56
1:E:146:TYR:HD1	1:E:148:VAL:HG22	1.68	0.56
3:D:30:ASN:ND2	3:D:30:ASN:H	2.01	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG22	1:B:194:PRO:HG2	1.88	0.56
3:A:261:ARG:HD2	3:A:318:PHE:CD2	2.40	0.56
3:A:528:CYS:HA	3:A:540:ILE:HD13	1.87	0.56
3:A:905:ALA:HB3	3:A:906:GLN:NE2	2.20	0.56
3:A:1052:LEU:HD12	3:A:1053:GLN:HB2	1.86	0.56
2:F:149:ILE:HG22	2:F:156:ASN:O	2.05	0.56
3:D:116:ASP:HB2	3:D:119:CYS:SG	2.46	0.56
3:D:195:LYS:C	3:D:197:SER:H	2.08	0.56
3:D:762:TRP:HH2	3:D:772:VAL:HG22	1.68	0.56
3:D:938:GLY:O	3:D:941:MET:N	2.35	0.56
3:D:975:GLN:HG2	3:D:1002:PHE:CE1	2.40	0.56
2:C:138:PHE:HA	2:C:141:LYS:NZ	2.21	0.56
3:A:821:GLN:HA	3:D:597:ARG:HH21	1.71	0.56
3:D:847:ASN:O	3:D:848:PHE:C	2.42	0.56
2:C:66:THR:HG22	2:C:67:ALA:N	2.21	0.56
3:A:70:SER:C	3:A:72:ASN:H	2.09	0.56
3:A:362:GLU:O	3:A:364:GLU:N	2.36	0.56
3:A:372:TYR:O	3:A:373:TRP:C	2.43	0.56
3:A:622:ILE:HG21	3:A:633:PHE:CD2	2.40	0.56
3:A:798:PRO:HG3	3:A:844:HIS:CE1	2.40	0.56
1:E:18:ASN:CG	1:E:108:ILE:HD11	2.26	0.56
3:D:55:GLU:HG2	3:D:56:HIS:ND1	2.21	0.56
3:D:178:VAL:HG11	3:D:194:LEU:HB3	1.88	0.56
3:D:256:ASN:OD1	3:D:257:VAL:HG23	2.05	0.56
3:D:632:THR:HA	3:D:697:ARG:NH2	2.20	0.56
3:D:1004:LEU:HD21	3:D:1042:LEU:HD22	1.86	0.56
1:B:244:VAL:CG1	1:B:245:LEU:HD13	2.34	0.56
3:A:116:ASP:C	3:A:118:THR:H	2.09	0.56
3:A:534:LYS:HE2	3:A:577:HIS:HB2	1.87	0.56
3:A:594:LYS:HE2	3:A:594:LYS:HA	1.87	0.56
3:D:134:LEU:O	3:D:138:LEU:HG	2.06	0.56
1:B:202:PHE:O	1:B:203:ARG:C	2.43	0.56
3:A:62:ARG:NH2	3:A:79:GLY:HA2	2.20	0.56
3:A:962:LEU:HD13	3:A:968:VAL:HB	1.87	0.56
3:D:632:THR:CA	3:D:697:ARG:HH22	2.17	0.56
3:D:983:LYS:HE2	3:D:991:ASP:HA	1.87	0.56
2:C:45:VAL:HG22	2:C:46:GLU:N	2.21	0.56
3:A:30:ASN:ND2	3:A:30:ASN:H	2.02	0.56
3:A:117:PRO:O	3:A:118:THR:OG1	2.22	0.56
2:C:81:ILE:HD11	3:A:77:TYR:CD1	2.42	0.56
3:A:95:PRO:HG2	3:A:98:GLN:HE21	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:CZ	1:B:70:THR:H	2.19	0.55
3:A:77:TYR:O	3:A:78:TYR:C	2.44	0.55
1:E:45:ARG:NH1	1:E:49:LEU:CD2	2.69	0.55
1:E:110:VAL:HB	1:E:285:LEU:HD11	1.88	0.55
3:D:227:GLU:HG2	3:D:263:VAL:CG1	2.36	0.55
3:D:261:ARG:HD2	3:D:318:PHE:CD2	2.41	0.55
3:D:847:ASN:O	3:D:849:PHE:N	2.39	0.55
3:A:46:ALA:O	3:A:50:LEU:HD12	2.06	0.55
3:D:704:HIS:HD2	3:D:766:SER:CA	2.19	0.55
3:A:290:THR:HG21	3:A:325:PHE:CE2	2.41	0.55
3:A:637:VAL:HG12	3:A:641:ILE:HD12	1.88	0.55
1:E:58:VAL:HG22	1:E:194:PRO:HG2	1.88	0.55
3:A:142:TRP:CZ3	3:A:197:SER:HB3	2.42	0.55
3:A:421:VAL:HG11	3:A:476:MET:HG2	1.87	0.55
3:A:704:HIS:HD2	3:A:766:SER:CA	2.20	0.55
1:E:4:LEU:HD23	3:D:522:LYS:HG3	1.87	0.55
3:D:925:HIS:O	3:D:928:SER:HB3	2.06	0.55
1:B:107:LEU:HB3	1:B:276:LEU:HD13	1.89	0.55
1:B:152:SER:O	1:B:225:PRO:CD	2.54	0.55
2:C:155:TYR:HE1	3:A:429:GLU:OE2	1.90	0.55
3:A:672:ALA:HB1	3:A:679:LEU:HD11	1.89	0.55
3:A:914:PHE:CE1	3:A:918:TYR:HD1	2.24	0.55
3:D:99:CYS:HA	3:D:102:ILE:HD12	1.87	0.55
3:D:859:CYS:C	3:D:861:PRO:HD2	2.27	0.55
1:B:260:HIS:O	1:B:261:LYS:C	2.43	0.55
3:A:56:HIS:O	3:A:58:ASP:N	2.40	0.55
3:A:95:PRO:HG2	3:A:98:GLN:HB3	1.89	0.55
1:E:240:SER:O	1:E:241:LEU:C	2.43	0.55
3:D:972:MET:O	3:D:976:ASP:HB2	2.07	0.55
1:B:98:ALA:CA	1:B:145:GLY:H	2.19	0.55
1:B:351:ASP:O	3:A:715:LEU:HD12	2.06	0.55
3:A:30:ASN:HB3	3:A:47:GLN:HE21	1.69	0.55
3:A:790:ARG:NH1	3:D:647:GLN:HB2	2.21	0.55
3:D:594:LYS:HE2	3:D:594:LYS:HA	1.88	0.55
3:D:747:SER:O	3:D:750:THR:HB	2.07	0.55
2:C:84:GLN:O	2:C:85:CYS:HB3	2.07	0.55
3:A:128:GLY:O	3:A:132:MET:HB2	2.07	0.55
3:A:962:LEU:CD1	3:A:968:VAL:HB	2.36	0.55
3:A:1003:SER:C	3:A:1005:ASN:H	2.09	0.55
1:E:114:LEU:HD12	1:E:118:TRP:CG	2.41	0.55
1:E:204:PHE:O	1:E:207:MET:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:66:ILE:HG22	3:D:76:LYS:HD2	1.86	0.55
3:D:247:ILE:O	3:D:251:ILE:HG13	2.05	0.55
3:D:432:VAL:HG23	3:D:432:VAL:O	2.06	0.55
3:D:515:ARG:HH11	3:D:515:ARG:CG	2.19	0.55
3:D:552:PRO:O	3:D:556:ARG:HG3	2.07	0.55
2:C:122:ASN:HA	2:C:149:ILE:O	2.07	0.55
2:C:139:HIS:O	2:C:143:ASN:N	2.40	0.55
3:A:638:GLY:HA3	3:A:701:ALA:HB3	1.89	0.55
2:F:28:LYS:O	2:F:32:THR:HG23	2.07	0.55
3:D:179:PHE:CE2	3:D:235:TRP:CE2	2.95	0.55
3:D:225:THR:CA	3:D:228:THR:HG22	2.34	0.55
3:D:383:GLU:OE1	3:D:405:ARG:HB2	2.07	0.55
3:D:559:TRP:HH2	3:D:610:PHE:HB2	1.72	0.55
3:D:737:GLU:OE1	3:D:794:ALA:HB1	2.07	0.55
3:A:55:GLU:HG2	3:A:56:HIS:ND1	2.22	0.55
3:A:616:ASN:OD1	3:A:656:LYS:HE3	2.06	0.55
2:F:66:THR:HG22	2:F:67:ALA:N	2.22	0.55
3:D:17:LEU:HD23	3:D:22:LYS:HZ1	1.71	0.55
3:D:616:ASN:OD1	3:D:656:LYS:HE3	2.06	0.55
3:D:870:GLN:O	3:D:873:LEU:N	2.39	0.55
1:B:352:HIS:ND1	1:B:352:HIS:N	2.49	0.54
1:E:13:ILE:HD11	3:D:572:PHE:CZ	2.42	0.54
3:D:866:ILE:HB	3:D:867:PRO:CD	2.37	0.54
3:D:962:LEU:O	3:D:963:ASN:HB3	2.07	0.54
2:C:101:VAL:HB	2:C:102:PRO:HD3	1.89	0.54
3:A:280:GLU:HG3	3:A:336:LEU:CD1	2.37	0.54
3:A:515:ARG:HH11	3:A:515:ARG:CG	2.19	0.54
3:A:639:TYR:CE1	3:A:701:ALA:HA	2.42	0.54
3:A:816:THR:HG23	3:A:859:CYS:SG	2.47	0.54
1:E:152:SER:O	1:E:225:PRO:CD	2.54	0.54
3:D:280:GLU:HG3	3:D:336:LEU:CD1	2.37	0.54
3:D:521:ILE:CG2	3:D:547:ILE:HG21	2.36	0.54
1:B:351:ASP:OD2	3:A:712:ARG:HA	2.08	0.54
3:A:26:ASN:O	3:A:29:ASP:HB2	2.07	0.54
3:A:276:VAL:CG2	3:A:280:GLU:HA	2.37	0.54
2:F:98:TYR:HA	2:F:101:VAL:HG23	1.88	0.54
3:D:26:ASN:O	3:D:29:ASP:HB2	2.07	0.54
3:D:95:PRO:HG2	3:D:98:GLN:HB3	1.90	0.54
1:B:255:GLY:C	1:B:256:LEU:HD23	2.28	0.54
3:A:378:ALA:O	3:A:382:ARG:HG3	2.07	0.54
3:A:383:GLU:OE1	3:A:405:ARG:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:676:VAL:O	3:A:676:VAL:HG12	2.07	0.54
1:E:175:TYR:HB2	1:E:182:TYR:CD1	2.42	0.54
1:E:237:THR:O	1:E:238:PRO:C	2.45	0.54
2:F:81:ILE:HG22	2:F:82:GLN:HG3	1.89	0.54
3:D:417:ARG:NE	3:D:464:LEU:O	2.34	0.54
3:D:626:GLN:HB2	3:D:627:PRO:HD2	1.89	0.54
3:A:940:THR:OG1	3:A:1012:LYS:HE3	2.08	0.54
3:D:271:ILE:O	3:D:274:VAL:HG23	2.07	0.54
3:D:306:LEU:O	3:D:308:TYR:N	2.40	0.54
3:D:988:HIS:H	3:D:988:HIS:CD2	2.24	0.54
1:B:4:LEU:HD22	3:A:521:ILE:CD1	2.38	0.54
2:C:110:ARG:NH2	3:A:176:GLU:OE1	2.40	0.54
3:A:983:LYS:HE2	3:A:991:ASP:HA	1.89	0.54
1:E:14:SER:HB2	1:E:16:ASP:OD2	2.07	0.54
1:E:159:ASN:HB2	1:E:223:LEU:HD11	1.90	0.54
2:F:146:TYR:C	2:F:146:TYR:CD2	2.81	0.54
2:F:159:LYS:N	2:F:160:PRO:CD	2.71	0.54
3:A:239:GLY:O	3:A:244:THR:HG23	2.08	0.54
3:A:517:LEU:O	3:A:518:VAL:C	2.43	0.54
3:A:704:HIS:HD2	3:A:766:SER:CB	2.21	0.54
1:E:4:LEU:O	1:E:7:LYS:N	2.40	0.54
1:E:202:PHE:O	1:E:203:ARG:C	2.46	0.54
1:E:209:SER:O	1:E:210:LYS:HD2	2.06	0.54
3:D:227:GLU:HG2	3:D:263:VAL:HG11	1.90	0.54
3:D:287:PHE:CD2	3:D:337:LEU:HD11	2.42	0.54
3:A:337:LEU:HD23	3:A:343:LEU:HB3	1.89	0.54
3:A:847:ASN:O	3:A:850:LEU:N	2.41	0.54
3:D:378:ALA:O	3:D:382:ARG:HG3	2.07	0.54
3:D:433:VAL:HG13	3:D:434:GLU:N	2.22	0.54
3:A:178:VAL:CG1	3:A:194:LEU:HB3	2.37	0.54
1:E:142:THR:HG23	1:E:148:VAL:HG21	1.88	0.54
2:F:29:ARG:HB3	2:F:157:PHE:HZ	1.73	0.54
2:C:15:LEU:HD22	2:C:23:LYS:HB3	1.89	0.54
3:A:20:SER:HB2	3:A:22:LYS:HD3	1.90	0.54
3:A:127:ILE:HG22	3:A:131:ASN:HD21	1.72	0.54
3:A:304:ILE:HG13	3:A:356:LEU:HB3	1.90	0.54
3:A:405:ARG:O	3:A:408:LEU:HB2	2.08	0.54
3:A:632:THR:HA	3:A:697:ARG:NH2	2.22	0.54
3:A:131:ASN:ND2	3:A:166:ASN:HD21	2.05	0.53
1:E:348:HIS:CD2	3:D:708:ILE:O	2.61	0.53
3:D:30:ASN:HB3	3:D:47:GLN:HE21	1.71	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:668:ILE:HG22	3:D:668:ILE:O	2.08	0.53
3:A:819:ILE:N	3:A:820:PRO:HD2	2.22	0.53
3:A:973:PHE:C	3:A:973:PHE:HD1	2.10	0.53
2:F:156:ASN:HB3	2:F:159:LYS:HG3	1.88	0.53
3:D:133:ILE:O	3:D:136:GLN:HB2	2.08	0.53
2:C:75:LEU:N	2:C:75:LEU:CD1	2.72	0.53
3:A:569:LEU:HD21	3:A:587:THR:CG2	2.34	0.53
3:A:819:ILE:HD12	3:A:855:VAL:HG21	1.89	0.53
3:A:964:PRO:HD2	3:A:968:VAL:HG21	1.91	0.53
2:C:146:TYR:C	2:C:146:TYR:CD2	2.82	0.53
3:A:218:ASN:OD1	3:A:218:ASN:O	2.27	0.53
3:A:247:ILE:O	3:A:251:ILE:HG13	2.07	0.53
3:A:293:GLN:O	3:A:296:GLN:HB3	2.08	0.53
3:A:871:PHE:CZ	3:A:875:LEU:HD11	2.44	0.53
3:A:1033:LEU:O	3:A:1034:PHE:C	2.47	0.53
1:E:173:CYS:SG	1:E:184:VAL:HG22	2.49	0.53
3:D:304:ILE:HG13	3:D:356:LEU:HB3	1.91	0.53
3:D:574:HIS:HD2	3:D:624:ASP:HB2	1.73	0.53
3:D:746:ARG:HH11	3:D:746:ARG:CG	2.12	0.53
3:D:905:ALA:HB3	3:D:906:GLN:HE22	1.72	0.53
3:D:1047:GLU:O	3:D:1051:LYS:HE2	2.08	0.53
3:A:179:PHE:CE2	3:A:235:TRP:CE2	2.96	0.53
3:A:859:CYS:C	3:A:861:PRO:HD2	2.29	0.53
3:A:953:VAL:HG11	3:A:974:ILE:HD13	1.89	0.53
3:D:272:ALA:HB1	3:D:329:PHE:HD1	1.74	0.53
3:A:51:THR:O	3:A:51:THR:HG22	2.09	0.53
3:A:238:LEU:HD22	3:A:242:PHE:CE2	2.40	0.53
2:F:85:CYS:HB2	2:F:164:LEU:HD22	1.91	0.53
3:D:819:ILE:HD12	3:D:855:VAL:HG21	1.91	0.53
3:D:914:PHE:CE1	3:D:918:TYR:HD1	2.26	0.53
3:D:1014:HIS:O	3:D:1017:ASP:HB3	2.08	0.53
1:B:3:GLU:HB3	3:A:522:LYS:NZ	2.24	0.53
1:B:51:LYS:NZ	1:B:264:HIS:HB2	2.23	0.53
2:C:81:ILE:HG22	2:C:82:GLN:HG3	1.91	0.53
3:A:35:LEU:O	3:A:36:TYR:HD1	1.91	0.53
3:A:168:MET:HE2	3:A:171:LEU:HD12	1.90	0.53
1:E:1:LEU:HD13	3:D:558:HIS:CD2	2.43	0.53
2:F:155:TYR:HE1	3:D:429:GLU:OE2	1.92	0.53
3:D:16:LEU:C	3:D:17:LEU:HD12	2.29	0.53
3:D:628:GLN:HA	3:D:631:HIS:HD2	1.74	0.53
3:A:615:LEU:CD2	3:A:618:ILE:HD11	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:417:ARG:NE	3:A:464:LEU:O	2.36	0.53
3:A:1004:LEU:HD21	3:A:1042:LEU:HD22	1.90	0.53
3:D:238:LEU:HD22	3:D:242:PHE:CE2	2.40	0.53
1:B:24:HIS:C	1:B:26:ARG:H	2.11	0.53
2:C:36:GLU:OE2	2:C:38:LYS:HE2	2.08	0.53
3:A:733:GLN:HB2	3:A:792:VAL:HG11	1.92	0.53
3:A:943:ALA:HB2	3:A:1015:LEU:HD12	1.89	0.53
