Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 02:31 AM EST

PDB ID	:	3O6X
Title	:	Crystal Structure of the type III Glutamine Synthetase from Bacteroides fragilis
Authors	:	van Rooyen, J.M.; Belrhali, H.; Abratt, V.R.; Sewell, B.T.
Deposited on	:	2010-07-29
Resolution	:	3.50 Å(reported)

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

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

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

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

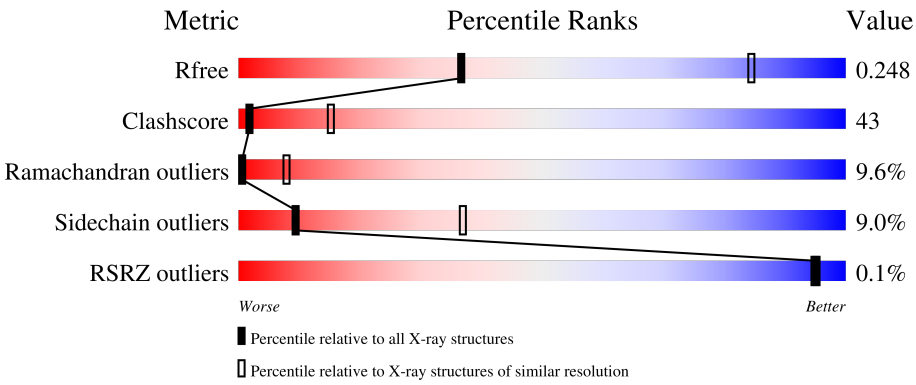
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	729	30% 45% 12% • 12%
1	B	729	33% 45% 10% • 12%
1	C	729	33% 44% 10% • 12%
1	D	729	32% 45% 9% • 12%
1	E	729	33% 45% 9% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	729	34% 43% 10% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	A	6001	-	-	X	-
5	CL	A	730	-	-	X	-
5	CL	B	6001	-	-	X	-
5	CL	C	6001	-	-	X	-
5	CL	D	6001	-	-	X	-
5	CL	E	6001	-	-	X	-
5	CL	F	6001	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30996 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	638	5120	3253	889	948	30	250	0	0
1	B	638	5120	3253	889	948	30	250	0	0
1	C	638	5120	3253	889	948	30	250	0	0
1	D	638	5120	3253	889	948	30	250	0	0
1	E	638	5120	3253	889	948	30	250	0	0
1	F	638	5120	3253	889	948	30	250	0	0

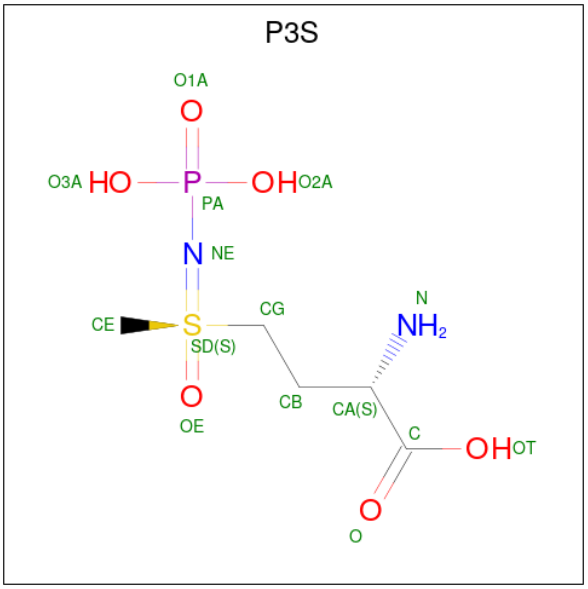
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLY	VAL	conflict	UNP Q5LGP1
A	531	LEU	PRO	conflict	UNP Q5LGP1
B	152	GLY	VAL	conflict	UNP Q5LGP1
B	531	LEU	PRO	conflict	UNP Q5LGP1
C	152	GLY	VAL	conflict	UNP Q5LGP1
C	531	LEU	PRO	conflict	UNP Q5LGP1
D	152	GLY	VAL	conflict	UNP Q5LGP1
D	531	LEU	PRO	conflict	UNP Q5LGP1
E	152	GLY	VAL	conflict	UNP Q5LGP1
E	531	LEU	PRO	conflict	UNP Q5LGP1
F	152	GLY	VAL	conflict	UNP Q5LGP1
F	531	LEU	PRO	conflict	UNP Q5LGP1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
			Total	Mg		
2	B	2	2	2	0	0
			Total	Mg		
2	C	2	2	2	0	0
			Total	Mg		
2	D	2	2	2	0	0
			Total	Mg		
2	E	2	2	2	0	0
			Total	Mg		
2	F	2	2	2	0	0

- Molecule 3 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: $C_5H_{13}N_2O_6PS$).