1:E:4:LEU:HD11	3:D:518:VAL:HG13	1.89	0.53
1:E:258:PHE:O	1:E:273:VAL:HA	2.08	0.53
2:F:137:VAL:HG12	2:F:140:ARG:NH1	2.24	0.53
3:D:749:ARG:O	3:D:753:ARG:HG3	2.09	0.53
1:B:106:TRP:HZ3	1:B:276:LEU:HA	1.74	0.52
3:A:66:ILE:HG22	3:A:76:LYS:HD2	1.90	0.52
3:D:46:ALA:O	3:D:50:LEU:HD12	2.09	0.52
3:D:517:LEU:HD11	3:D:551:TYR:CG	2.44	0.52
3:D:819:ILE:N	3:D:820:PRO:HD2	2.23	0.52
3:D:997:PHE:CD1	3:D:1014:HIS:NE2	2.77	0.52
3:D:1034:PHE:O	3:D:1035:LEU:O	2.27	0.52
2:C:92:VAL:CG2	2:C:129:ARG:HG3	2.39	0.52
3:A:20:SER:O	3:A:22:LYS:N	2.42	0.52
3:A:821:GLN:HA	3:D:597:ARG:NH2	2.24	0.52
2:F:15:LEU:CD2	2:F:23:LYS:HG2	2.39	0.52
1:B:46:LEU:HD22	1:B:50:GLN:NE2	2.23	0.52
1:B:183:TYR:HA	1:B:229:VAL:O	2.10	0.52
2:C:35:PHE:HE2	2:C:37:LYS:HG2	1.74	0.52
3:A:249:THR:O	3:A:253:LYS:HB3	2.10	0.52
3:A:388:THR:O	3:A:389:SER:C	2.47	0.52
3:A:860:PHE:HE1	3:A:900:LEU:HG	1.74	0.52
3:D:77:TYR:O	3:D:78:TYR:C	2.48	0.52
3:D:389:SER:C	3:D:391:SER:H	2.10	0.52
1:B:4:LEU:O	1:B:7:LYS:N	2.42	0.52
1:B:119:ILE:CD1	1:B:259:TYR:HB2	2.37	0.52
3:A:860:PHE:N	3:A:861:PRO:CD	2.71	0.52
1:E:98:ALA:HA	1:E:145:GLY:H	1.73	0.52
3:A:56:HIS:C	3:A:58:ASP:N	2.61	0.52
3:A:276:VAL:O	3:A:277:SER:C	2.47	0.52
3:A:870:GLN:O	3:A:873:LEU:N	2.42	0.52
3:A:953:VAL:CG1	3:A:974:ILE:HD13	2.39	0.52
3:A:970:ASN:N	3:A:970:ASN:ND2	2.56	0.52
3:A:974:ILE:O	3:A:975:GLN:C	2.47	0.52
1:E:237:THR:O	1:E:240:SER:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:103:LYS:HE3	3:D:146:TRP:CD1	2.44	0.52
3:D:128:GLY:O	3:D:132:MET:HB2	2.10	0.52
3:D:168:MET:SD	3:D:225:THR:HG23	2.49	0.52
3:D:293:GLN:O	3:D:296:GLN:HB3	2.10	0.52
3:D:324:LEU:CD2	3:D:368:ILE:HD13	2.40	0.52
1:B:169:THR:HG22	1:B:171:LEU:HD21	1.91	0.52
3:D:615:LEU:HA	3:D:618:ILE:HG13	1.89	0.52
1:E:98:ALA:CA	1:E:145:GLY:H	2.22	0.52
2:F:75:LEU:O	2:F:78:GLY:N	2.40	0.52
3:D:816:THR:HG23	3:D:859:CYS:SG	2.49	0.52
3:A:271:ILE:O	3:A:274:VAL:HG23	2.09	0.52
3:A:1052:LEU:HD12	3:A:1053:GLN:N	2.25	0.52
3:D:28:LEU:O	3:D:32:VAL:HG23	2.09	0.52
2:C:119:LEU:HD23	2:C:146:TYR:HD1	1.74	0.52
1:E:146:TYR:CE2	3:D:626:GLN:NE2	2.78	0.52
3:D:56:HIS:O	3:D:58:ASP:N	2.43	0.52
3:D:434:GLU:O	3:D:435:ASN:O	2.28	0.52
3:D:678:ILE:C	3:D:680:LYS:H	2.12	0.52
3:A:210:GLN:O	3:A:211:PHE:C	2.49	0.52
3:D:95:PRO:HG2	3:D:98:GLN:CB	2.40	0.52
3:D:134:LEU:O	3:D:134:LEU:HD12	2.10	0.52
3:D:882:PHE:HA	3:D:890:ALA:HA	1.91	0.52
3:D:948:TYR:C	3:D:948:TYR:CD1	2.83	0.52
3:D:1004:LEU:HD21	3:D:1042:LEU:CD2	2.39	0.52
3:A:30:ASN:HB2	3:A:48:GLU:OE2	2.10	0.51
3:A:95:PRO:HG2	3:A:98:GLN:CB	2.40	0.51
3:A:133:ILE:O	3:A:136:GLN:HB2	2.10	0.51
3:A:621:ILE:HG22	3:A:622:ILE:HG23	1.92	0.51
3:A:695:ASN:HD21	3:A:709:GLN:HE21	1.58	0.51
3:A:798:PRO:HG2	3:A:843:GLU:OE1	2.09	0.51
3:D:29:ASP:O	3:D:33:ASN:ND2	2.43	0.51
3:D:74:ASN:O	3:D:77:TYR:CB	2.58	0.51
3:D:163:LEU:O	3:D:163:LEU:HD23	2.10	0.51
3:D:417:ARG:O	3:D:421:VAL:HG23	2.10	0.51
1:B:237:THR:O	1:B:240:SER:N	2.43	0.51
3:A:406:ARG:O	3:A:407:GLN:C	2.48	0.51
3:A:833:MET:HB3	3:A:841:TYR:HD1	1.75	0.51
3:A:882:PHE:HA	3:A:890:ALA:HA	1.91	0.51
1:E:6:LEU:C	1:E:6:LEU:HD23	2.30	0.51
1:E:107:LEU:HB3	1:E:276:LEU:HD13	1.92	0.51
3:D:860:PHE:N	3:D:861:PRO:CD	2.72	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:PHE:N	1:B:234:PHE:CD1	2.78	0.51
1:B:357:MET:CG	3:A:719:ASN:HD21	2.23	0.51
2:C:31:LEU:HG	2:C:31:LEU:O	2.10	0.51
3:A:647:GLN:O	3:A:651:GLU:HG3	2.10	0.51
1:E:58:VAL:HA	1:E:194:PRO:HG2	1.91	0.51
3:D:600:VAL:HG11	3:D:640:MET:O	2.11	0.51
2:C:42:THR:OG1	4:C:217:GTP:O1G	2.25	0.51
2:C:92:VAL:HG23	2:C:129:ARG:HG3	1.92	0.51
1:E:63:ARG:HH22	1:E:70:THR:HG23	1.76	0.51
1:E:175:TYR:C	1:E:175:TYR:CD2	2.83	0.51
3:D:430:VAL:O	3:D:430:VAL:CG1	2.58	0.51
3:D:768:ASP:HB3	3:D:771:MET:HE3	1.92	0.51
1:B:4:LEU:HD11	3:A:518:VAL:CG1	2.35	0.51
1:B:142:THR:HG23	1:B:148:VAL:HG21	1.91	0.51
1:B:280:MET:O	1:B:284:VAL:HG23	2.10	0.51
2:C:13:LEU:HB2	2:C:85:CYS:SG	2.51	0.51
3:A:306:LEU:O	3:A:308:TYR:N	2.43	0.51
3:A:509:HIS:HB2	3:A:512:ASP:OD2	2.11	0.51
3:A:521:ILE:HG22	3:A:547:ILE:HG21	1.92	0.51
2:F:31:LEU:C	2:F:32:THR:HG22	2.31	0.51
3:D:804:MET:HA	3:D:807:ILE:HG12	1.93	0.51
1:B:215:GLU:HG2	1:B:216:GLY:H	1.75	0.51
2:C:117:ILE:HG23	2:C:144:LEU:HD22	1.91	0.51
3:A:74:ASN:O	3:A:77:TYR:N	2.44	0.51
3:A:223:HIS:NE2	3:A:263:VAL:HG21	2.25	0.51
3:A:406:ARG:HA	3:A:409:TYR:HD2	1.74	0.51
3:D:347:LEU:O	3:D:351:LEU:HB2	2.09	0.51
3:D:517:LEU:O	3:D:518:VAL:C	2.46	0.51
1:B:240:SER:O	1:B:241:LEU:C	2.47	0.51
2:C:47:VAL:O	2:C:47:VAL:HG23	2.09	0.51
3:A:678:ILE:C	3:A:680:LYS:H	2.12	0.51
2:F:98:TYR:HE1	2:F:136:ILE:HG23	1.75	0.51
1:B:357:MET:HG3	3:A:719:ASN:HD21	1.75	0.51
3:A:157:SER:HB3	3:A:164:CYS:HB2	1.92	0.51
3:A:432:VAL:O	3:A:433:VAL:HB	2.10	0.51
3:D:238:LEU:CD2	3:D:242:PHE:HE2	2.23	0.51
1:B:41:GLU:HG3	1:B:109:ASP:CB	2.35	0.51
1:B:357:MET:CG	3:A:719:ASN:ND2	2.74	0.51
3:A:654:ILE:HG22	3:A:654:ILE:O	2.10	0.51
3:A:912:GLN:OE1	3:A:958:ILE:HG12	2.11	0.51
3:A:914:PHE:CD1	3:A:918:TYR:HD1	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1006:GLN:HB2	3:A:1049:LYS:HG2	1.91	0.51
1:E:119:ILE:CD1	1:E:259:TYR:HB2	2.39	0.51
3:D:51:THR:O	3:D:51:THR:HG22	2.11	0.51
3:D:672:ALA:HB1	3:D:679:LEU:HD11	1.93	0.51
3:D:871:PHE:CE2	3:D:875:LEU:HD11	2.46	0.51
3:D:875:LEU:HD21	3:D:914:PHE:CE1	2.46	0.51
3:D:906:GLN:NE2	3:D:906:GLN:N	2.58	0.51
3:A:1038:ARG:HA	3:A:1041:ALA:CB	2.40	0.51
3:D:134:LEU:HD23	3:D:170:ILE:HD12	1.94	0.51
3:D:970:ASN:N	3:D:970:ASN:ND2	2.58	0.51
1:B:175:TYR:CD2	1:B:175:TYR:C	2.84	0.50
3:A:257:VAL:O	3:A:257:VAL:HG12	2.11	0.50
3:A:299:PRO:HD2	3:A:302:THR:CG2	2.41	0.50
1:E:281:VAL:HG13	1:E:282:SER:H	1.76	0.50
3:D:30:ASN:N	3:D:30:ASN:HD22	2.07	0.50
3:D:44:ARG:O	3:D:47:GLN:HG2	2.11	0.50
3:D:95:PRO:CG	3:D:98:GLN:HE21	2.24	0.50
3:D:491:TRP:CH2	3:D:535:ASP:HB3	2.46	0.50
3:D:912:GLN:OE1	3:D:958:ILE:HG12	2.11	0.50
1:B:180:GLN:OE1	3:A:684:THR:HG22	2.10	0.50
3:A:44:ARG:O	3:A:47:GLN:HG2	2.11	0.50
3:A:95:PRO:CG	3:A:98:GLN:HE21	2.24	0.50
3:A:103:LYS:HE3	3:A:146:TRP:CD1	2.46	0.50
3:A:123:GLU:C	3:A:125:VAL:N	2.63	0.50
3:A:225:THR:CA	3:A:228:THR:HG22	2.39	0.50
1:E:122:VAL:HG22	1:E:256:LEU:HD22	1.93	0.50
3:D:150:ILE:O	3:D:154:VAL:HG23	2.11	0.50
3:D:436:ASP:O	3:D:436:ASP:OD2	2.28	0.50
1:B:98:ALA:HB1	1:B:144:SER:HA	1.93	0.50
1:B:234:PHE:HB3	1:B:235:PRO:HD2	1.94	0.50
3:A:803:THR:O	3:A:807:ILE:HG12	2.11	0.50
2:F:122:ASN:HA	2:F:149:ILE:O	2.12	0.50
3:D:139:LYS:HD2	3:D:186:ILE:HD11	1.93	0.50
3:D:841:TYR:O	3:D:845:ARG:HG3	2.12	0.50
3:A:378:ALA:HB1	3:A:382:ARG:NH1	2.26	0.50
3:A:823:PHE:O	3:A:827:PHE:HB3	2.11	0.50
2:F:132:LYS:O	2:F:135:SER:N	2.38	0.50
3:D:249:THR:O	3:D:253:LYS:HB3	2.11	0.50
3:D:569:LEU:HD11	3:D:587:THR:HG21	1.94	0.50
1:B:138:THR:HG22	1:B:151:PHE:CZ	2.45	0.50
1:B:152:SER:O	1:B:225:PRO:HD3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:ILE:CG1	2:C:118:VAL:N	2.74	0.50
3:A:28:LEU:O	3:A:32:VAL:HG23	2.11	0.50
3:A:101:GLY:O	3:A:105:TYR:HB2	2.10	0.50
3:A:280:GLU:HG3	3:A:336:LEU:HD13	1.92	0.50
3:A:1043:ARG:HA	3:A:1043:ARG:CZ	2.41	0.50
3:D:123:GLU:C	3:D:125:VAL:H	2.13	0.50
3:D:142:TRP:CZ3	3:D:197:SER:HB3	2.46	0.50
3:D:178:VAL:CG1	3:D:194:LEU:HB3	2.41	0.50
1:B:351:ASP:HB2	1:B:352:HIS:CE1	2.46	0.50
3:A:406:ARG:C	3:A:408:LEU:N	2.62	0.50
3:A:736:GLY:C	3:A:738:MET:N	2.64	0.50
2:F:31:LEU:HB3	2:F:50:LEU:CD2	2.39	0.50
2:F:38:LYS:HD2	3:D:840:GLU:HA	1.92	0.50
3:D:290:THR:HG21	3:D:325:PHE:CE2	2.46	0.50
3:D:539:ILE:HG22	3:D:540:ILE:N	2.27	0.50
3:D:569:LEU:HD21	3:D:587:THR:CG2	2.38	0.50
3:D:709:GLN:O	3:D:712:ARG:HB3	2.11	0.50
3:D:870:GLN:O	3:D:873:LEU:HB3	2.11	0.50
3:A:168:MET:SD	3:A:225:THR:HG23	2.51	0.50
3:A:552:PRO:O	3:A:556:ARG:HG3	2.11	0.50
3:A:1046:GLN:HE22	3:A:1049:LYS:NZ	2.10	0.50
1:E:1:LEU:CD2	3:D:558:HIS:HD2	2.24	0.50
3:D:123:GLU:OE1	3:D:123:GLU:HA	2.11	0.50
3:D:1038:ARG:O	3:D:1041:ALA:HB3	2.12	0.50
1:B:39:GLN:O	1:B:39:GLN:HG2	2.11	0.50
1:B:357:MET:CB	3:A:719:ASN:HD21	2.24	0.50
2:C:31:LEU:C	2:C:32:THR:CG2	2.80	0.50
2:C:31:LEU:O	2:C:32:THR:HG22	2.12	0.50
3:A:749:ARG:O	3:A:753:ARG:HG3	2.12	0.50
1:E:41:GLU:HG3	1:E:109:ASP:CB	2.36	0.50
1:E:176:ASN:OD1	1:E:179:ASN:HB2	2.12	0.50
2:F:47:VAL:HG12	2:F:64:TRP:CG	2.47	0.50
1:B:122:VAL:HG22	1:B:256:LEU:HD22	1.94	0.50
3:A:615:LEU:HA	3:A:618:ILE:HG13	1.92	0.50
1:E:234:PHE:HB3	1:E:235:PRO:HD2	1.94	0.50
3:D:393:LEU:HD23	3:D:394:LEU:H	1.77	0.50
3:D:879:ILE:HD12	3:D:879:ILE:N	2.27	0.50
3:D:962:LEU:O	3:D:963:ASN:CB	2.59	0.50
3:D:1004:LEU:HD12	3:D:1014:HIS:HB2	1.93	0.50
3:A:15:GLN:HG2	3:A:16:LEU:O	2.12	0.49
3:A:276:VAL:HG23	3:A:283:PHE:CD2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:924:GLN:NE2	3:A:977:TYR:OH	2.45	0.49
1:E:234:PHE:N	1:E:234:PHE:CD1	2.79	0.49
3:D:300:LEU:HB3	3:D:352:HIS:CE1	2.47	0.49
3:D:676:VAL:O	3:D:676:VAL:HG12	2.11	0.49
3:D:974:ILE:N	3:D:974:ILE:HD12	2.27	0.49
1:B:106:TRP:CZ3	1:B:276:LEU:HA	2.46	0.49
1:B:119:ILE:HD11	1:B:259:TYR:CB	2.40	0.49
3:A:72:ASN:O	3:A:75:THR:N	2.44	0.49
3:A:129:LYS:O	3:A:133:ILE:HG13	2.12	0.49
3:A:948:TYR:CD1	3:A:948:TYR:C	2.85	0.49
2:F:45:VAL:HG22	2:F:46:GLU:N	2.27	0.49
2:F:117:ILE:CG1	2:F:118:VAL:N	2.75	0.49
3:D:142:TRP:N	3:D:143:PRO:HD2	2.27	0.49
3:D:276:VAL:O	3:D:276:VAL:HG13	2.10	0.49
3:D:637:VAL:HG12	3:D:641:ILE:HD12	1.93	0.49
3:D:716:ASP:O	3:D:717:MET:C	2.51	0.49
3:D:963:ASN:N	3:D:964:PRO:CD	2.75	0.49
1:B:149:ASN:HD22	1:B:150:ARG:H	1.60	0.49
3:A:56:HIS:N	3:A:57:PRO:CD	2.75	0.49
3:A:96:ARG:HH22	3:A:145:HIS:HB3	1.76	0.49
3:A:526:GLY:O	3:A:530:GLN:HG3	2.12	0.49
3:A:528:CYS:CB	3:A:540:ILE:HG21	2.26	0.49
3:A:559:TRP:HH2	3:A:610:PHE:HB2	1.77	0.49
3:A:697:ARG:NH2	3:A:697:ARG:HG3	2.26	0.49
3:A:945:ILE:O	3:A:949:MET:HG3	2.12	0.49
3:D:63:VAL:O	3:D:76:LYS:HE3	2.13	0.49
3:A:424:MET:HA	3:A:457:MET:CE	2.41	0.49
1:E:25:PRO:HG2	1:E:108:ILE:HD13	1.95	0.49
3:D:28:LEU:O	3:D:28:LEU:HD23	2.11	0.49
3:D:865:ALA:O	3:D:866:ILE:HG23	2.11	0.49
1:B:18:ASN:CG	1:B:108:ILE:HD11	2.33	0.49
2:C:75:LEU:HD11	3:A:49:VAL:HG22	1.95	0.49
3:A:163:LEU:O	3:A:163:LEU:HD23	2.13	0.49
3:A:739:VAL:O	3:A:742:GLN:HG2	2.12	0.49
3:D:526:GLY:O	3:D:530:GLN:HG3	2.13	0.49
3:A:29:ASP:O	3:A:33:ASN:ND2	2.45	0.49
3:A:313:ASP:HA	3:A:316:GLN:HG3	1.94	0.49
3:A:329:PHE:CE1	3:A:333:HIS:HD2	2.30	0.49
3:A:514:LYS:O	3:A:515:ARG:C	2.49	0.49
3:A:547:ILE:HG22	3:A:548:VAL:N	2.26	0.49
3:A:997:PHE:CD1	3:A:1014:HIS:NE2	2.80	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:TRP:CZ3	1:E:276:LEU:HA	2.48	0.49
3:D:966:ASN:HB3	3:D:967:PRO:HD3	1.94	0.49
1:B:69:TRP:HB3	1:B:95:LYS:HE3	1.94	0.49
1:B:155:LEU:HG	1:B:217:LEU:HD11	1.95	0.49
1:B:220:LYS:C	1:B:221:THR:HG23	2.33	0.49
3:A:709:GLN:O	3:A:712:ARG:HB3	2.12	0.49
3:A:1036:GLU:O	3:A:1037:GLU:C	2.51	0.49
3:D:365:ILE:HG22	3:D:366:PHE:N	2.28	0.49
3:D:962:LEU:C	3:D:964:PRO:HD3	2.33	0.49
3:D:1035:LEU:O	3:D:1037:GLU:N	2.46	0.49
3:A:552:PRO:HA	3:A:555:LEU:HD12	1.95	0.49
3:A:1004:LEU:HD21	3:A:1042:LEU:CD2	2.42	0.49
3:D:157:SER:HB3	3:D:164:CYS:HB2	1.94	0.49
3:D:639:TYR:CE1	3:D:701:ALA:HA	2.48	0.49
1:B:160:ARG:NE	1:B:160:ARG:CA	2.68	0.49
2:C:123:LYS:C	2:C:125:ASP:H	2.15	0.49
3:A:30:ASN:N	3:A:30:ASN:HD22	2.09	0.49
3:A:153:ILE:HA	3:A:156:ALA:CB	2.43	0.49
3:A:255:LEU:HD12	3:A:268:LEU:CD1	2.42	0.49
3:A:450:SER:O	3:A:453:LEU:N	2.46	0.49
3:A:650:GLN:O	3:A:654:ILE:HG13	2.12	0.49
3:A:766:SER:H	3:A:810:LYS:HZ3	1.60	0.49
2:F:70:GLU:OE2	3:D:1023:LYS:NZ	2.43	0.49
3:D:676:VAL:HG13	3:D:679:LEU:HD12	1.94	0.49
3:A:146:TRP:CE3	3:A:149:PHE:HB2	2.47	0.49
3:A:276:VAL:O	3:A:278:GLN:N	2.46	0.49
3:A:458:ARG:HG3	3:A:503:SER:HB2	1.94	0.49
3:A:804:MET:HA	3:A:807:ILE:HG12	1.95	0.49
3:A:1008:ILE:HG13	3:A:1009:PRO:HD3	1.94	0.49
3:D:297:MET:O	3:D:299:PRO:HD3	2.13	0.49
3:D:875:LEU:O	3:D:878:ILE:N	2.45	0.49
3:A:127:ILE:CG2	3:A:131:ASN:HD21	2.26	0.48
3:A:279:TYR:O	3:A:283:PHE:CD2	2.66	0.48
1:E:11:LEU:HG	3:D:572:PHE:CZ	2.48	0.48
1:E:210:LYS:HD2	1:E:210:LYS:N	2.22	0.48
3:D:299:PRO:HD2	3:D:302:THR:CG2	2.43	0.48
1:B:236:CYS:HA	1:B:241:LEU:HD21	1.94	0.48
2:C:47:VAL:HG12	2:C:64:TRP:CG	2.48	0.48
2:C:156:ASN:HB3	2:C:159:LYS:HG3	1.93	0.48
3:A:962:LEU:HB3	3:A:964:PRO:CD	2.30	0.48
1:E:1:LEU:HG	1:E:2:ASN:HD22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:TRP:HZ3	1:E:276:LEU:HA	1.79	0.48
2:F:178:ALA:O	2:F:179:MET:CB	2.61	0.48
3:D:279:TYR:O	3:D:283:PHE:CD2	2.65	0.48
3:D:400:PHE:O	3:D:400:PHE:CD1	2.66	0.48
3:D:406:ARG:NH2	3:D:467:LEU:O	2.46	0.48
3:D:833:MET:HB3	3:D:841:TYR:HD1	1.75	0.48
3:D:897:LEU:O	3:D:901:LEU:HG	2.13	0.48
3:A:672:ALA:HA	3:A:675:ASN:O	2.12	0.48
1:E:39:GLN:O	1:E:39:GLN:HG2	2.12	0.48
2:F:77:ASP:HA	2:F:80:TYR:CE2	2.45	0.48
3:D:218:ASN:O	3:D:222:VAL:HG23	2.13	0.48
3:D:284:GLU:CG	3:D:336:LEU:HD11	2.42	0.48
3:D:420:MET:O	3:D:424:MET:HB2	2.14	0.48
3:A:286:LEU:HD12	3:A:286:LEU:C	2.32	0.48
3:A:672:ALA:CB	3:A:678:ILE:HD11	2.37	0.48
3:A:786:ILE:HD13	3:D:645:THR:HG21	1.94	0.48
3:A:1036:GLU:O	3:A:1039:GLU:N	2.46	0.48
1:E:351:ASP:OD2	1:E:351:ASP:N	2.40	0.48
3:D:405:ARG:O	3:D:408:LEU:HB2	2.13	0.48
3:D:840:GLU:O	3:D:845:ARG:NH1	2.46	0.48
3:D:879:ILE:HG12	3:D:925:HIS:CD2	2.48	0.48
3:D:1021:GLN:HE22	3:D:1033:LEU:HD13	1.79	0.48
3:D:1035:LEU:O	3:D:1038:ARG:N	2.46	0.48
2:C:13:LEU:HD12	2:C:14:VAL:O	2.12	0.48
2:C:75:LEU:CD1	3:A:49:VAL:HG22	2.44	0.48
2:C:159:LYS:N	2:C:160:PRO:CD	2.77	0.48
4:C:217:GTP:O3B	4:C:217:GTP:O1A	2.32	0.48
3:A:134:LEU:HD23	3:A:170:ILE:HD12	1.96	0.48
3:A:430:VAL:O	3:A:430:VAL:CG1	2.61	0.48
3:A:879:ILE:HG12	3:A:925:HIS:CD2	2.48	0.48
3:A:988:HIS:CD2	3:A:988:HIS:N	2.81	0.48
1:E:130:LEU:HD11	1:E:170:ILE:CG2	2.43	0.48
2:F:117:ILE:HG23	2:F:144:LEU:HD22	1.94	0.48
3:D:15:GLN:C	3:D:16:LEU:HD12	2.34	0.48
3:D:334:GLY:C	3:D:336:LEU:H	2.16	0.48
3:D:424:MET:HA	3:D:457:MET:CE	2.41	0.48
3:D:1003:SER:O	3:D:1005:ASN:N	2.47	0.48
3:A:232:PHE:O	3:A:236:ILE:HG23	2.14	0.48
3:A:324:LEU:CD2	3:A:368:ILE:HD13	2.44	0.48
3:A:334:GLY:C	3:A:336:LEU:H	2.16	0.48
3:D:272:ALA:HB1	3:D:329:PHE:CD1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:LEU:HD23	1:B:1:LEU:H	1.79	0.48
2:C:81:ILE:HD11	3:A:77:TYR:CG	2.49	0.48
3:A:188:GLN:NE2	3:A:1013:GLU:HG3	2.28	0.48
3:D:188:GLN:NE2	3:D:1013:GLU:HG3	2.29	0.48
3:A:259:MET:C	3:A:261:ARG:H	2.16	0.48
3:A:551:TYR:O	3:A:554:PHE:HB3	2.14	0.48
3:A:769:PRO:CG	3:A:770:GLN:N	2.77	0.48
3:A:894:LEU:HA	3:A:894:LEU:HD23	1.48	0.48
3:D:122:LYS:O	3:D:123:GLU:O	2.32	0.48
3:D:611:ILE:O	3:D:614:ILE:HB	2.14	0.48
3:D:802:SER:O	3:D:806:ILE:HG13	2.13	0.48
3:D:1022:ILE:CG1	3:D:1023:LYS:N	2.76	0.48
2:C:29:ARG:HB3	2:C:157:PHE:HZ	1.79	0.48
3:A:383:GLU:OE2	3:A:405:ARG:HG3	2.14	0.48
3:A:600:VAL:HG11	3:A:640:MET:O	2.14	0.48
3:A:962:LEU:O	3:A:963:ASN:HB2	2.14	0.48
1:E:146:TYR:CD1	1:E:146:TYR:C	2.88	0.48
3:D:280:GLU:HG3	3:D:336:LEU:HD13	1.94	0.48
3:D:924:GLN:NE2	3:D:977:TYR:OH	2.47	0.48
1:B:1:LEU:HD22	3:A:514:LYS:NZ	2.28	0.48
1:B:60:HIS:CE1	1:B:100:GLN:HE22	2.32	0.48
2:C:24:THR:OG1	4:C:217:GTP:O1G	2.32	0.48
3:A:139:LYS:HD2	3:A:186:ILE:HD11	1.96	0.48
3:A:329:PHE:CE1	3:A:333:HIS:CD2	3.02	0.48
3:A:334:GLY:C	3:A:336:LEU:N	2.66	0.48
3:A:376:LEU:HG	3:A:380:LEU:HD12	1.95	0.48
3:A:517:LEU:HD11	3:A:551:TYR:CG	2.49	0.48
3:D:504:ILE:O	3:D:504:ILE:HD12	2.14	0.48
1:B:58:VAL:HA	1:B:194:PRO:CG	2.44	0.47
3:A:150:ILE:O	3:A:154:VAL:HG23	2.14	0.47
3:A:271:ILE:C	3:A:273:GLY:H	2.17	0.47
3:A:687:GLN:O	3:A:691:ILE:HB	2.14	0.47
3:A:831:LEU:HD13	3:A:848:PHE:CZ	2.49	0.47
3:D:127:ILE:HG22	3:D:128:GLY:N	2.29	0.47
3:D:157:SER:HB3	3:D:164:CYS:CB	2.44	0.47
3:D:329:PHE:CE1	3:D:333:HIS:HD2	2.30	0.47
1:B:142:THR:C	1:B:144:SER:N	2.67	0.47
3:A:56:HIS:HB3	3:A:82:ILE:CG2	2.44	0.47
3:A:246:LEU:O	3:A:249:THR:N	2.46	0.47
3:A:736:GLY:C	3:A:738:MET:H	2.16	0.47
3:A:865:ALA:O	3:A:866:ILE:HG23	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:PHE:O	2:F:141:LYS:HD2	2.14	0.47
3:D:56:HIS:N	3:D:57:PRO:CD	2.77	0.47
3:D:62:ARG:HH12	3:D:82:ILE:HD13	1.79	0.47
3:D:102:ILE:O	3:D:105:TYR:N	2.47	0.47
3:D:578:ASP:OD2	3:D:578:ASP:N	2.47	0.47
3:D:894:LEU:HB3	3:D:941:MET:HE2	1.96	0.47
1:B:55:LEU:H	1:B:55:LEU:CD1	2.09	0.47
1:B:98:ALA:CB	1:B:144:SER:HA	2.44	0.47
3:A:268:LEU:O	3:A:269:THR:C	2.53	0.47
3:D:491:TRP:CD2	3:D:539:ILE:HD12	2.49	0.47
3:D:547:ILE:HG22	3:D:548:VAL:N	2.28	0.47
1:B:18:ASN:ND2	1:B:36:SER:OG	2.47	0.47
1:B:247:MET:HB2	1:B:249:PHE:CE1	2.49	0.47
3:A:55:GLU:HB3	3:A:57:PRO:HD3	1.97	0.47
3:A:239:GLY:HA2	3:A:243:GLU:OE2	2.13	0.47
3:A:768:ASP:HB3	3:A:771:MET:HE3	1.96	0.47
3:A:871:PHE:CE2	3:A:875:LEU:HD11	2.49	0.47
3:A:964:PRO:O	3:A:968:VAL:HG22	2.13	0.47
1:E:284:VAL:CG1	1:E:285:LEU:HD13	2.44	0.47
3:D:80:LEU:HB3	3:D:133:ILE:HD11	1.95	0.47
3:D:129:LYS:O	3:D:133:ILE:HG13	2.14	0.47
3:D:615:LEU:CD2	3:D:618:ILE:HD11	2.43	0.47
1:B:48:GLU:C	1:B:50:GLN:H	2.16	0.47
2:C:88:ILE:HD11	2:C:117:ILE:CD1	2.44	0.47
2:C:88:ILE:HD11	2:C:117:ILE:HD11	1.97	0.47
3:A:491:TRP:CH2	3:A:535:ASP:HB3	2.49	0.47
3:A:975:GLN:HG3	3:A:998:VAL:CG1	2.44	0.47
3:A:1004:LEU:HD12	3:A:1014:HIS:HB2	1.96	0.47
2:F:123:LYS:C	2:F:125:ASP:H	2.17	0.47
3:D:30:ASN:HB2	3:D:48:GLU:OE2	2.15	0.47
3:D:50:LEU:C	3:D:52:HIS:H	2.18	0.47
3:D:179:PHE:CE2	3:D:235:TRP:CD2	3.02	0.47
3:D:376:LEU:HG	3:D:380:LEU:HD12	1.96	0.47
3:D:887:ARG:CD	3:D:937:ALA:HB3	2.37	0.47
3:D:1003:SER:C	3:D:1005:ASN:N	2.67	0.47
1:B:155:LEU:HD11	1:B:228:PHE:CZ	2.49	0.47
3:A:875:LEU:HD21	3:A:914:PHE:HE1	1.80	0.47
3:A:898:PHE:HD2	3:A:945:ILE:HG12	1.80	0.47
1:E:119:ILE:HD11	1:E:259:TYR:CB	2.43	0.47
1:E:200:THR:OG1	1:E:263:THR:HG23	2.14	0.47
2:F:16:VAL:HG23	2:F:88:ILE:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:56:HIS:C	3:D:58:ASP:N	2.67	0.47
3:D:153:ILE:HA	3:D:156:ALA:CB	2.45	0.47
3:D:282:GLN:OE1	3:D:282:GLN:N	2.47	0.47
3:D:313:ASP:HA	3:D:316:GLN:HG3	1.96	0.47
3:D:484:VAL:CG1	3:D:530:GLN:OE1	2.54	0.47
3:D:860:PHE:CE1	3:D:900:LEU:HG	2.47	0.47
3:D:1049:LYS:C	3:D:1051:LYS:H	2.18	0.47
1:B:13:ILE:CG2	3:A:575:GLU:OE1	2.59	0.47
2:C:98:TYR:HE1	2:C:136:ILE:HG23	1.79	0.47
3:A:100:GLU:O	3:A:103:LYS:HB3	2.15	0.47
3:A:122:LYS:O	3:A:123:GLU:O	2.32	0.47
3:A:146:TRP:N	3:A:147:PRO:CD	2.77	0.47
3:A:656:LYS:O	3:A:656:LYS:HG2	2.13	0.47
3:A:668:ILE:HG22	3:A:668:ILE:O	2.14	0.47
3:A:973:PHE:CD1	3:A:974:ILE:N	2.81	0.47
1:E:122:VAL:HG11	1:E:249:PHE:CE2	2.49	0.47
1:E:183:TYR:HA	1:E:229:VAL:O	2.14	0.47
1:E:244:VAL:HG13	1:E:245:LEU:CD1	2.39	0.47
2:F:124:VAL:HG21	2:F:155:TYR:CD2	2.50	0.47
2:F:140:ARG:NH2	3:D:371:GLU:OE1	2.39	0.47
3:D:344:ARG:NE	3:D:408:LEU:HD21	2.30	0.47
3:D:406:ARG:HA	3:D:409:TYR:HD2	1.78	0.47
3:D:915:TYR:HA	3:D:919:PHE:HB2	1.96	0.47
3:D:1047:GLU:HA	3:D:1050:HIS:NE2	2.29	0.47
1:B:1:LEU:HG	1:B:2:ASN:N	2.30	0.47
3:A:63:VAL:O	3:A:76:LYS:HE3	2.15	0.47
3:A:731:ALA:HB1	3:A:739:VAL:HG11	1.95	0.47
1:E:13:ILE:HD11	3:D:572:PHE:CE2	2.49	0.47
1:E:25:PRO:HG2	1:E:108:ILE:CD1	2.45	0.47
3:D:23:LEU:HD11	3:D:26:ASN:CB	2.44	0.47
3:D:239:GLY:O	3:D:244:THR:HG23	2.15	0.47