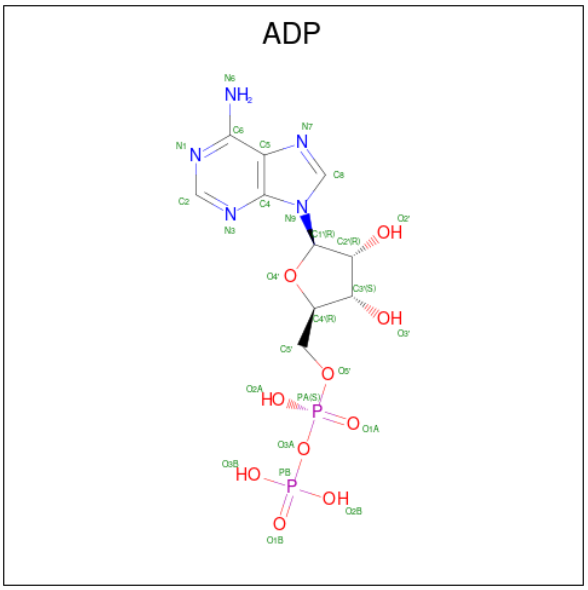
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	15	5	2	6	1	1	0	0
			Total	C	N	O	P	S		
3	B	1	15	5	2	6	1	1	0	0
			Total	C	N	O	P	S		
3	C	1	15	5	2	6	1	1	0	0
			Total	C	N	O	P	S		
3	D	1	15	5	2	6	1	1	0	0
			Total	C	N	O	P	S		
3	E	1	15	5	2	6	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	F	1	15	5	2	6	1	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	27	10	5	10	2	0	0
4	B	1	27	10	5	10	2	0	0
4	C	1	27	10	5	10	2	0	0
4	D	1	27	10	5	10	2	0	0
4	E	1	27	10	5	10	2	0	0
4	F	1	27	10	5	10	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	3	3	3	0	0
5	B	2	2	2	0	0

Continued on next page...

Continued from previous page...