3:D:255:LEU:HD23	3:D:255:LEU:O	2.14	0.47
3:D:704:HIS:HD2	3:D:766:SER:HA	1.80	0.47
3:D:769:PRO:CG	3:D:770:GLN:N	2.78	0.47
3:D:847:ASN:O	3:D:850:LEU:N	2.47	0.47
1:B:63:ARG:NH1	1:B:95:LYS:HZ2	2.05	0.47
1:B:146:TYR:CD1	1:B:146:TYR:C	2.89	0.47
3:A:168:MET:HE2	3:A:168:MET:HA	1.97	0.47
3:A:378:ALA:HB1	3:A:382:ARG:HH12	1.79	0.47
3:A:578:ASP:OD2	3:A:578:ASP:N	2.48	0.47
2:F:23:LYS:O	2:F:27:VAL:HG13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:GLU:OE2	3:D:103:LYS:HD3	2.14	0.47
3:D:127:ILE:O	3:D:130:LEU:N	2.48	0.47
3:D:146:TRP:CE3	3:D:149:PHE:HB2	2.49	0.47
3:D:257:VAL:O	3:D:257:VAL:HG12	2.15	0.47
3:D:458:ARG:O	3:D:462:VAL:HG23	2.15	0.47
2:C:26:PHE:CZ	2:C:30:HIS:CE1	3.03	0.47
2:C:138:PHE:O	2:C:141:LYS:HD2	2.15	0.47
3:D:718:LEU:HA	3:D:718:LEU:HD23	1.56	0.47
1:B:47:LEU:HA	1:B:47:LEU:HD23	1.62	0.46
1:B:114:LEU:HD12	1:B:118:TRP:CG	2.50	0.46
1:B:188:MET:HE3	1:B:265:TYR:CE1	2.50	0.46
1:B:352:HIS:HA	1:B:353:PRO:HD3	1.79	0.46
2:C:155:TYR:O	2:C:156:ASN:C	2.54	0.46
3:A:142:TRP:HH2	3:A:197:SER:C	2.19	0.46
3:A:747:SER:O	3:A:750:THR:HB	2.15	0.46
1:E:52:SER:O	1:E:53:LYS:C	2.54	0.46
3:D:102:ILE:O	3:D:103:LYS:C	2.54	0.46
3:D:123:GLU:C	3:D:125:VAL:N	2.68	0.46
3:D:258:PRO:O	3:D:261:ARG:HB3	2.15	0.46
3:D:378:ALA:HB1	3:D:382:ARG:NH1	2.30	0.46
1:B:63:ARG:NH1	1:B:95:LYS:HZ1	2.10	0.46
1:B:142:THR:C	1:B:144:SER:H	2.18	0.46
3:A:351:LEU:HA	3:A:351:LEU:HD23	1.55	0.46
3:A:704:HIS:CD2	3:A:767:ASN:N	2.83	0.46
3:A:840:GLU:O	3:A:845:ARG:NH1	2.47	0.46
3:A:918:TYR:O	3:A:922:ILE:HG13	2.15	0.46
3:D:660:LEU:O	3:D:661:PRO:C	2.51	0.46
2:C:12:LYS:O	2:C:12:LYS:HG2	2.15	0.46
2:C:98:TYR:HA	2:C:101:VAL:HG23	1.96	0.46
3:A:28:LEU:O	3:A:28:LEU:HD23	2.15	0.46
3:A:66:ILE:HD13	3:A:66:ILE:H	1.80	0.46
3:A:93:ILE:HG23	3:A:1027:GLY:HA3	1.96	0.46
3:A:219:ALA:CB	3:A:220:PRO:HD3	2.43	0.46
3:A:240:TYR:O	3:A:244:THR:HG21	2.15	0.46
3:A:287:PHE:CD2	3:A:337:LEU:HD11	2.50	0.46
3:A:935:HIS:ND1	3:A:935:HIS:N	2.63	0.46
3:A:952:LEU:O	3:A:952:LEU:HD23	2.15	0.46
2:F:81:ILE:HD11	3:D:77:TYR:CG	2.51	0.46
2:F:155:TYR:O	2:F:156:ASN:C	2.54	0.46
3:D:101:GLY:O	3:D:105:TYR:HB2	2.14	0.46
3:D:521:ILE:HG22	3:D:547:ILE:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:627:PRO:O	3:D:631:HIS:CD2	2.69	0.46
3:D:752:LYS:O	3:D:755:THR:HB	2.15	0.46
1:B:25:PRO:HG2	1:B:108:ILE:CD1	2.45	0.46
2:C:45:VAL:HG22	2:C:46:GLU:H	1.79	0.46
2:C:50:LEU:O	2:C:60:LYS:HA	2.16	0.46
3:A:240:TYR:O	3:A:244:THR:CG2	2.63	0.46
3:A:272:ALA:HB1	3:A:329:PHE:HD1	1.80	0.46
3:A:465:THR:O	3:A:469:TYR:HB3	2.16	0.46
3:A:875:LEU:O	3:A:876:ASP:C	2.53	0.46
3:A:906:GLN:NE2	3:A:906:GLN:N	2.63	0.46
1:E:240:SER:O	1:E:242:CYS:N	2.49	0.46
2:F:64:TRP:HE3	2:F:79:TYR:HB3	1.78	0.46
2:F:75:LEU:N	2:F:75:LEU:CD1	2.79	0.46
2:F:83:ALA:O	2:F:115:ILE:HG21	2.15	0.46
3:D:406:ARG:C	3:D:408:LEU:N	2.65	0.46
3:D:660:LEU:HD12	3:D:660:LEU:N	2.30	0.46
1:B:277:ARG:HG2	1:B:280:MET:HE3	1.98	0.46
2:C:83:ALA:O	2:C:115:ILE:HG21	2.16	0.46
2:C:124:VAL:HG21	2:C:155:TYR:CD2	2.51	0.46
3:A:189:VAL:HG11	3:A:1038:ARG:HG3	1.97	0.46
3:A:269:THR:HG22	3:A:270:GLU:N	2.29	0.46
2:F:31:LEU:O	2:F:32:THR:HG22	2.15	0.46
3:D:246:LEU:O	3:D:249:THR:N	2.47	0.46
3:D:286:LEU:HD12	3:D:286:LEU:C	2.35	0.46
3:A:297:MET:O	3:A:299:PRO:HD3	2.16	0.46
3:A:724:LEU:HD12	3:A:751:VAL:HB	1.97	0.46
3:A:813:GLY:HA2	3:A:816:THR:OG1	2.16	0.46
3:A:964:PRO:HB2	3:A:968:VAL:CG1	2.46	0.46
3:D:317:ASN:O	3:D:318:PHE:C	2.52	0.46
3:D:894:LEU:HA	3:D:894:LEU:HD23	1.48	0.46
2:C:15:LEU:CD2	2:C:23:LYS:HG2	2.45	0.46
2:C:156:ASN:ND2	2:C:159:LYS:HE3	2.31	0.46
3:A:25:ILE:H	3:A:25:ILE:CD1	2.25	0.46
3:A:87:ILE:HG23	3:A:91:TRP:CE3	2.50	0.46
3:A:229:LEU:O	3:A:233:LEU:HG	2.15	0.46
3:A:718:LEU:HA	3:A:718:LEU:HD23	1.48	0.46
3:A:819:ILE:N	3:A:820:PRO:CD	2.79	0.46
3:A:914:PHE:CE1	3:A:918:TYR:CD1	3.04	0.46
3:A:938:GLY:O	3:A:939:LEU:C	2.53	0.46
3:D:87:ILE:HG23	3:D:91:TRP:CE3	2.51	0.46
3:D:259:MET:C	3:D:261:ARG:H	2.17	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:467:LEU:O	3:D:468:ASP:HB2	2.16	0.46
3:D:816:THR:HG23	3:D:859:CYS:CB	2.46	0.46
2:C:153:SER:HB2	3:A:431:LEU:HD21	1.98	0.46
3:A:167:ASN:HA	3:A:170:ILE:HG13	1.98	0.46
3:A:676:VAL:HG13	3:A:679:LEU:HD12	1.97	0.46
1:E:13:ILE:HG22	3:D:537:LYS:CB	2.45	0.46
3:D:56:HIS:HB3	3:D:82:ILE:CG2	2.45	0.46
3:D:144:LYS:HB2	3:D:145:HIS:CD2	2.50	0.46
3:D:879:ILE:HD12	3:D:879:ILE:H	1.81	0.46
2:C:73:GLY:HA3	2:C:76:ARG:NH2	2.31	0.46
3:A:142:TRP:N	3:A:143:PRO:HD2	2.31	0.46
3:A:402:ILE:H	3:A:402:ILE:HG12	1.48	0.46
3:A:1007:ASP:OD1	3:A:1010:ALA:HB2	2.16	0.46
1:E:238:PRO:HA	1:E:241:LEU:HD12	1.96	0.46
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.79	0.46
3:D:378:ALA:HA	3:D:463:TYR:CE2	2.51	0.46
3:D:887:ARG:O	3:D:891:ASP:HB2	2.16	0.46
3:D:973:PHE:O	3:D:973:PHE:HD1	1.99	0.46
3:A:109:LEU:O	3:A:112:LYS:HG3	2.16	0.46
3:A:258:PRO:O	3:A:261:ARG:HB3	2.16	0.46
1:E:247:MET:HB2	1:E:249:PHE:CE1	2.51	0.46
2:F:146:TYR:CD2	2:F:147:TYR:N	2.84	0.46
3:D:223:HIS:HD2	3:D:223:HIS:O	1.99	0.46
3:D:269:THR:HG22	3:D:270:GLU:N	2.30	0.46
1:B:93:LEU:HA	1:B:94:PRO:HD3	1.74	0.45
1:B:280:MET:O	1:B:283:ASP:HB2	2.14	0.45
2:C:42:THR:OG1	4:C:217:GTP:PG	2.74	0.45
2:C:45:VAL:CG2	2:C:46:GLU:H	2.29	0.45
3:A:282:GLN:OE1	3:A:282:GLN:N	2.48	0.45
3:A:704:HIS:HD2	3:A:766:SER:HA	1.80	0.45
2:F:45:VAL:CG2	2:F:46:GLU:N	2.78	0.45
3:D:480:LEU:HB2	3:D:497:LEU:HD21	1.98	0.45
3:D:801:LEU:HD11	3:D:830:THR:HG21	1.97	0.45
3:D:950:PHE:O	3:D:953:VAL:HB	2.16	0.45
1:B:60:HIS:HE1	1:B:100:GLN:HE22	1.63	0.45
1:B:107:LEU:HB2	1:B:274:GLY:CA	2.44	0.45
3:A:107:VAL:O	3:A:111:ILE:CG1	2.50	0.45
3:A:150:ILE:HG23	3:A:151:SER:N	2.28	0.45
3:A:467:LEU:O	3:A:468:ASP:HB2	2.16	0.45
1:E:277:ARG:HH22	3:D:620:THR:HG21	1.80	0.45
2:F:139:HIS:N	2:F:139:HIS:ND1	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:55:GLU:HB3	3:D:57:PRO:HD3	1.98	0.45
3:D:195:LYS:O	3:D:197:SER:N	2.49	0.45
3:D:675:ASN:ND2	3:D:677:ASP:HB2	2.31	0.45
3:D:964:PRO:HG2	3:D:968:VAL:CB	2.46	0.45
1:B:154:LEU:HD13	1:B:215:GLU:CG	2.46	0.45
3:A:102:ILE:O	3:A:105:TYR:N	2.49	0.45
3:A:559:TRP:O	3:A:559:TRP:CG	2.69	0.45
3:A:1003:SER:C	3:A:1005:ASN:N	2.69	0.45
3:A:1032:ASP:OD1	3:A:1032:ASP:N	2.49	0.45
2:F:71:LYS:HE2	3:D:932:ASP:OD1	2.17	0.45
3:D:329:PHE:CE1	3:D:333:HIS:CD2	3.05	0.45
3:D:334:GLY:C	3:D:336:LEU:N	2.68	0.45
3:D:378:ALA:HB1	3:D:382:ARG:HH12	1.80	0.45
3:D:656:LYS:O	3:D:656:LYS:HG2	2.16	0.45
3:D:675:ASN:C	3:D:677:ASP:H	2.20	0.45
3:D:1008:ILE:HG13	3:D:1009:PRO:HD3	1.97	0.45
3:D:1022:ILE:HG13	3:D:1023:LYS:N	2.31	0.45
3:A:344:ARG:NE	3:A:408:LEU:HD21	2.32	0.45
3:A:930:VAL:HG11	3:A:1015:LEU:HD22	1.97	0.45
3:A:1003:SER:O	3:A:1005:ASN:N	2.50	0.45
1:E:348:HIS:NE2	3:D:708:ILE:O	2.49	0.45
2:F:153:SER:HB2	3:D:431:LEU:HD21	1.99	0.45
3:D:113:THR:HG22	3:D:119:CYS:SG	2.57	0.45
3:D:130:LEU:O	3:D:131:ASN:C	2.54	0.45
3:D:647:GLN:O	3:D:651:GLU:HG3	2.16	0.45
3:D:715:LEU:O	3:D:718:LEU:HB2	2.17	0.45
3:D:746:ARG:HG2	3:D:746:ARG:NH1	2.15	0.45
3:D:785:LEU:HD11	3:D:804:MET:HG2	1.97	0.45
3:D:819:ILE:N	3:D:820:PRO:CD	2.80	0.45
3:A:103:LYS:O	3:A:107:VAL:HG23	2.15	0.45
3:A:946:LEU:HA	3:A:946:LEU:HD12	1.61	0.45
3:A:966:ASN:N	3:A:967:PRO:CD	2.80	0.45
1:E:152:SER:O	1:E:225:PRO:HD2	2.16	0.45
2:F:84:GLN:O	2:F:168:LEU:HD21	2.17	0.45
2:F:171:ASP:C	2:F:171:ASP:OD1	2.55	0.45
3:D:172:LYS:O	3:D:175:SER:HB3	2.16	0.45
3:D:271:ILE:C	3:D:273:GLY:H	2.19	0.45
1:B:245:LEU:HA	1:B:245:LEU:HD12	1.55	0.45
1:B:281:VAL:HG13	1:B:282:SER:N	2.30	0.45
3:A:122:LYS:HD2	3:A:122:LYS:HA	1.59	0.45
3:A:378:ALA:HA	3:A:463:TYR:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:406:ARG:NH2	3:A:467:LEU:O	2.50	0.45
3:A:458:ARG:O	3:A:462:VAL:HG23	2.16	0.45
3:A:632:THR:N	3:A:697:ARG:HH22	2.15	0.45
3:A:691:ILE:CG2	3:A:692:LEU:N	2.79	0.45
3:A:847:ASN:O	3:A:849:PHE:N	2.50	0.45
2:F:106:ARG:O	2:F:110:ARG:HG3	2.15	0.45
1:B:54:ARG:H	1:B:55:LEU:HD12	1.82	0.45
1:B:277:ARG:CG	1:B:280:MET:HE3	2.47	0.45
3:A:118:THR:HG22	3:A:121:GLU:HG3	1.99	0.45
3:A:195:LYS:C	3:A:197:SER:N	2.69	0.45
3:A:563:LYS:HE2	3:A:606:GLU:OE2	2.16	0.45
3:A:837:ASP:O	3:A:845:ARG:NH2	2.49	0.45
3:A:847:ASN:O	3:A:848:PHE:C	2.55	0.45
1:E:1:LEU:O	1:E:4:LEU:CD1	2.64	0.45
3:D:406:ARG:O	3:D:407:GLN:C	2.54	0.45
3:D:736:GLY:C	3:D:738:MET:N	2.69	0.45
3:D:837:ASP:O	3:D:845:ARG:NH2	2.49	0.45
1:B:107:LEU:O	1:B:276:LEU:HD11	2.17	0.45
3:A:50:LEU:C	3:A:52:HIS:H	2.21	0.45
3:A:372:TYR:O	3:A:375:HIS:N	2.50	0.45
3:A:950:PHE:O	3:A:953:VAL:HB	2.16	0.45
1:E:277:ARG:CG	1:E:280:MET:HE3	2.47	0.45
3:D:121:GLU:C	3:D:123:GLU:N	2.61	0.45
3:D:509:HIS:HB2	3:D:512:ASP:OD2	2.17	0.45
3:D:918:TYR:O	3:D:922:ILE:HG13	2.17	0.45
3:D:988:HIS:CD2	3:D:988:HIS:N	2.84	0.45
1:B:284:VAL:O	1:B:284:VAL:HG12	2.17	0.45
3:A:60:TRP:CD1	3:A:60:TRP:N	2.76	0.45
3:A:250:LEU:HA	3:A:250:LEU:HD23	1.71	0.45
3:A:300:LEU:HB3	3:A:352:HIS:CE1	2.52	0.45
3:A:396:GLY:O	3:A:397:SER:O	2.34	0.45
3:A:628:GLN:O	3:A:631:HIS:HB2	2.17	0.45
3:D:19:PHE:CD1	3:D:19:PHE:C	2.89	0.45
3:D:304:ILE:HG12	3:D:356:LEU:HB3	1.99	0.45
3:D:351:LEU:HA	3:D:351:LEU:HD23	1.47	0.45
3:D:551:TYR:O	3:D:554:PHE:HB3	2.17	0.45
3:D:843:GLU:O	3:D:844:HIS:C	2.54	0.45
3:D:914:PHE:CD1	3:D:918:TYR:HD1	2.34	0.45
1:B:69:TRP:CE3	1:B:95:LYS:HD3	2.52	0.45
1:B:111:PRO:CD	1:B:114:LEU:HD13	2.45	0.45
3:A:27:LEU:HA	3:A:30:ASN:OD1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:223:HIS:HD2	3:A:223:HIS:O	2.00	0.45
3:A:268:LEU:HD23	3:A:268:LEU:HA	1.80	0.45
3:A:423:ARG:O	3:A:424:MET:C	2.53	0.45
3:A:729:SER:OG	3:A:792:VAL:HG13	2.17	0.45
3:D:66:ILE:HD13	3:D:66:ILE:H	1.82	0.45
3:D:116:ASP:HB2	3:D:119:CYS:CB	2.45	0.45
3:D:186:ILE:HG22	3:D:187:THR:O	2.17	0.45
3:D:195:LYS:C	3:D:197:SER:N	2.70	0.45
3:D:559:TRP:O	3:D:559:TRP:CG	2.70	0.45
3:D:930:VAL:HG11	3:D:1015:LEU:HD22	1.98	0.45
3:D:952:LEU:O	3:D:952:LEU:HD23	2.17	0.45
1:E:152:SER:O	1:E:225:PRO:HD3	2.16	0.44
2:F:26:PHE:CZ	2:F:30:HIS:CE1	3.05	0.44
2:F:108:LEU:CD1	2:F:112:CYS:SG	3.05	0.44
3:D:60:TRP:CD1	3:D:60:TRP:N	2.76	0.44
3:D:898:PHE:HD2	3:D:945:ILE:HG12	1.83	0.44
1:B:41:GLU:CG	1:B:109:ASP:HB3	2.36	0.44
1:B:237:THR:O	1:B:238:PRO:C	2.55	0.44
2:C:45:VAL:CG2	2:C:46:GLU:N	2.80	0.44
3:A:304:ILE:HG12	3:A:356:LEU:HB3	1.99	0.44
3:A:332:GLU:HG3	3:A:332:GLU:O	2.17	0.44
3:A:362:GLU:C	3:A:364:GLU:H	2.19	0.44
3:A:515:ARG:CG	3:A:515:ARG:NH1	2.79	0.44
3:A:539:ILE:HG22	3:A:540:ILE:N	2.33	0.44
3:A:643:ALA:O	3:A:645:THR:HG23	2.17	0.44
3:A:834:ILE:HG21	3:A:845:ARG:HA	1.99	0.44
3:A:1007:ASP:O	3:A:1010:ALA:HB3	2.18	0.44
2:F:45:VAL:CG2	2:F:46:GLU:H	2.30	0.44
2:F:94:SER:HB3	2:F:97:THR:CG2	2.47	0.44
3:D:190:LYS:O	3:D:194:LEU:HD13	2.16	0.44
3:D:337:LEU:CD2	3:D:343:LEU:HB3	2.46	0.44
3:D:503:SER:O	3:D:505:SER:N	2.49	0.44
3:D:721:TYR:CE2	3:D:784:VAL:HG22	2.52	0.44
2:C:85:CYS:HB2	2:C:164:LEU:HD22	1.99	0.44
3:A:19:PHE:O	3:A:20:SER:OG	2.33	0.44
3:A:102:ILE:H	3:A:102:ILE:HG13	1.55	0.44
3:A:855:VAL:O	3:A:859:CYS:HB2	2.17	0.44
1:E:260:HIS:O	1:E:262:GLN:N	2.50	0.44
3:D:129:LYS:O	3:D:132:MET:HB3	2.16	0.44
3:D:680:LYS:HB3	3:D:680:LYS:HE2	1.86	0.44
1:B:172:ASP:HB2	1:B:188:MET:CE	2.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:N	1:B:212:PRO:CD	2.80	0.44
3:A:736:GLY:O	3:A:738:MET:N	2.51	0.44
3:A:915:TYR:HA	3:A:919:PHE:HB2	1.98	0.44
1:E:4:LEU:HD22	3:D:521:ILE:CD1	2.46	0.44
1:E:142:THR:C	1:E:144:SER:H	2.19	0.44
3:D:72:ASN:O	3:D:75:THR:N	2.50	0.44
3:D:78:TYR:CE2	3:D:82:ILE:HD11	2.52	0.44
3:D:103:LYS:O	3:D:107:VAL:HG23	2.16	0.44
3:D:223:HIS:NE2	3:D:263:VAL:HG21	2.32	0.44
3:D:255:LEU:HD12	3:D:268:LEU:CD1	2.47	0.44
3:D:509:HIS:O	3:D:510:GLU:C	2.56	0.44
3:D:592:ALA:O	3:D:596:ARG:HB3	2.17	0.44
3:D:974:ILE:O	3:D:975:GLN:C	2.54	0.44
2:C:122:ASN:O	2:C:123:LYS:CB	2.60	0.44
3:A:116:ASP:C	3:A:118:THR:N	2.71	0.44
3:A:157:SER:HB3	3:A:164:CYS:CB	2.47	0.44
3:A:329:PHE:CD1	3:A:333:HIS:HD2	2.35	0.44
3:D:831:LEU:HD12	3:D:834:ILE:HD11	1.99	0.44
3:D:879:ILE:HA	3:D:882:PHE:CE2	2.52	0.44
3:D:900:LEU:HD23	3:D:900:LEU:C	2.37	0.44
2:C:88:ILE:HD13	2:C:88:ILE:N	2.33	0.44
3:A:179:PHE:CE2	3:A:235:TRP:CD2	3.05	0.44
3:A:654:ILE:O	3:A:654:ILE:CG2	2.64	0.44
3:A:735:ASN:HB2	3:A:739:VAL:CG2	2.48	0.44
3:A:870:GLN:O	3:A:873:LEU:HB3	2.18	0.44
1:E:142:THR:C	1:E:144:SER:N	2.70	0.44
1:E:277:ARG:HG2	1:E:280:MET:HE3	2.00	0.44
2:F:50:LEU:O	2:F:60:LYS:HA	2.17	0.44
3:D:55:GLU:CG	3:D:56:HIS:H	2.31	0.44
3:D:887:ARG:HD2	3:D:887:ARG:HA	1.76	0.44
3:D:912:GLN:H	3:D:912:GLN:HG2	1.57	0.44
3:A:98:GLN:O	3:A:102:ILE:HG13	2.18	0.44
3:A:279:TYR:O	3:A:283:PHE:HD2	2.01	0.44
3:A:426:LYS:HG3	3:A:499:TRP:CH2	2.53	0.44
3:A:659:LEU:HD23	3:A:659:LEU:HA	1.77	0.44
3:A:963:ASN:N	3:A:964:PRO:CD	2.80	0.44
1:E:1:LEU:HD22	3:D:558:HIS:CD2	2.45	0.44
2:F:92:VAL:CG2	2:F:129:ARG:HG3	2.47	0.44
3:D:465:THR:O	3:D:469:TYR:HB3	2.18	0.44
3:D:515:ARG:CG	3:D:515:ARG:NH1	2.79	0.44
3:D:672:ALA:CB	3:D:678:ILE:HD11	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:OG1	1:B:263:THR:HG23	2.17	0.44
2:C:138:PHE:O	2:C:139:HIS:C	2.56	0.44
2:C:139:HIS:N	2:C:139:HIS:ND1	2.66	0.44
3:A:786:ILE:O	3:A:789:GLN:HB3	2.17	0.44
3:A:801:LEU:HD11	3:A:830:THR:HG21	1.99	0.44
1:E:211:LEU:N	1:E:212:PRO:CD	2.81	0.44
3:D:172:LYS:O	3:D:176:GLU:HG3	2.18	0.44
2:C:171:ASP:C	2:C:171:ASP:OD1	2.56	0.44
3:A:32:VAL:O	3:A:36:TYR:HB2	2.17	0.44
3:A:88:LYS:HE2	3:A:136:GLN:NE2	2.33	0.44
3:A:721:TYR:CE2	3:A:784:VAL:HG22	2.53	0.44
3:A:879:ILE:HD12	3:A:879:ILE:N	2.33	0.44
1:E:114:LEU:HD12	1:E:118:TRP:CD1	2.53	0.44
3:D:137:ILE:O	3:D:140:GLN:HB2	2.18	0.44
3:D:643:ALA:O	3:D:645:THR:HG23	2.18	0.44
3:D:920:CYS:HB3	3:D:977:TYR:HE2	1.81	0.44
1:B:1:LEU:HD22	3:A:514:LYS:HE3	2.00	0.43
3:A:622:ILE:HD13	3:A:630:VAL:HG23	2.00	0.43
3:A:735:ASN:HB2	3:A:739:VAL:HG22	1.99	0.43
1:E:103:LEU:HD21	1:E:143:LYS:HD3	2.00	0.43
1:E:149:ASN:HD22	1:E:150:ARG:H	1.66	0.43
3:D:138:LEU:C	3:D:140:GLN:H	2.19	0.43
3:D:672:ALA:HA	3:D:675:ASN:O	2.17	0.43
2:C:132:LYS:O	2:C:133:ALA:C	2.54	0.43
3:A:504:ILE:HD12	3:A:504:ILE:O	2.19	0.43
3:A:516:PHE:O	3:A:519:THR:HB	2.18	0.43
3:A:552:PRO:O	3:A:553:ARG:C	2.55	0.43
3:A:833:MET:HE3	3:A:841:TYR:CE1	2.53	0.43
3:A:962:LEU:HA	3:A:973:PHE:HE2	1.84	0.43
1:E:236:CYS:HA	1:E:241:LEU:HD21	2.00	0.43
3:D:973:PHE:CD1	3:D:973:PHE:C	2.92	0.43
1:B:63:ARG:NH1	1:B:70:THR:N	2.66	0.43
1:B:214:GLU:O	1:B:215:GLU:C	2.57	0.43
2:C:23:LYS:HE3	4:C:217:GTP:O1B	2.18	0.43
3:A:44:ARG:HD3	3:A:44:ARG:HA	1.81	0.43
3:A:379:GLU:OE2	3:A:382:ARG:NH2	2.37	0.43
3:A:592:ALA:O	3:A:596:ARG:HB3	2.18	0.43
1:E:13:ILE:HG22	3:D:537:LYS:HB3	2.00	0.43
1:E:124:PRO:HB3	1:E:251:PHE:CD2	2.53	0.43
1:E:146:TYR:CE1	1:E:147:CYS:O	2.72	0.43
1:E:202:PHE:O	1:E:205:TYR:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:ARG:HB3	2:F:157:PHE:CZ	2.53	0.43
3:D:450:SER:O	3:D:453:LEU:N	2.51	0.43
3:A:134:LEU:O	3:A:134:LEU:HD12	2.18	0.43
3:A:229:LEU:O	3:A:229:LEU:HD22	2.17	0.43
3:A:822:ILE:O	3:A:824:ASP:N	2.51	0.43
3:D:25:ILE:H	3:D:25:ILE:CD1	2.27	0.43
3:D:559:TRP:CH2	3:D:610:PHE:HB2	2.53	0.43
1:B:175:TYR:HB2	1:B:182:TYR:CD1	2.53	0.43
1:B:278:PRO:O	1:B:281:VAL:HG12	2.18	0.43
2:C:53:HIS:HB2	2:C:179:MET:O	2.18	0.43
2:C:171:ASP:OD1	2:C:174:LEU:N	2.52	0.43
3:A:22:LYS:HD2	3:A:22:LYS:HA	1.64	0.43
3:A:62:ARG:HH12	3:A:82:ILE:HD13	1.84	0.43
3:A:503:SER:O	3:A:505:SER:N	2.50	0.43
3:A:816:THR:HG23	3:A:859:CYS:CB	2.48	0.43
3:A:1007:ASP:OD2	3:A:1009:PRO:HD2	2.18	0.43
2:F:119:LEU:HD23	2:F:146:TYR:HD1	1.84	0.43
3:D:217:GLN:H	3:D:217:GLN:HG3	1.70	0.43
3:D:384:SER:CB	3:D:403:PRO:HG2	2.48	0.43
3:D:516:PHE:O	3:D:519:THR:HB	2.19	0.43
3:D:946:LEU:HA	3:D:946:LEU:HD12	1.57	0.43
1:B:98:ALA:CB	1:B:145:GLY:H	2.32	0.43
2:C:138:PHE:HA	2:C:141:LYS:HZ1	1.84	0.43
3:A:142:TRP:HZ3	3:A:197:SER:HB3	1.83	0.43
3:A:516:PHE:CE1	3:A:520:VAL:CG2	3.00	0.43
3:A:887:ARG:CD	3:A:937:ALA:HB3	2.35	0.43
3:A:954:GLU:O	3:A:955:GLU:HG3	2.19	0.43
1:E:158:GLY:O	1:E:159:ASN:HB3	2.18	0.43
3:D:150:ILE:HG23	3:D:151:SER:N	2.30	0.43
3:D:247:ILE:H	3:D:247:ILE:HG13	1.63	0.43
3:D:516:PHE:CE1	3:D:520:VAL:CG2	3.01	0.43
3:D:635:GLU:OE1	3:D:697:ARG:HD2	2.19	0.43
3:D:778:PRO:O	3:D:781:LEU:HB2	2.19	0.43
3:A:138:LEU:C	3:A:140:GLN:H	2.20	0.43
3:A:259:MET:C	3:A:261:ARG:N	2.72	0.43
3:A:879:ILE:HA	3:A:882:PHE:CE2	2.53	0.43
3:A:894:LEU:HB3	3:A:941:MET:HE2	2.01	0.43
3:A:904:VAL:CG1	3:A:911:ALA:HA	2.49	0.43
3:A:926:ILE:HG21	3:A:946:LEU:HD13	2.01	0.43
1:E:138:THR:HG22	1:E:151:PHE:CZ	2.53	0.43
2:F:134:LYS:HG3	2:F:135:SER:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:448:THR:O	3:D:449:ASP:C	2.57	0.43
3:D:997:PHE:CD1	3:D:1014:HIS:CE1	3.01	0.43
2:C:23:LYS:O	2:C:27:VAL:HG13	2.19	0.43
3:A:287:PHE:HB2	3:A:329:PHE:CE2	2.54	0.43
3:A:730:ALA:O	3:A:731:ALA:C	2.57	0.43
3:A:899:THR:HG23	3:A:903:ASN:HD21	1.81	0.43
3:D:30:ASN:CB	3:D:47:GLN:NE2	2.79	0.43
3:D:777:VAL:O	3:D:780:LEU:HB2	2.18	0.43
3:D:823:PHE:O	3:D:827:PHE:HB3	2.18	0.43
3:D:831:LEU:HD13	3:D:848:PHE:CZ	2.54	0.43
3:D:935:HIS:N	3:D:935:HIS:ND1	2.67	0.43
1:B:34:TYR:HB3	1:B:35:SER:H	1.74	0.43
1:B:55:LEU:HD13	1:B:57:TYR:HE2	1.76	0.43
1:B:103:LEU:CD1	1:B:268:GLY:HA2	2.49	0.43
1:B:173:CYS:SG	1:B:184:VAL:HG22	2.59	0.43
1:B:238:PRO:HA	1:B:241:LEU:HD12	1.99	0.43
1:B:350:PRO:HB2	1:B:351:ASP:H	1.61	0.43
3:A:30:ASN:CB	3:A:47:GLN:NE2	2.80	0.43
3:A:186:ILE:HG22	3:A:187:THR:O	2.19	0.43
3:A:317:ASN:O	3:A:318:PHE:C	2.55	0.43
3:A:778:PRO:N	3:A:779:PRO:CD	2.82	0.43
3:A:802:SER:O	3:A:806:ILE:HG13	2.18	0.43
3:A:962:LEU:HD13	3:A:968:VAL:CB	2.48	0.43
1:E:278:PRO:O	1:E:281:VAL:HG12	2.18	0.43
2:F:47:VAL:HG11	2:F:64:TRP:CE2	2.54	0.43
3:D:55:GLU:HG2	3:D:56:HIS:H	1.84	0.43
3:D:100:GLU:O	3:D:103:LYS:HB3	2.19	0.43
3:D:625:LEU:HB3	3:D:629:GLN:HB2	2.01	0.43
1:B:195:PHE:HA	1:B:198:CYS:SG	2.59	0.43
1:B:240:SER:O	1:B:242:CYS:N	2.52	0.43
3:A:137:ILE:O	3:A:140:GLN:HB2	2.19	0.43
3:A:238:LEU:CD2	3:A:242:PHE:HE2	2.27	0.43
3:A:420:MET:O	3:A:424:MET:HB2	2.19	0.43
3:A:823:PHE:HD1	3:A:823:PHE:HA	1.72	0.43
3:D:17:LEU:HD23	3:D:22:LYS:HZ2	1.84	0.43
3:D:306:LEU:C	3:D:308:TYR:N	2.72	0.43
1:B:7:LYS:HD2	3:A:522:LYS:CG	2.49	0.42
2:C:64:TRP:HE3	2:C:79:TYR:HB3	1.82	0.42
3:A:286:LEU:HD12	3:A:290:THR:HG1	1.84	0.42
3:A:443:GLU:OE1	3:A:443:GLU:HA	2.19	0.42
3:A:509:HIS:O	3:A:510:GLU:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:964:PRO:HB2	3:A:968:VAL:HG11	2.00	0.42
1:E:155:LEU:HG	1:E:217:LEU:HD11	2.01	0.42
1:E:240:SER:C	1:E:242:CYS:N	2.73	0.42
2:F:156:ASN:HB3	2:F:159:LYS:CG	2.48	0.42
3:D:372:TYR:O	3:D:373:TRP:C	2.57	0.42
3:D:875:LEU:O	3:D:876:ASP:C	2.57	0.42
3:D:1007:ASP:OD1	3:D:1010:ALA:HB2	2.19	0.42
1:B:69:TRP:CD2	1:B:95:LYS:O	2.73	0.42
3:A:27:LEU:HD23	3:A:75:THR:HG23	2.01	0.42
3:A:66:ILE:HG22	3:A:76:LYS:NZ	2.33	0.42
3:A:323:SER:O	3:A:327:CYS:HB3	2.19	0.42
3:A:365:ILE:HG22	3:A:366:PHE:N	2.34	0.42
3:A:637:VAL:HG12	3:A:641:ILE:CD1	2.49	0.42
1:E:1:LEU:HD21	1:E:2:ASN:ND2	2.35	0.42