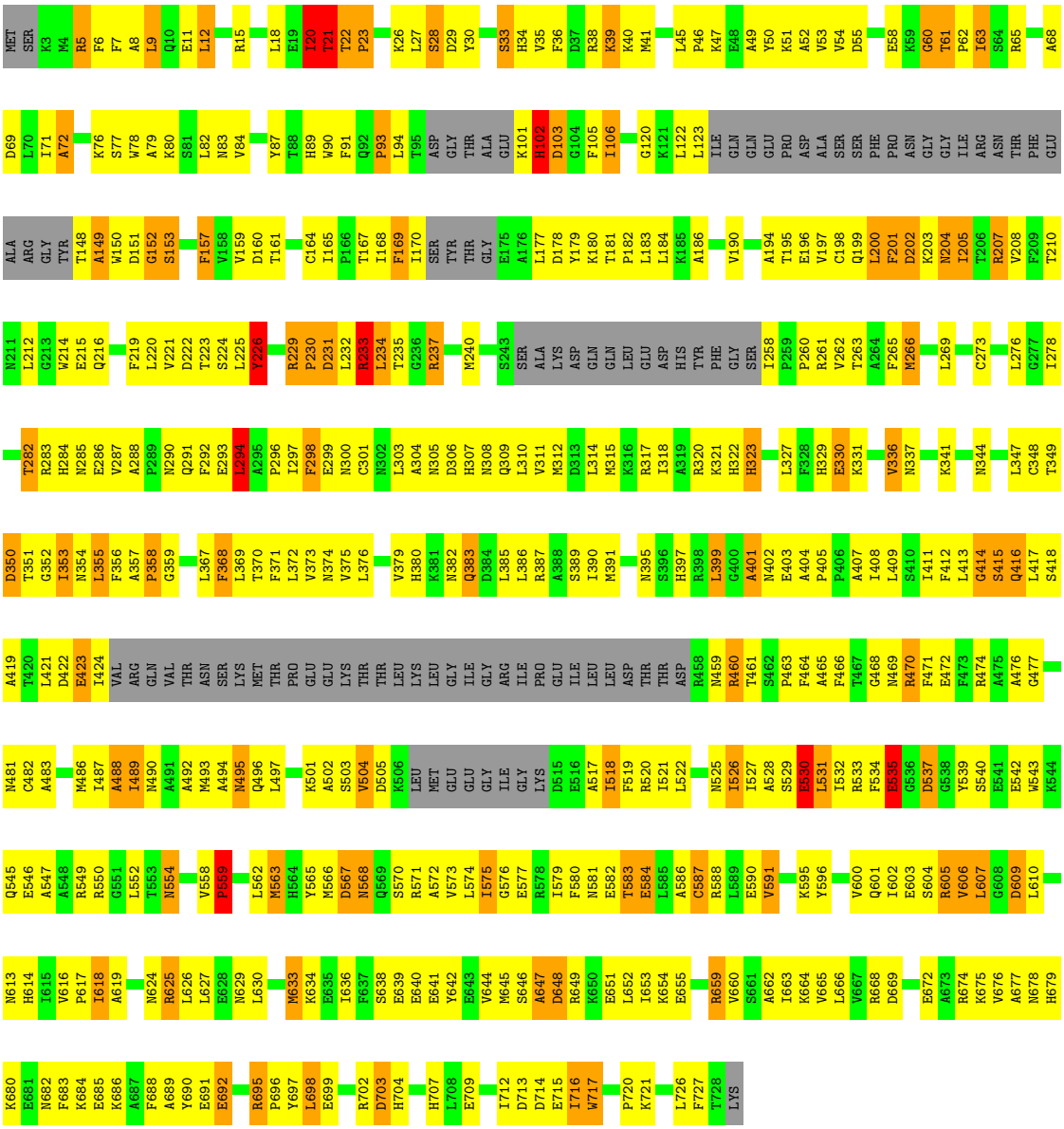
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	C	2	2	2	0	0
5	D	2	2	2	0	0
5	E	2	2	2	0	0
5	F	1	1	1	0	0