3:D:362:GLU:C	3:D:364:GLU:H	2.22	0.42
3:D:443:GLU:OE1	3:D:443:GLU:HA	2.19	0.42
3:D:525:LEU:HD12	3:D:525:LEU:HA	1.82	0.42
3:D:563:LYS:HE2	3:D:606:GLU:OE2	2.18	0.42
3:D:575:GLU:O	3:D:581:GLN:HG3	2.19	0.42
3:D:697:ARG:O	3:D:698:ALA:C	2.57	0.42
3:D:841:TYR:O	3:D:842:PRO:C	2.56	0.42
2:C:26:PHE:CE1	2:C:30:HIS:CE1	3.07	0.42
3:A:195:LYS:O	3:A:197:SER:N	2.53	0.42
3:A:715:LEU:O	3:A:718:LEU:HB2	2.19	0.42
3:A:887:ARG:O	3:A:891:ASP:HB2	2.19	0.42
3:D:222:VAL:HG11	3:D:254:PHE:HE1	1.84	0.42
2:C:35:PHE:CE2	2:C:37:LYS:HG2	2.54	0.42
2:C:73:GLY:HA3	2:C:76:ARG:CZ	2.50	0.42
3:A:565:VAL:O	3:A:565:VAL:CG1	2.63	0.42
3:A:675:ASN:C	3:A:677:ASP:H	2.23	0.42
1:E:122:VAL:HG11	1:E:249:PHE:CZ	2.54	0.42
2:F:15:LEU:HD22	2:F:23:LYS:CB	2.49	0.42
3:D:27:LEU:HA	3:D:30:ASN:OD1	2.18	0.42
3:D:142:TRP:HH2	3:D:197:SER:C	2.23	0.42
3:D:228:THR:O	3:D:232:PHE:CD2	2.72	0.42
3:D:265:LEU:HD11	3:D:325:PHE:HB2	2.02	0.42
3:D:470:VAL:O	3:D:474:ILE:HG13	2.18	0.42
3:D:914:PHE:CE1	3:D:918:TYR:CD1	3.07	0.42
3:D:938:GLY:O	3:D:939:LEU:C	2.57	0.42
1:B:52:SER:O	1:B:53:LYS:C	2.57	0.42
1:B:63:ARG:NH1	1:B:70:THR:HB	2.24	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:THR:HG21	2:C:89:MET:HB3	2.01	0.42
2:C:84:GLN:O	2:C:168:LEU:HD21	2.19	0.42
3:A:55:GLU:CG	3:A:56:HIS:H	2.33	0.42
3:A:80:LEU:HD21	3:A:126:TYR:CE1	2.54	0.42
3:A:579:GLY:C	3:A:581:GLN:N	2.72	0.42
1:E:107:LEU:O	1:E:276:LEU:HD11	2.20	0.42
1:E:245:LEU:HA	1:E:245:LEU:HD12	1.57	0.42
2:F:75:LEU:HD11	3:D:49:VAL:HG22	2.02	0.42
3:D:279:TYR:O	3:D:283:PHE:HD2	2.02	0.42
3:D:422:SER:O	3:D:496:THR:HG21	2.20	0.42
3:D:611:ILE:HG23	3:D:612:ASP:N	2.32	0.42
3:D:704:HIS:CD2	3:D:766:SER:HA	2.55	0.42
3:D:724:LEU:HD12	3:D:751:VAL:HB	2.00	0.42
3:D:962:LEU:HD23	3:D:968:VAL:HG11	2.00	0.42
3:D:1007:ASP:O	3:D:1010:ALA:HB3	2.20	0.42
2:C:177:VAL:HG22	2:C:178:ALA:N	2.35	0.42
3:A:80:LEU:HB3	3:A:133:ILE:HD11	2.00	0.42
3:A:127:ILE:O	3:A:130:LEU:HB2	2.20	0.42
3:A:222:VAL:HG11	3:A:254:PHE:HE1	1.85	0.42
3:A:272:ALA:HB1	3:A:329:PHE:CD1	2.55	0.42
3:A:433:VAL:O	3:A:433:VAL:CG1	2.66	0.42
3:A:785:LEU:HD11	3:A:804:MET:HG2	2.01	0.42
3:A:843:GLU:O	3:A:844:HIS:C	2.57	0.42
3:A:862:ALA:O	3:A:865:ALA:N	2.52	0.42
3:A:920:CYS:HB3	3:A:977:TYR:HE2	1.84	0.42
3:A:939:LEU:HD21	3:A:1016:ARG:HH11	1.83	0.42
2:F:47:VAL:O	2:F:47:VAL:HG23	2.18	0.42
3:D:138:LEU:C	3:D:140:GLN:N	2.72	0.42
3:D:430:VAL:O	3:D:430:VAL:HG13	2.20	0.42
3:D:500:ALA:O	3:D:503:SER:OG	2.32	0.42
3:D:637:VAL:HG12	3:D:641:ILE:CD1	2.50	0.42
3:D:766:SER:H	3:D:810:LYS:HZ3	1.65	0.42
3:D:1029:ASP:HB3	3:D:1030:THR:H	1.63	0.42
1:B:96:HIS:HB3	1:B:97:TYR:H	1.65	0.42
2:C:117:ILE:HG12	2:C:118:VAL:N	2.34	0.42
3:A:78:TYR:CE2	3:A:82:ILE:HD11	2.54	0.42
3:A:255:LEU:C	3:A:257:VAL:H	2.23	0.42
3:A:406:ARG:O	3:A:408:LEU:N	2.52	0.42
3:A:470:VAL:O	3:A:474:ILE:HG13	2.19	0.42
3:A:1038:ARG:HH21	3:A:1042:LEU:CD2	2.33	0.42
1:E:3:GLU:O	1:E:7:LYS:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LEU:HD11	1:E:228:PHE:CZ	2.55	0.42
3:D:127:ILE:N	3:D:127:ILE:HD12	2.35	0.42
3:D:133:ILE:O	3:D:136:GLN:N	2.52	0.42
3:D:401:ASP:O	3:D:403:PRO:HD3	2.20	0.42
1:B:153:SER:N	1:B:158:GLY:O	2.44	0.42
2:C:38:LYS:HA	3:A:842:PRO:CG	2.50	0.42
2:C:155:TYR:CD1	3:A:445:MET:SD	3.12	0.42
3:A:94:LEU:HB2	3:A:99:CYS:SG	2.60	0.42
3:A:102:ILE:O	3:A:103:LYS:C	2.58	0.42
3:A:716:ASP:O	3:A:717:MET:C	2.58	0.42
3:A:970:ASN:O	3:A:971:GLN:C	2.58	0.42
1:E:4:LEU:C	1:E:7:LYS:H	2.23	0.42
2:F:132:LYS:O	2:F:133:ALA:C	2.56	0.42
3:D:16:LEU:HB3	3:D:17:LEU:H	1.62	0.42
3:D:146:TRP:N	3:D:147:PRO:CD	2.82	0.42
3:D:687:GLN:O	3:D:691:ILE:HB	2.20	0.42
1:B:24:HIS:C	1:B:26:ARG:N	2.72	0.42
1:B:241:LEU:HA	1:B:244:VAL:HG12	2.02	0.42
2:C:42:THR:H	4:C:217:GTP:PG	2.43	0.42
3:A:149:PHE:CZ	3:A:153:ILE:HD13	2.54	0.42
3:A:422:SER:O	3:A:496:THR:HG21	2.20	0.42
3:A:704:HIS:CD2	3:A:766:SER:HA	2.55	0.42
3:A:850:LEU:O	3:A:853:GLN:HB3	2.20	0.42
3:A:887:ARG:HD2	3:A:887:ARG:HA	1.79	0.42
1:E:18:ASN:ND2	1:E:108:ILE:HD11	2.35	0.42
1:E:58:VAL:HA	1:E:194:PRO:CG	2.50	0.42
1:E:93:LEU:HA	1:E:94:PRO:HD3	1.61	0.42
2:F:146:TYR:CG	2:F:147:TYR:N	2.87	0.42
3:D:98:GLN:O	3:D:102:ILE:HG13	2.19	0.42
3:D:178:VAL:O	3:D:178:VAL:HG12	2.20	0.42
3:D:681:ASP:HA	3:D:682:PRO:HD3	1.95	0.42
3:D:722:LYS:HD3	3:D:783:ALA:HA	2.02	0.42
3:D:953:VAL:O	3:D:955:GLU:N	2.53	0.42
1:B:60:HIS:CD2	1:B:93:LEU:HB3	2.55	0.42
1:B:101:LEU:N	1:B:101:LEU:HD23	2.34	0.42
2:C:44:GLY:HA3	3:A:45:MET:HE1	2.01	0.42
3:A:125:VAL:O	3:A:126:TYR:C	2.58	0.42
3:A:306:LEU:C	3:A:308:TYR:N	2.73	0.42
3:A:531:LYS:HD3	3:A:531:LYS:HA	1.81	0.42
3:A:777:VAL:O	3:A:780:LEU:HB2	2.20	0.42
3:A:939:LEU:HD12	3:A:939:LEU:HA	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1032:ASP:O	3:A:1034:PHE:CE1	2.73	0.42
1:E:41:GLU:CG	1:E:109:ASP:HB3	2.38	0.42
1:E:48:GLU:H	1:E:48:GLU:HG2	1.55	0.42
1:E:122:VAL:O	1:E:122:VAL:HG12	2.19	0.42
2:F:13:LEU:HD12	2:F:14:VAL:O	2.18	0.42
3:D:695:ASN:HD22	3:D:695:ASN:HA	1.54	0.42
3:D:926:ILE:HG21	3:D:946:LEU:HD13	2.02	0.42
1:B:1:LEU:HD22	3:A:514:LYS:CE	2.50	0.41
1:B:8:LEU:HG	1:B:8:LEU:O	2.20	0.41
3:A:91:TRP:CZ3	3:A:102:ILE:HD13	2.55	0.41
3:A:334:GLY:O	3:A:337:LEU:N	2.50	0.41
1:E:10:GLY:HA3	1:E:34:TYR:CE1	2.55	0.41
1:E:111:PRO:CD	1:E:114:LEU:HD13	2.48	0.41
3:D:514:LYS:O	3:D:515:ARG:C	2.58	0.41
3:D:707:VAL:CG1	3:D:708:ILE:N	2.83	0.41
3:D:729:SER:OG	3:D:792:VAL:HG13	2.20	0.41
3:D:732:ILE:HA	3:D:739:VAL:HG21	2.02	0.41
3:A:165:GLN:HA	3:A:221:LEU:HD13	2.01	0.41
3:A:255:LEU:HD12	3:A:268:LEU:HD12	2.02	0.41
3:A:262:ASN:OD1	3:A:318:PHE:HA	2.20	0.41
3:A:534:LYS:CE	3:A:577:HIS:HB2	2.48	0.41
3:A:575:GLU:O	3:A:581:GLN:HG3	2.20	0.41
3:A:608:MET:HA	3:A:609:PRO:HD3	1.62	0.41
3:A:695:ASN:HD22	3:A:695:ASN:HA	1.57	0.41
3:A:1029:ASP:O	3:A:1030:THR:C	2.58	0.41
1:E:175:TYR:CD2	1:E:175:TYR:O	2.73	0.41
2:F:28:LYS:O	2:F:29:ARG:C	2.58	0.41
3:D:125:VAL:O	3:D:126:TYR:C	2.58	0.41
3:D:168:MET:CE	3:D:171:LEU:HD12	2.49	0.41
3:D:287:PHE:HB2	3:D:329:PHE:CE2	2.55	0.41
3:D:423:ARG:HG3	3:D:423:ARG:HH11	1.86	0.41
3:D:970:ASN:O	3:D:971:GLN:C	2.58	0.41
1:B:105:GLU:O	1:B:106:TRP:C	2.59	0.41
1:B:111:PRO:CG	1:B:114:LEU:HD13	2.51	0.41
1:B:260:HIS:O	1:B:262:GLN:N	2.53	0.41
2:C:167:LYS:HA	2:C:167:LYS:HD2	1.92	0.41
3:A:90:ARG:O	3:A:91:TRP:C	2.59	0.41
3:A:607:VAL:HG22	3:A:608:MET:HG2	2.02	0.41
3:A:1038:ARG:HH21	3:A:1042:LEU:HD21	1.83	0.41
2:F:98:TYR:CE1	2:F:136:ILE:HG23	2.54	0.41
3:D:80:LEU:HD21	3:D:126:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:329:PHE:CD1	3:D:333:HIS:HD2	2.37	0.41
3:D:330:LEU:HB2	3:D:372:TYR:CE1	2.55	0.41
3:D:964:PRO:HG2	3:D:968:VAL:CG1	2.50	0.41
3:A:133:ILE:O	3:A:136:GLN:N	2.53	0.41
3:A:962:LEU:HB2	3:A:973:PHE:HD2	1.85	0.41
1:E:244:VAL:HA	1:E:247:MET:HG3	2.02	0.41
2:F:132:LYS:O	2:F:134:LYS:N	2.53	0.41
3:D:90:ARG:O	3:D:91:TRP:C	2.59	0.41
3:D:91:TRP:CZ3	3:D:102:ILE:HD13	2.55	0.41
3:D:347:LEU:HD23	3:D:347:LEU:C	2.41	0.41
3:D:388:THR:HG21	3:D:402:ILE:HD13	2.02	0.41
3:D:813:GLY:HA2	3:D:816:THR:OG1	2.21	0.41
3:D:939:LEU:HD21	3:D:1016:ARG:HH11	1.84	0.41
3:D:954:GLU:O	3:D:955:GLU:HG3	2.20	0.41
1:B:103:LEU:HD21	1:B:143:LYS:HD3	2.03	0.41
1:B:176:ASN:OD1	1:B:179:ASN:N	2.54	0.41
1:B:244:VAL:HG13	1:B:245:LEU:CD1	2.40	0.41
1:B:244:VAL:HA	1:B:247:MET:HG3	2.03	0.41
2:C:77:ASP:HA	2:C:80:TYR:CE2	2.52	0.41
3:A:227:GLU:O	3:A:230:LEU:HB3	2.20	0.41
3:A:244:THR:C	3:A:246:LEU:H	2.24	0.41
3:A:551:TYR:N	3:A:552:PRO:CD	2.83	0.41
3:A:742:GLN:HB2	3:A:743:PRO:HD2	2.03	0.41
3:A:864:LEU:HD23	3:A:864:LEU:HA	1.81	0.41
1:E:119:ILE:HD13	1:E:119:ILE:H	1.85	0.41
2:F:141:LYS:HD2	2:F:141:LYS:H	1.86	0.41
3:D:427:PRO:HD3	3:D:499:TRP:CD2	2.55	0.41
3:D:667:SER:O	3:D:671:GLN:HG3	2.21	0.41
3:D:695:ASN:HD21	3:D:709:GLN:HE21	1.67	0.41
2:C:13:LEU:HD12	2:C:13:LEU:O	2.20	0.41
2:C:141:LYS:HD2	2:C:141:LYS:H	1.85	0.41
3:A:144:LYS:C	3:A:145:HIS:CD2	2.94	0.41
3:A:430:VAL:O	3:A:430:VAL:HG13	2.20	0.41
3:A:626:GLN:HB2	3:A:627:PRO:HD2	2.02	0.41
3:A:721:TYR:CD2	3:A:784:VAL:HG22	2.56	0.41
1:E:98:ALA:CB	1:E:145:GLY:H	2.34	0.41
1:E:226:PHE:HZ	3:D:683:GLU:OE1	2.03	0.41
1:E:348:HIS:N	3:D:707:VAL:HG13	2.36	0.41
2:F:35:PHE:CE2	2:F:37:LYS:HG2	2.55	0.41
2:F:66:THR:HG22	2:F:67:ALA:H	1.84	0.41
3:D:259:MET:C	3:D:261:ARG:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:552:PRO:O	3:D:553:ARG:C	2.58	0.41
3:D:622:ILE:HD13	3:D:630:VAL:HG23	2.03	0.41
3:D:1008:ILE:C	3:D:1008:ILE:CD1	2.86	0.41
2:C:71:LYS:HE2	3:A:932:ASP:OD1	2.20	0.41
3:A:594:LYS:HE2	3:A:594:LYS:CA	2.49	0.41
3:A:871:PHE:O	3:A:872:LYS:C	2.57	0.41
3:A:1015:LEU:HA	3:A:1015:LEU:HD23	1.82	0.41
3:A:1040:THR:HA	3:A:1043:ARG:CG	2.49	0.41
1:E:245:LEU:HD21	1:E:281:VAL:HG11	2.03	0.41
3:D:631:HIS:CE1	3:D:693:LYS:CB	3.02	0.41
3:D:744:LEU:HD12	3:D:744:LEU:O	2.21	0.41
3:D:911:ALA:O	3:D:914:PHE:HB3	2.21	0.41
1:B:130:LEU:HD11	1:B:170:ILE:CG2	2.51	0.41
3:A:172:LYS:O	3:A:175:SER:HB3	2.20	0.41
3:A:372:TYR:O	3:A:374:ASN:N	2.53	0.41
3:A:949:MET:O	3:A:952:LEU:HB3	2.20	0.41
1:E:262:GLN:HE21	1:E:262:GLN:HB2	1.66	0.41
2:F:86:ALA:C	2:F:87:ILE:HG13	2.41	0.41
3:D:93:ILE:CG2	3:D:1027:GLY:HA3	2.51	0.41
3:D:697:ARG:NH2	3:D:697:ARG:HG3	2.35	0.41
3:D:823:PHE:HD1	3:D:823:PHE:HA	1.72	0.41
3:D:906:GLN:N	3:D:906:GLN:CD	2.72	0.41
3:D:997:PHE:HD1	3:D:1014:HIS:NE2	2.18	0.41
2:C:44:GLY:CA	3:A:45:MET:HE3	2.48	0.41
2:C:66:THR:HG22	2:C:67:ALA:H	1.84	0.41
2:C:106:ARG:O	2:C:110:ARG:HG3	2.20	0.41
2:C:146:TYR:CD2	2:C:147:TYR:N	2.89	0.41
3:A:23:LEU:HD11	3:A:26:ASN:CB	2.46	0.41
3:A:72:ASN:O	3:A:74:ASN:N	2.54	0.41
3:A:168:MET:HG3	3:A:225:THR:OG1	2.21	0.41
3:A:421:VAL:HG22	3:A:461:LEU:HD21	2.03	0.41
3:A:445:MET:HE2	3:A:445:MET:HB3	1.96	0.41
3:A:667:SER:O	3:A:671:GLN:HG3	2.21	0.41
3:A:975:GLN:HG3	3:A:998:VAL:HG12	2.03	0.41
1:E:61:ALA:HB1	1:E:168:TYR:HE1	1.86	0.41
1:E:154:LEU:HD23	1:E:154:LEU:HA	1.82	0.41
2:F:171:ASP:OD1	2:F:174:LEU:N	2.54	0.41
3:D:27:LEU:CD2	3:D:75:THR:HG23	2.51	0.41
3:D:161:GLU:O	3:D:164:CYS:HB3	2.20	0.41
3:D:198:MET:O	3:D:202:PHE:HB2	2.21	0.41
3:D:240:TYR:O	3:D:244:THR:CG2	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:391:SER:HA	3:D:392:PRO:HD3	1.73	0.41
3:D:516:PHE:O	3:D:520:VAL:HG23	2.21	0.41
3:D:531:LYS:HA	3:D:531:LYS:HD3	1.84	0.41
3:D:552:PRO:HA	3:D:555:LEU:HD12	2.03	0.41
3:D:847:ASN:C	3:D:849:PHE:N	2.75	0.41
3:D:850:LEU:O	3:D:853:GLN:HB3	2.21	0.41
3:D:853:GLN:O	3:D:857:SER:OG	2.36	0.41
3:D:983:LYS:HE2	3:D:991:ASP:OD1	2.21	0.41
3:D:1007:ASP:OD2	3:D:1009:PRO:HD2	2.21	0.41
1:B:25:PRO:HG2	1:B:108:ILE:HD13	2.03	0.41
1:B:48:GLU:C	1:B:50:GLN:N	2.73	0.41
1:B:355:CYS:O	1:B:356:LEU:CB	2.69	0.41
2:C:9:VAL:HG22	2:C:58:PRO:O	2.21	0.41
3:A:164:CYS:O	3:A:165:GLN:C	2.59	0.41
3:A:247:ILE:H	3:A:247:ILE:HG13	1.59	0.41
3:A:583:MET:SD	3:A:583:MET:C	3.00	0.41
3:A:660:LEU:HB2	3:A:661:PRO:HD3	2.03	0.41
3:A:746:ARG:NH1	3:A:746:ARG:CG	2.76	0.41
3:A:911:ALA:O	3:A:914:PHE:HB3	2.21	0.41
1:E:2:ASN:N	1:E:2:ASN:HD22	2.19	0.41
1:E:63:ARG:NH1	1:E:72:MET:CB	2.81	0.41
1:E:122:VAL:HG21	1:E:249:PHE:CZ	2.56	0.41
2:F:35:PHE:HE2	2:F:37:LYS:HG2	1.86	0.41
3:D:14:ARG:CG	3:D:14:ARG:NH1	2.75	0.41
3:D:55:GLU:HG2	3:D:56:HIS:N	2.36	0.41
3:D:165:GLN:HA	3:D:221:LEU:HD13	2.03	0.41
3:D:229:LEU:O	3:D:233:LEU:HG	2.21	0.41
3:D:247:ILE:HG21	3:D:286:LEU:HB2	2.03	0.41
3:D:615:LEU:HA	3:D:618:ILE:CG1	2.51	0.41
1:B:208:HIS:CD2	1:B:208:HIS:N	2.90	0.40
3:A:138:LEU:C	3:A:140:GLN:N	2.74	0.40
3:A:347:LEU:O	3:A:351:LEU:HB2	2.20	0.40
3:A:970:ASN:O	3:A:973:PHE:HB3	2.21	0.40
1:E:13:ILE:HD12	1:E:13:ILE:HG21	1.85	0.40
1:E:63:ARG:NH1	1:E:70:THR:H	2.19	0.40
1:E:169:THR:HG22	1:E:171:LEU:HD21	2.02	0.40
1:E:208:HIS:CD2	1:E:208:HIS:N	2.90	0.40
1:E:216:GLY:O	1:E:219:GLU:N	2.54	0.40
1:E:255:GLY:O	1:E:256:LEU:HD23	2.20	0.40
2:F:156:ASN:ND2	2:F:159:LYS:HE3	2.36	0.40
3:D:149:PHE:CZ	3:D:153:ILE:HD13	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:268:LEU:O	3:D:269:THR:C	2.59	0.40
3:D:287:PHE:HZ	3:D:350:ALA:CB	2.34	0.40
3:D:588:PHE:CE2	3:D:636:ALA:HB1	2.56	0.40
3:D:839:GLU:O	3:D:840:GLU:C	2.59	0.40
3:D:948:TYR:CE1	3:D:952:LEU:HD12	2.56	0.40
1:B:105:GLU:O	1:B:274:GLY:HA2	2.20	0.40
1:B:240:SER:C	1:B:242:CYS:N	2.75	0.40
1:B:241:LEU:C	1:B:244:VAL:HG12	2.42	0.40
3:A:130:LEU:O	3:A:131:ASN:C	2.59	0.40
3:A:219:ALA:HB3	3:A:220:PRO:CD	2.41	0.40
3:A:326:LEU:HD23	3:A:326:LEU:HA	1.89	0.40
3:A:997:PHE:CD1	3:A:1014:HIS:CE1	3.05	0.40
1:E:102:MET:SD	1:E:265:TYR:HA	2.61	0.40
2:F:75:LEU:CD1	3:D:49:VAL:HG22	2.51	0.40
3:D:127:ILE:O	3:D:130:LEU:HB2	2.21	0.40
3:D:594:LYS:HE2	3:D:594:LYS:CA	2.50	0.40
3:D:672:ALA:O	3:D:676:VAL:HG22	2.22	0.40
3:D:786:ILE:O	3:D:789:GLN:HB3	2.21	0.40
3:D:855:VAL:O	3:D:859:CYS:HB2	2.21	0.40
3:D:938:GLY:O	3:D:940:THR:N	2.54	0.40
3:D:1013:GLU:OE1	3:D:1013:GLU:HA	2.14	0.40
1:B:7:LYS:HD2	3:A:522:LYS:HG3	2.04	0.40
1:B:257:LEU:CD1	1:B:275:TRP:HB2	2.52	0.40
2:C:13:LEU:HD12	2:C:14:VAL:C	2.42	0.40
2:C:37:LYS:HA	4:C:217:GTP:O2'	2.21	0.40
3:A:287:PHE:HZ	3:A:350:ALA:CB	2.35	0.40
2:F:138:PHE:HA	2:F:141:LYS:HZ2	1.86	0.40
2:F:164:LEU:HA	2:F:164:LEU:HD23	1.91	0.40
3:D:164:CYS:O	3:D:165:GLN:C	2.59	0.40
3:D:227:GLU:HG2	3:D:263:VAL:HG13	2.03	0.40
3:D:402:ILE:H	3:D:402:ILE:HG12	1.56	0.40
2:C:38:LYS:HA	3:A:842:PRO:HG3	2.04	0.40
3:A:55:GLU:HG2	3:A:56:HIS:H	1.86	0.40
3:A:660:LEU:O	3:A:661:PRO:C	2.57	0.40
3:A:672:ALA:O	3:A:676:VAL:HG22	2.22	0.40
3:A:973:PHE:O	3:A:976:ASP:CB	2.69	0.40
2:F:135:SER:O	2:F:137:VAL:HG22	2.21	0.40
3:D:94:LEU:HB2	3:D:99:CYS:SG	2.62	0.40
3:D:219:ALA:HB3	3:D:220:PRO:CD	2.41	0.40
3:D:251:ILE:HG22	3:D:293:GLN:HG3	2.04	0.40
3:D:328:THR:HG23	3:D:331:LYS:NZ	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:HIS:CD2	3:D:766:SER:CB	3.00	0.40
1:B:24:HIS:HA	1:B:25:PRO:HD3	1.97	0.40
1:B:51:LYS:HZ1	1:B:264:HIS:N	2.19	0.40
1:B:254:ASP:O	1:B:277:ARG:NE	2.49	0.40
1:B:260:HIS:CE1	1:B:262:GLN:CG	3.00	0.40
2:C:16:VAL:HG23	2:C:88:ILE:HA	2.03	0.40
3:A:232:PHE:HD2	3:A:232:PHE:HA	1.71	0.40
3:A:255:LEU:O	3:A:255:LEU:HD23	2.21	0.40
3:A:437:GLN:HB2	3:A:439:GLU:HG3	2.02	0.40
3:A:729:SER:O	3:A:730:ALA:C	2.59	0.40
3:A:745:ILE:HD13	3:A:745:ILE:HA	1.84	0.40
3:A:958:ILE:O	3:A:958:ILE:HG13	2.21	0.40
3:A:997:PHE:HD1	3:A:1014:HIS:NE2	2.19	0.40
1:E:107:LEU:HB2	1:E:274:GLY:CA	2.47	0.40
2:F:92:VAL:HG23	2:F:129:ARG:HG3	2.03	0.40
3:D:15:GLN:O	3:D:16:LEU:HD12	2.21	0.40
3:D:27:LEU:HD23	3:D:75:THR:HG23	2.04	0.40
3:D:102:ILE:HG13	3:D:102:ILE:H	1.60	0.40
3:D:383:GLU:OE2	3:D:405:ARG:HG3	2.21	0.40
3:D:407:GLN:HE21	3:D:407:GLN:HB3	1.66	0.40
3:D:736:GLY:O	3:D:737:GLU:C	2.60	0.40
3:D:745:ILE:HD13	3:D:745:ILE:HA	1.83	0.40
3:D:1008:ILE:O	3:D:1012:LYS:HB2	2.21	0.40
3:D:1043:ARG:HA	3:D:1043:ARG:HD2	1.72	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	B	262/361 (73%)	206 (79%)	38 (14%)	18 (7%)	1 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	267/361 (74%)	211 (79%)	39 (15%)	17 (6%)	1	12
2	C	169/176 (96%)	139 (82%)	23 (14%)	7 (4%)	3	22
2	F	169/176 (96%)	138 (82%)	24 (14%)	7 (4%)	3	22
3	A	1037/1073 (97%)	760 (73%)	206 (20%)	71 (7%)	1	11
3	D	1037/1073 (97%)	755 (73%)	220 (21%)	62 (6%)	1	13
All	All	2941/3220 (91%)	2209 (75%)	550 (19%)	182 (6%)	1	13

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	B	145	GLY
1	B	180	GLN
1	B	217	LEU
2	C	76	ARG
3	A	55	GLU
3	A	114	SER
3	A	123	GLU
3	A	127	ILE
3	A	200	ASN
3	A	326	LEU
3	A	397	SER
3	A	433	VAL
3	A	450	SER
3	A	468	ASP
3	A	486	GLY
3	A	939	LEU
3	A	963	ASN
3	A	1028	GLU
1	E	39	GLN
1	E	145	GLY
1	E	180	GLN
1	E	217	LEU
2	F	76	ARG
3	D	42	GLN
3	D	55	GLU
3	D	123	GLU
3	D	127	ILE
3	D	200	ASN
3	D	326	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	363	THR
3	D	392	PRO
3	D	435	ASN
3	D	450	SER
3	D	468	ASP
3	D	627	PRO
3	D	848	PHE
3	D	939	LEU
3	D	963	ASN
3	D	1029	ASP
3	D	1035	LEU
3	D	1036	GLU
1	B	53	LYS
2	C	32	THR
2	C	87	ILE
3	A	115	SER
3	A	118	THR
3	A	125	VAL
3	A	269	THR
3	A	277	SER
3	A	297	MET
3	A	307	ALA
3	A	388	THR
3	A	435	ASN
3	A	504	ILE
3	A	627	PRO
3	A	674	LYS
3	A	730	ALA
3	A	743	PRO
3	A	769	PRO
3	A	823	PHE
3	A	843	GLU
3	A	848	PHE
3	A	1027	GLY
3	A	1037	GLU
1	E	25	PRO
1	E	51	LYS
1	E	159	ASN
3	D	269	THR
3	D	297	MET
3	D	307	ALA
3	D	486	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	504	ILE
3	D	712	ARG
3	D	737	GLU
3	D	769	PRO
3	D	965	GLY
1	B	10	GLY
1	B	25	PRO
1	B	156	PRO
1	B	261	LYS
1	B	350	PRO
2	C	65	ASP
2	C	106	ARG
3	A	13	ALA
3	A	64	ASP
3	A	122	LYS
3	A	143	PRO
3	A	149	PHE
3	A	362	GLU
3	A	363	THR
3	A	530	GLN
3	A	712	ARG
3	A	737	GLU
3	A	781	LEU
3	A	954	GLU
1	E	53	LYS
1	E	156	PRO
2	F	32	THR
2	F	106	ARG
3	D	64	ASP
3	D	125	VAL
3	D	143	PRO
3	D	530	GLN
3	D	730	ALA
3	D	743	PRO
3	D	823	PHE
3	D	843	GLU
3	D	954	GLU
1	B	49	LEU
1	B	240	SER
3	A	124	LYS
3	A	246	LEU
3	A	268	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	392	PRO
3	A	679	LEU
3	A	961	PRO
1	E	191	ARG
1	E	240	SER
1	E	242	CYS
1	E	261	LYS
2	F	87	ILE
3	D	21	GLN
3	D	65	THR
3	D	77	TYR
3	D	122	LYS
3	D	149	PHE
3	D	196	ASP
3	D	217	GLN
3	D	246	LEU
3	D	268	LEU
3	D	362	GLU
3	D	679	LEU
3	D	781	LEU
3	D	820	PRO
1	B	241	LEU
1	B	242	CYS
1	B	356	LEU
1	B	358	GLU
2	C	85	CYS
3	A	21	GLN
3	A	65	THR
3	A	77	TYR
3	A	91	TRP
3	A	341	LEU
3	A	510	GLU
3	A	807	ILE
3	A	820	PRO
3	A	899	THR
3	A	971	GLN
3	A	1005	ASN
1	E	18	ASN
2	F	85	CYS
3	D	91	TRP
3	D	341	LEU
3	D	510	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	899	THR
3	D	1037	GLU
1	B	18	ASN
1	B	267	PRO
3	A	482	ASN
1	E	241	LEU
1	E	267	PRO
2	F	65	ASP
3	D	235	TRP
3	D	335	GLN
3	A	258	PRO
3	A	484	VAL
3	A	540	ILE
3	D	807	ILE
3	D	961	PRO
3	D	1027	GLY
1	E	284	VAL
3	D	258	PRO
3	D	540	ILE
3	D	451	ILE
3	A	146	TRP
2	F	137	VAL
2	C	137	VAL
3	A	31	VAL
3	A	451	ILE
3	A	676	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	244/323 (76%)	199 (82%)	45 (18%)	1	7
1	E	247/323 (76%)	210 (85%)	37 (15%)	3	15
2	C	150/154 (97%)	129 (86%)	21 (14%)	3	17
2	F	150/154 (97%)	125 (83%)	25 (17%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	945/973 (97%)	838 (89%)	107 (11%)	6	25
3	D	945/973 (97%)	831 (88%)	114 (12%)	5	23
All	All	2681/2900 (92%)	2332 (87%)	349 (13%)	4	20

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	SER
1	B	1	LEU
1	B	6	LEU
1	B	7	LYS
1	B	13	ILE
1	B	39	GLN
1	B	46	LEU
1	B	53	LYS
1	B	54	ARG
1	B	55	LEU
1	B	70	THR
1	B	92	LYS
1	B	95	LYS
1	B	108	ILE
1	B	109	ASP
1	B	110	VAL
1	B	112	SER
1	B	119	ILE
1	B	123	CYS
1	B	139	SER
1	B	149	ASN
1	B	151	PHE
1	B	160	ARG
1	B	171	LEU
1	B	174	ILE
1	B	188	MET
1	B	198	CYS
1	B	201	ASP
1	B	215	GLU
1	B	222	LYS
1	B	234	PHE
1	B	241	LEU
1	B	245	LEU
1	B	246	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	257	LEU
1	B	262	GLN
1	B	269	SER
1	B	275	TRP
1	B	276	LEU
1	B	282	SER
1	B	283	ASP
1	B	352	HIS
1	B	355	CYS
1	B	356	LEU
1	B	357	MET
2	C	13	LEU
2	C	27	VAL
2	C	29	ARG
2	C	30	HIS
2	C	32	THR
2	C	51	VAL
2	C	75	LEU
2	C	76	ARG
2	C	77	ASP
2	C	88	ILE
2	C	95	ARG
2	C	97	THR
2	C	108	LEU
2	C	112	CYS
2	C	117	ILE