3 Residue-property plots (i)

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

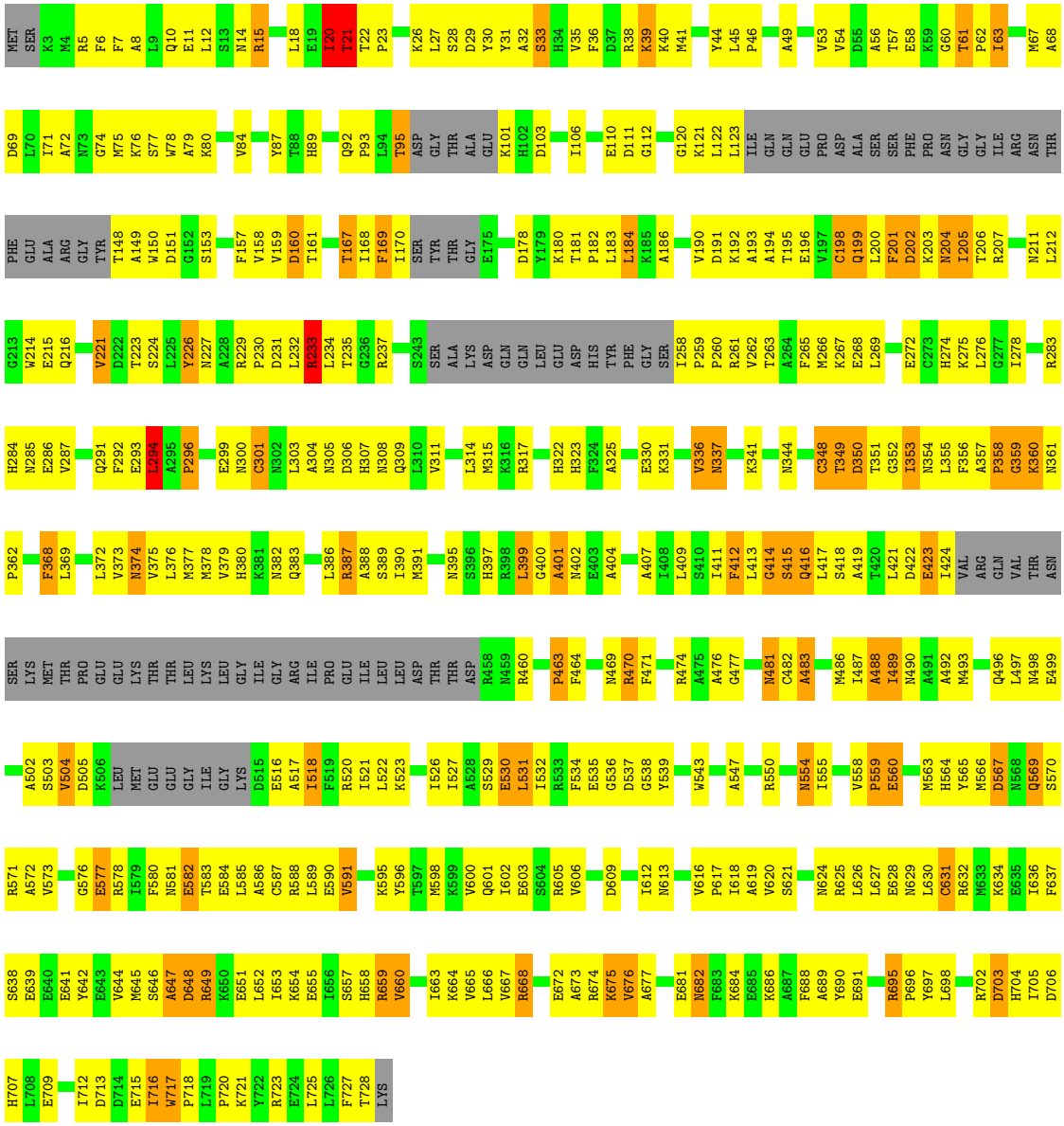
- Molecule 1: Glutamine synthetase

Chain A: 30% 45% 12% • 12%



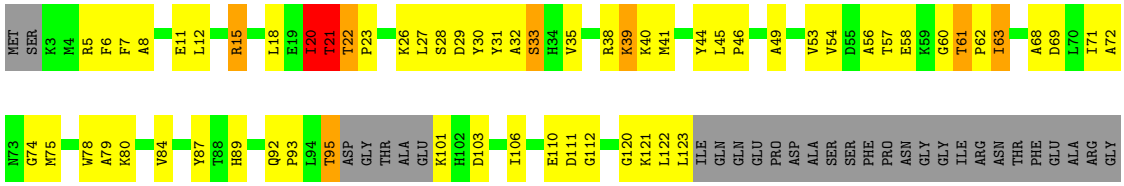
• Molecule 1: Glutamine synthetase

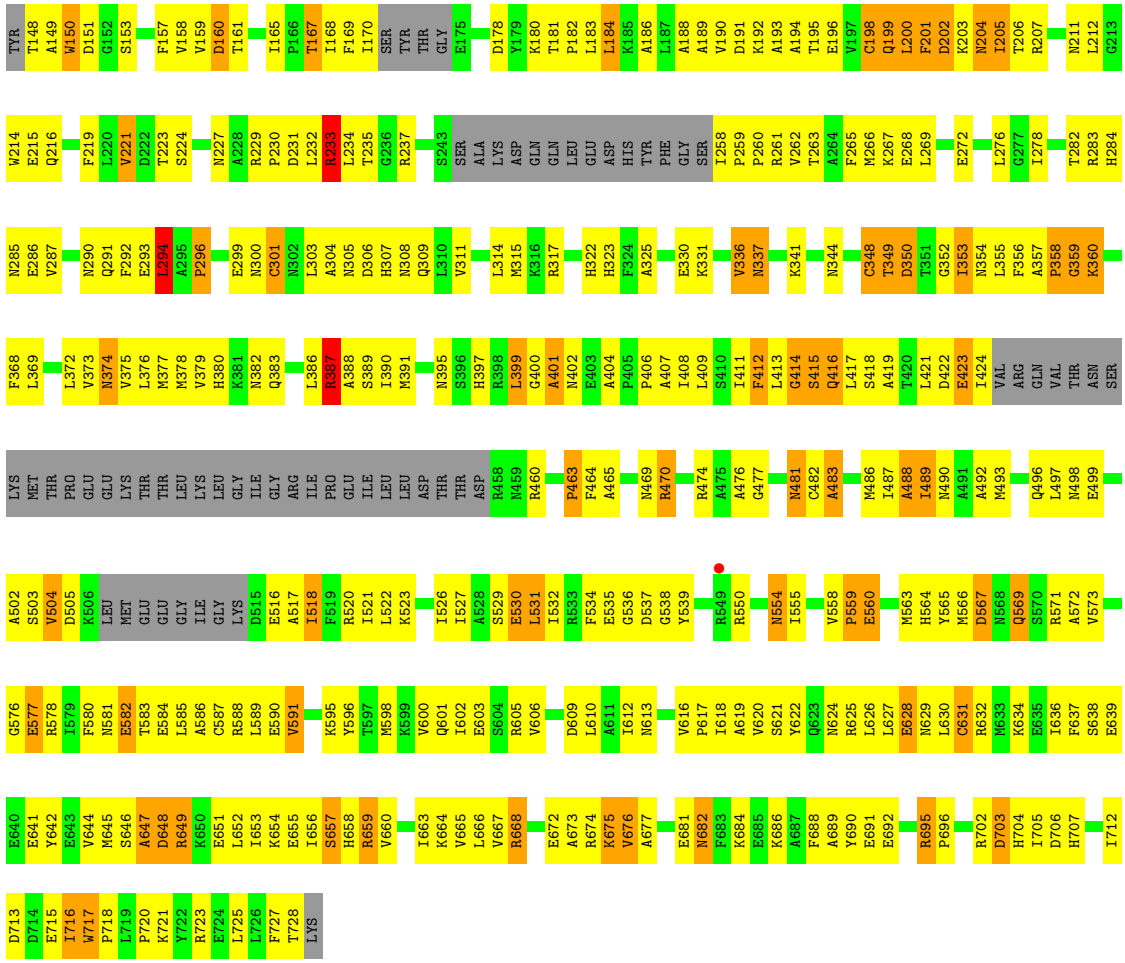
Chain B: 33% 45% 10% • 12%



• Molecule 1: Glutamine synthetase

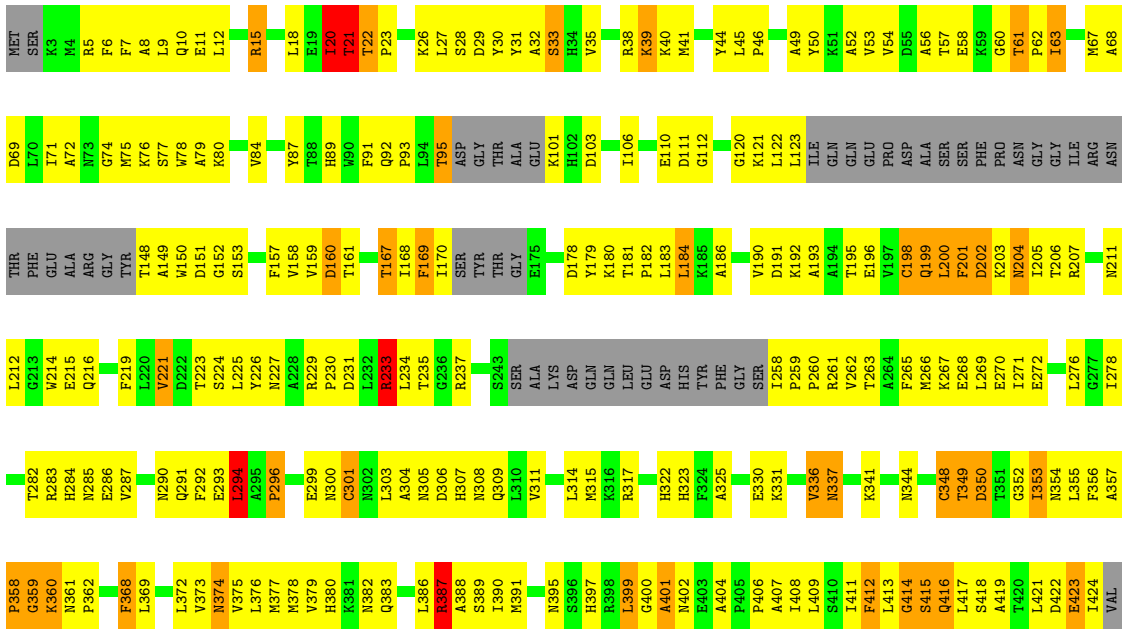