2	C	130	LYS
2	C	137	VAL
2	C	141	LYS
2	C	144	LEU
2	C	148	ASP
2	C	173	ASN
3	A	18	ASP
3	A	23	LEU
3	A	29	ASP
3	A	30	ASN
3	A	34	CYS
3	A	35	LEU
3	A	45	MET
3	A	60	TRP
3	A	66	ILE
3	A	73	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	80	LEU
3	A	109	LEU
3	A	146	TRP
3	A	148	THR
3	A	159	THR
3	A	160	SER
3	A	189	VAL
3	A	196	ASP
3	A	199	CYS
3	A	205	ILE
3	A	228	THR
3	A	229	LEU
3	A	231	ARG
3	A	232	PHE
3	A	263	VAL
3	A	265	LEU
3	A	277	SER
3	A	285	THR
3	A	286	LEU
3	A	294	LEU
3	A	313	ASP
3	A	314	ASP
3	A	323	SER
3	A	327	CYS
3	A	331	LYS
3	A	335	GLN
3	A	337	LEU
3	A	353	TYR
3	A	365	ILE
3	A	374	ASN
3	A	387	SER
3	A	388	THR
3	A	391	SER
3	A	393	LEU
3	A	398	GLN
3	A	406	ARG
3	A	422	SER
3	A	426	LYS
3	A	430	VAL
3	A	433	VAL
3	A	440	VAL
3	A	443	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	444	PHE
3	A	452	ASN
3	A	460	THR
3	A	487	THR
3	A	490	SER
3	A	515	ARG
3	A	525	LEU
3	A	539	ILE
3	A	569	LEU
3	A	578	ASP
3	A	597	ARG
3	A	606	GLU
3	A	607	VAL
3	A	613	GLU
3	A	617	ASN
3	A	659	LEU
3	A	662	ASN
3	A	684	THR
3	A	691	ILE
3	A	695	ASN
3	A	708	ILE
3	A	720	VAL
3	A	746	ARG
3	A	747	SER
3	A	749	ARG
3	A	771	MET
3	A	781	LEU
3	A	804	MET
3	A	816	THR
3	A	823	PHE
3	A	852	LEU
3	A	855	VAL
3	A	872	LYS
3	A	885	THR
3	A	887	ARG
3	A	907	GLU
3	A	916	GLN
3	A	920	CYS
3	A	928	SER
3	A	935	HIS
3	A	940	THR
3	A	946	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	948	TYR
3	A	962	LEU
3	A	969	ASN
3	A	970	ASN
3	A	973	PHE
3	A	976	ASP
3	A	988	HIS
3	A	1008	ILE
3	A	1013	GLU
3	A	1020	VAL
3	A	1032	ASP
3	A	1033	LEU
3	A	1053	GLN
1	E	1	LEU
1	E	4	LEU
1	E	8	LEU
1	E	13	ILE
1	E	14	SER
1	E	27	LEU
1	E	33	LYS
1	E	39	GLN
1	E	45	ARG
1	E	49	LEU
1	E	108	ILE
1	E	109	ASP
1	E	110	VAL
1	E	112	SER
1	E	119	ILE
1	E	123	CYS
1	E	139	SER
1	E	149	ASN
1	E	151	PHE
1	E	160	ARG
1	E	171	LEU
1	E	188	MET
1	E	198	CYS
1	E	201	ASP
1	E	209	SER
1	E	234	PHE
1	E	241	LEU
1	E	245	LEU
1	E	246	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	257	LEU
1	E	262	GLN
1	E	269	SER
1	E	275	TRP
1	E	276	LEU
1	E	282	SER
1	E	283	ASP
1	E	351	ASP
2	F	9	VAL
2	F	13	LEU
2	F	27	VAL
2	F	29	ARG
2	F	30	HIS
2	F	31	LEU
2	F	32	THR
2	F	38	LYS
2	F	43	LEU
2	F	51	VAL
2	F	75	LEU
2	F	76	ARG
2	F	77	ASP
2	F	88	ILE
2	F	95	ARG
2	F	97	THR
2	F	108	LEU
2	F	112	CYS
2	F	117	ILE
2	F	130	LYS
2	F	134	LYS
2	F	137	VAL
2	F	141	LYS
2	F	148	ASP
2	F	173	ASN
3	D	14	ARG
3	D	19	PHE
3	D	21	GLN
3	D	23	LEU
3	D	29	ASP
3	D	30	ASN
3	D	34	CYS
3	D	35	LEU
3	D	37	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	45	MET
3	D	58	ASP
3	D	60	TRP
3	D	66	ILE
3	D	70	SER
3	D	73	MET
3	D	80	LEU
3	D	109	LEU
3	D	112	LYS
3	D	113	THR
3	D	118	THR
3	D	119	CYS
3	D	146	TRP
3	D	148	THR
3	D	159	THR
3	D	160	SER
3	D	189	VAL
3	D	199	CYS
3	D	205	ILE
3	D	210	GLN
3	D	229	LEU
3	D	231	ARG
3	D	263	VAL
3	D	265	LEU
3	D	277	SER
3	D	286	LEU
3	D	294	LEU
3	D	313	ASP
3	D	314	ASP
3	D	323	SER
3	D	327	CYS
3	D	331	LYS
3	D	335	GLN
3	D	336	LEU
3	D	337	LEU
3	D	353	TYR
3	D	365	ILE
3	D	374	ASN
3	D	387	SER
3	D	389	SER
3	D	393	LEU
3	D	395	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	401	ASP
3	D	402	ILE
3	D	406	ARG
3	D	422	SER
3	D	426	LYS
3	D	430	VAL
3	D	433	VAL
3	D	437	GLN
3	D	443	GLU
3	D	444	PHE
3	D	452	ASN
3	D	460	THR
3	D	485	ASN
3	D	490	SER
3	D	515	ARG
3	D	525	LEU
3	D	539	ILE
3	D	569	LEU
3	D	578	ASP
3	D	606	GLU
3	D	607	VAL
3	D	613	GLU
3	D	617	ASN
3	D	659	LEU
3	D	662	ASN
3	D	684	THR
3	D	691	ILE
3	D	695	ASN
3	D	708	ILE
3	D	720	VAL
3	D	739	VAL
3	D	743	PRO
3	D	746	ARG
3	D	747	SER
3	D	749	ARG
3	D	771	MET
3	D	781	LEU
3	D	804	MET
3	D	823	PHE
3	D	852	LEU
3	D	855	VAL
3	D	857	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	872	LYS
3	D	885	THR
3	D	887	ARG
3	D	907	GLU
3	D	916	GLN
3	D	928	SER
3	D	935	HIS
3	D	940	THR
3	D	946	LEU
3	D	948	TYR
3	D	970	ASN
3	D	973	PHE
3	D	976	ASP
3	D	988	HIS
3	D	1008	ILE
3	D	1013	GLU
3	D	1020	VAL
3	D	1030	THR
3	D	1031	SER
3	D	1050	HIS
3	D	1053	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	50	GLN
1	B	60	HIS
1	B	149	ASN
1	B	180	GLN
1	B	199	GLN
1	B	208	HIS
1	B	262	GLN
2	C	30	HIS
2	C	103	ASN
2	C	156	ASN
3	A	26	ASN
3	A	30	ASN
3	A	47	GLN
3	A	98	GLN
3	A	131	ASN
3	A	204	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	317	ASN
3	A	321	ASN
3	A	333	HIS
3	A	335	GLN
3	A	374	ASN
3	A	399	HIS
3	A	407	GLN
3	A	437	GLN
3	A	543	ASN
3	A	574	HIS
3	A	617	ASN
3	A	626	GLN
3	A	628	GLN
3	A	631	HIS
3	A	650	GLN
3	A	695	ASN
3	A	704	HIS
3	A	719	ASN
3	A	727	ASN
3	A	742	GLN
3	A	767	ASN
3	A	775	ASN
3	A	853	GLN
3	A	858	HIS
3	A	888	ASN
3	A	903	ASN
3	A	906	GLN
3	A	916	GLN
3	A	924	GLN
3	A	963	ASN
3	A	970	ASN
3	A	988	HIS
3	A	993	GLN
3	A	1006	GLN
3	A	1046	GLN
1	E	2	ASN
1	E	18	ASN
1	E	60	HIS
1	E	149	ASN
1	E	199	GLN
1	E	208	HIS
1	E	260	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	262	GLN
2	F	103	ASN
2	F	156	ASN
3	D	26	ASN
3	D	30	ASN
3	D	43	GLN
3	D	47	GLN
3	D	98	GLN
3	D	131	ASN
3	D	145	HIS
3	D	204	GLN
3	D	210	GLN
3	D	223	HIS
3	D	317	ASN
3	D	321	ASN
3	D	333	HIS
3	D	335	GLN
3	D	407	GLN
3	D	437	GLN
3	D	483	GLN
3	D	574	HIS
3	D	617	ASN
3	D	626	GLN
3	D	628	GLN
3	D	631	HIS
3	D	695	ASN
3	D	704	HIS
3	D	742	GLN
3	D	767	ASN
3	D	775	ASN
3	D	853	GLN
3	D	858	HIS
3	D	888	ASN
3	D	903	ASN
3	D	906	GLN
3	D	916	GLN
3	D	924	GLN
3	D	970	ASN
3	D	988	HIS
3	D	993	GLN
3	D	1006	GLN
3	D	1021	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GTP	C	217	5	26,34,34	1.00	1 (3%)	33,54,54	2.16	9 (27%)
4	GTP	F	217	5	26,34,34	0.99	1 (3%)	33,54,54	2.06	10 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	217	5	-	9/18/38/38	0/3/3/3
4	GTP	F	217	5	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	217	GTP	C6-N1	3.04	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	217	GTP	C6-N1	2.99	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	217	GTP	C2-N3-C4	5.50	121.64	115.36
4	F	217	GTP	N3-C2-N1	-5.25	120.22	127.22
4	C	217	GTP	N3-C2-N1	-4.90	120.69	127.22
4	F	217	GTP	PA-O3A-PB	-4.73	116.60	132.83
4	C	217	GTP	C4-C5-N7	-4.38	104.83	109.40
4	C	217	GTP	PA-O3A-PB	-4.34	117.93	132.83
4	C	217	GTP	C5-C6-N1	-3.97	118.00	123.43
4	F	217	GTP	PB-O3B-PG	-3.64	120.32	132.83
4	F	217	GTP	C2-N3-C4	3.48	119.34	115.36
4	F	217	GTP	C5-C6-N1	-3.17	119.09	123.43
4	F	217	GTP	C1'-N9-C4	-3.05	121.29	126.64
4	C	217	GTP	O2'-C2'-C3'	-2.81	102.73	111.82
4	F	217	GTP	C6-N1-C2	2.75	120.30	115.93
4	C	217	GTP	C6-N1-C2	2.46	119.84	115.93
4	F	217	GTP	O2G-PG-O3B	2.45	112.85	104.64
4	F	217	GTP	N2-C2-N1	2.17	120.63	117.25
4	F	217	GTP	C4-C5-N7	-2.13	107.18	109.40
4	C	217	GTP	PB-O3B-PG	-2.08	125.70	132.83
4	C	217	GTP	O3'-C3'-C4'	-2.01	105.25	111.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

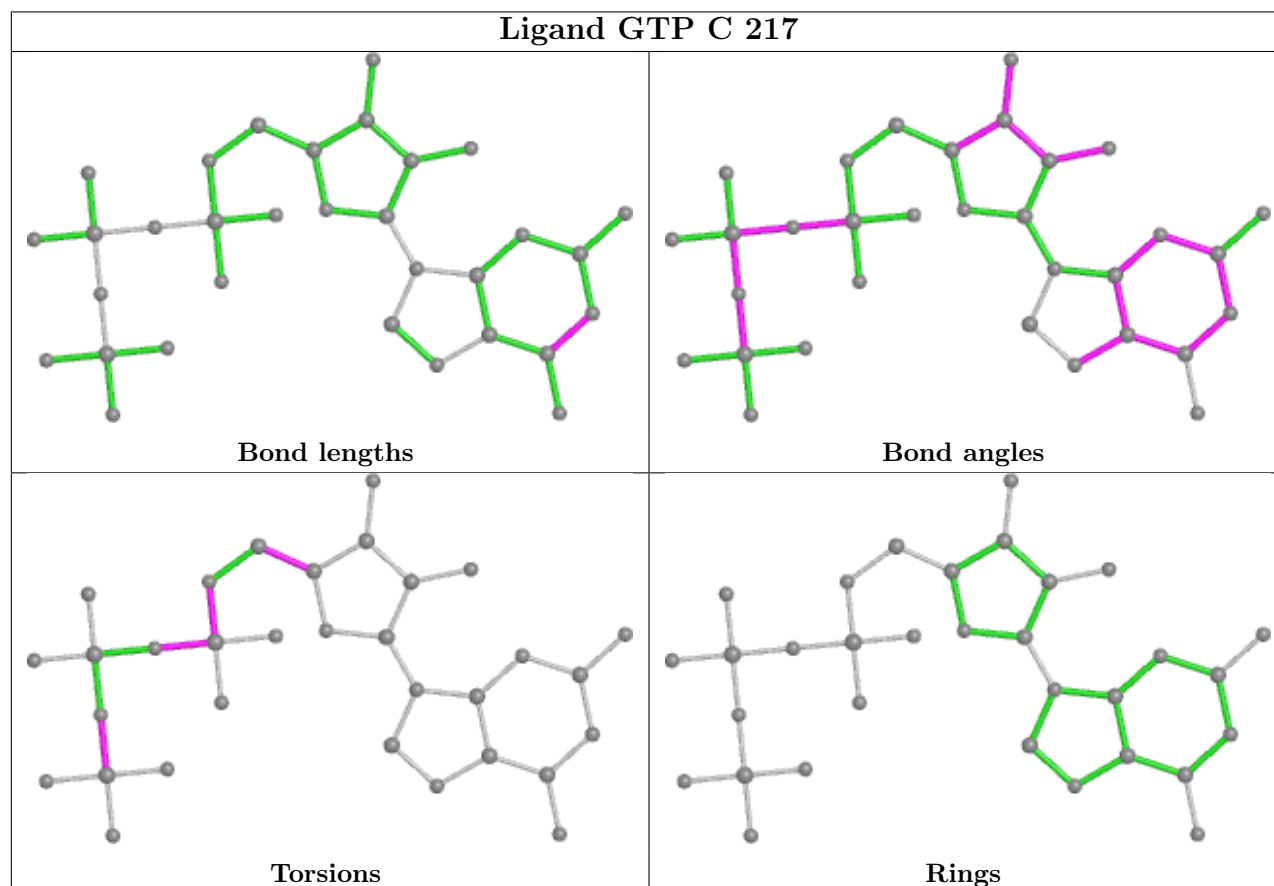
Mol	Chain	Res	Type	Atoms
4	C	217	GTP	PB-O3B-PG-O3G
4	C	217	GTP	C5'-O5'-PA-O1A
4	C	217	GTP	C5'-O5'-PA-O2A
4	C	217	GTP	C3'-C4'-C5'-O5'
4	C	217	GTP	O4'-C4'-C5'-O5'
4	F	217	GTP	O4'-C4'-C5'-O5'
4	C	217	GTP	C5'-O5'-PA-O3A
4	C	217	GTP	PB-O3B-PG-O1G
4	C	217	GTP	PB-O3A-PA-O1A
4	C	217	GTP	PB-O3A-PA-O2A

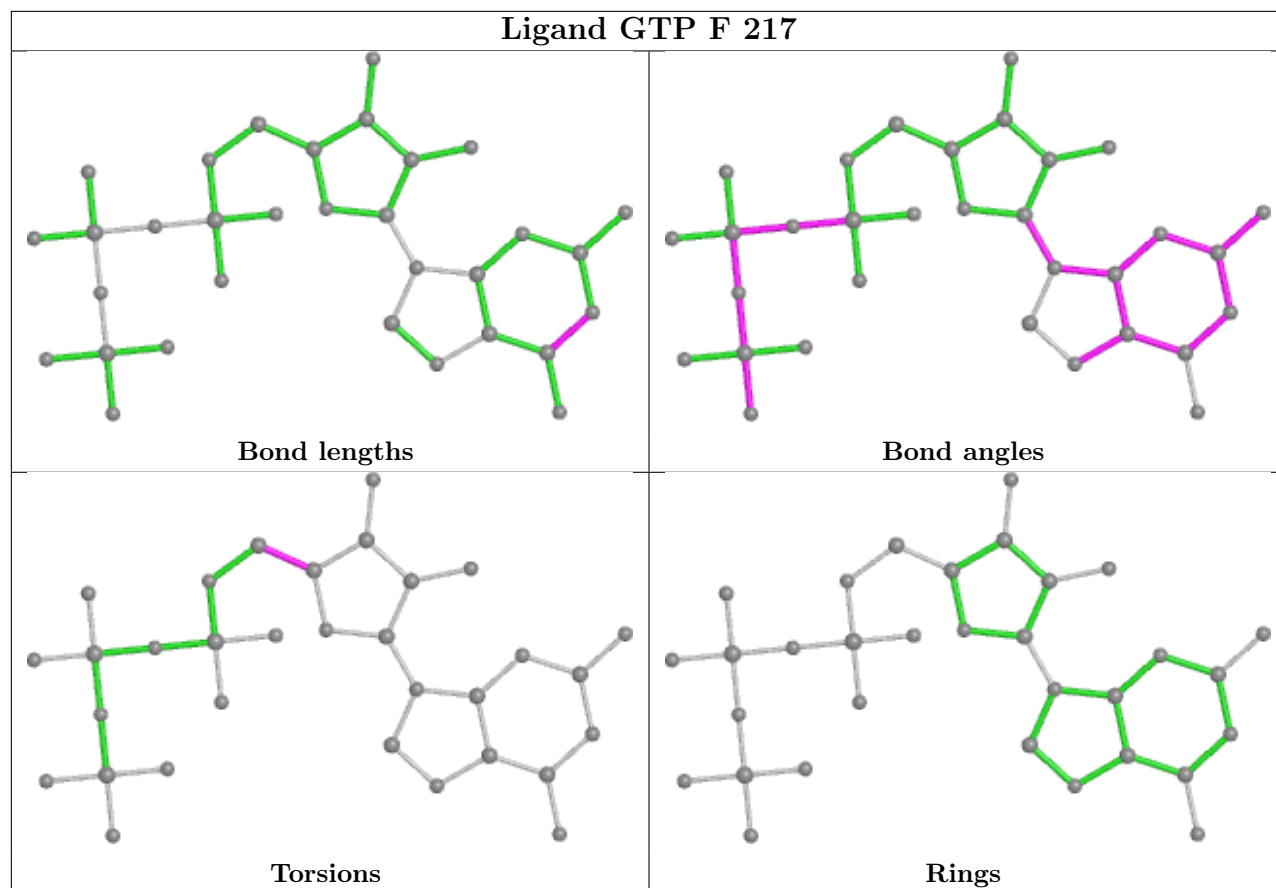
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	217	GTP	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	272/361 (75%)	-0.02	4 (1%) 73 72	7, 30, 72, 91	4 (1%)
1	E	277/361 (76%)	0.02	8 (2%) 51 50	7, 30, 80, 111	7 (2%)
2	C	171/176 (97%)	-0.14	0 100 100	10, 28, 58, 84	1 (0%)
2	F	171/176 (97%)	-0.25	0 100 100	10, 27, 56, 80	0
3	A	1041/1073 (97%)	-0.01	19 (1%) 68 67	4, 35, 90, 141	6 (0%)
3	D	1041/1073 (97%)	0.01	28 (2%) 54 53	5, 35, 89, 147	13 (1%)
All	All	2973/3220 (92%)	-0.02	59 (1%) 65 64	4, 32, 85, 147	31 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	70	SER	8.6
3	A	967	PRO	8.5
3	A	966	ASN	7.5
3	D	966	ASN	5.2
3	D	397	SER	5.0
3	D	965	GLY	4.4
1	E	352	HIS	4.3
3	D	71	GLN	4.1
3	D	1052	LEU	4.0
3	D	154	VAL	3.8
3	A	339	LYS	3.6
3	D	1032	ASP	3.6
1	E	45	ARG	3.5
3	A	391	SER	3.5
3	D	398	GLN	3.4
1	E	34	TYR	3.3
1	B	3	GLU	3.2
3	D	1026	ALA	3.0
3	D	155	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	296	GLN	2.9
3	A	332	GLU	2.9
3	A	397	SER	2.9
3	A	400	PHE	2.9
3	D	62	ARG	2.8
3	A	395	SER	2.8
3	D	395	SER	2.7
1	E	2	ASN	2.7
3	A	964	PRO	2.7
3	D	158	ARG	2.7
1	B	349	SER	2.6
3	A	120	VAL	2.6
3	D	1027	GLY	2.6
3	A	37	HIS	2.6
3	D	312	LYS	2.5
3	D	967	PRO	2.5
3	D	1021	GLN	2.5
3	D	487	THR	2.4
3	A	114	SER	2.4
1	E	3	GLU	2.4
3	D	119	CYS	2.4
3	D	980	ASN	2.4
3	D	56	HIS	2.3
3	A	200	ASN	2.3
1	E	6	LEU	2.2
3	A	64	ASP	2.2
3	D	203	SER	2.2
3	A	396	GLY	2.2
3	D	33	ASN	2.2
1	E	53	LYS	2.2
1	B	35	SER	2.2
3	A	62	ARG	2.1
3	A	160	SER	2.1
1	E	193	HIS	2.1
3	D	60	TRP	2.1
1	B	348	HIS	2.1
3	D	976	ASP	2.0
3	D	969	ASN	2.0
3	A	912	GLN	2.0
3	D	204	GLN	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](#)

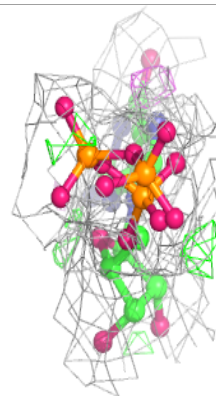
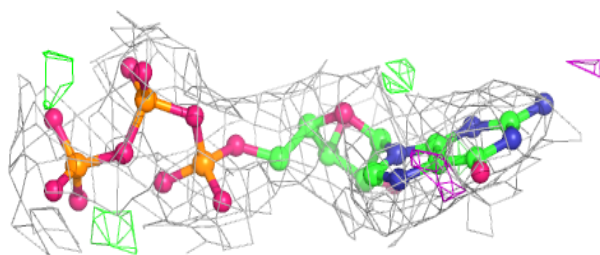
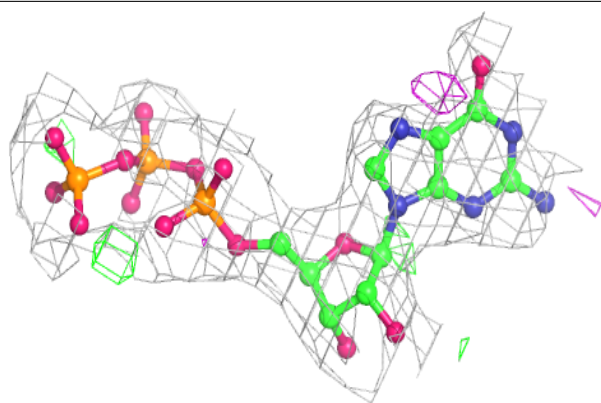
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GTP	C	217	32/32	0.94	0.19	10,21,47,63	0
4	GTP	F	217	32/32	0.96	0.17	7,18,30,35	0
5	MG	C	218	1/1	0.96	0.19	0,0,0,0	0
5	MG	F	218	1/1	0.96	0.13	6,6,6,6	0

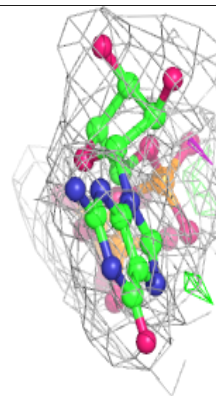
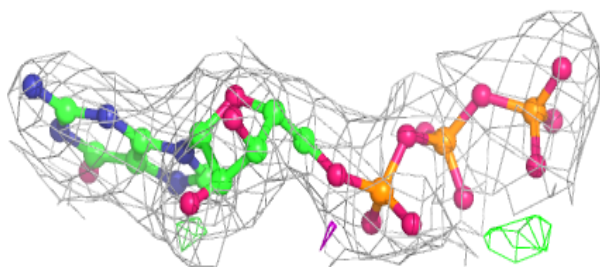
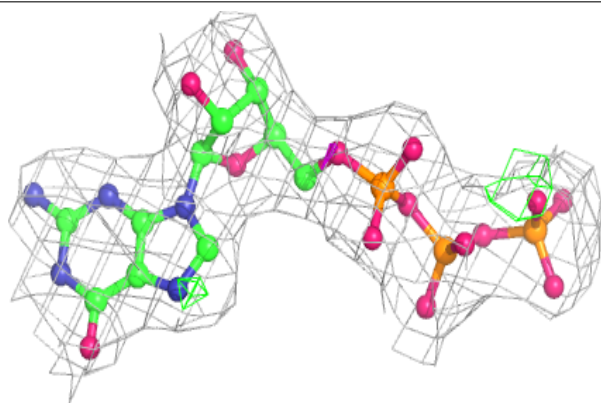
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP C 217:

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

**Electron density around GTP F 217:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.