Chain C: 33% 44% 10% • 12%

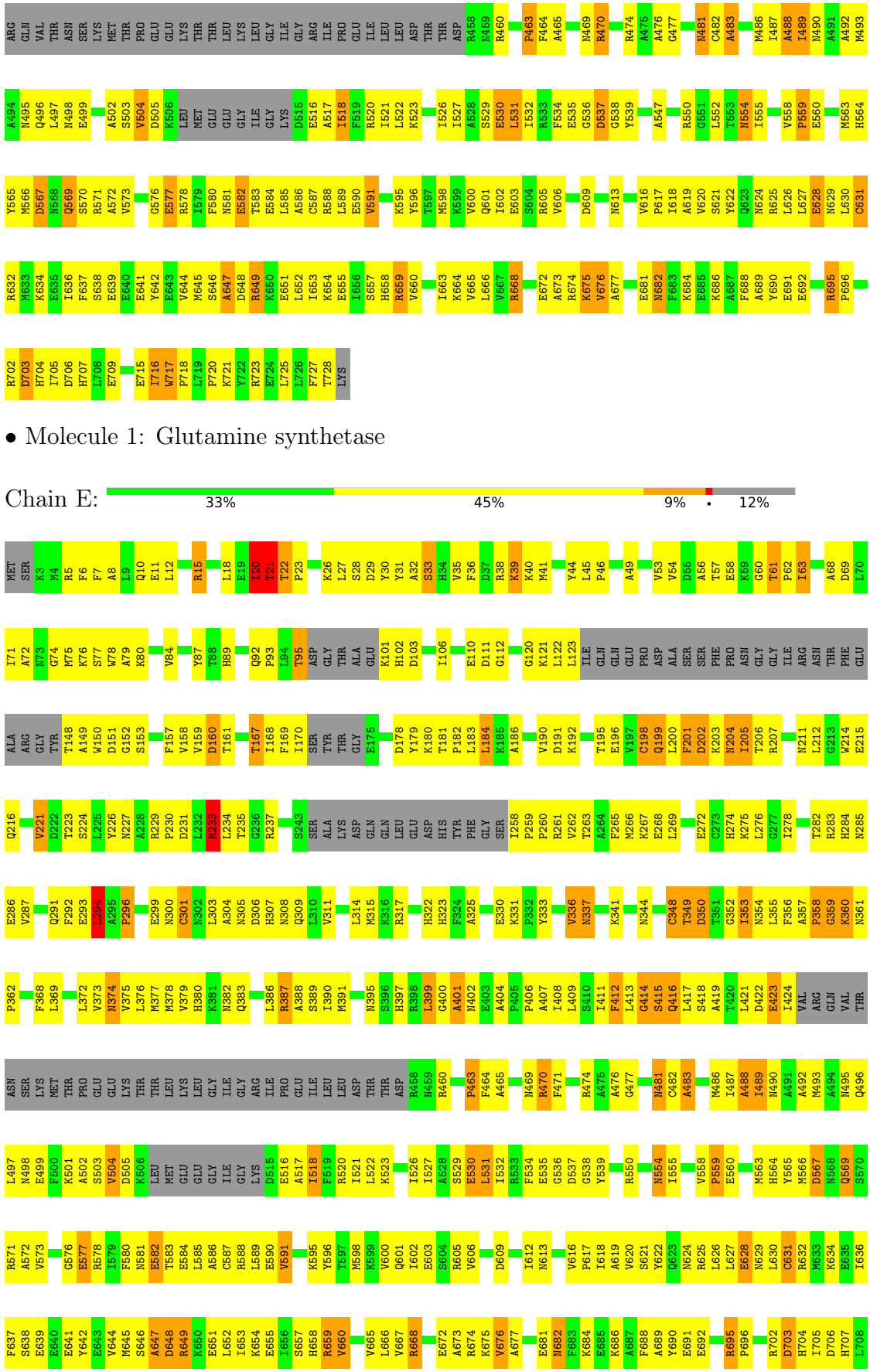




• Molecule 1: Glutamine synthetase

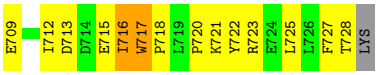
Chain D: 32% 45% 9% • 12%





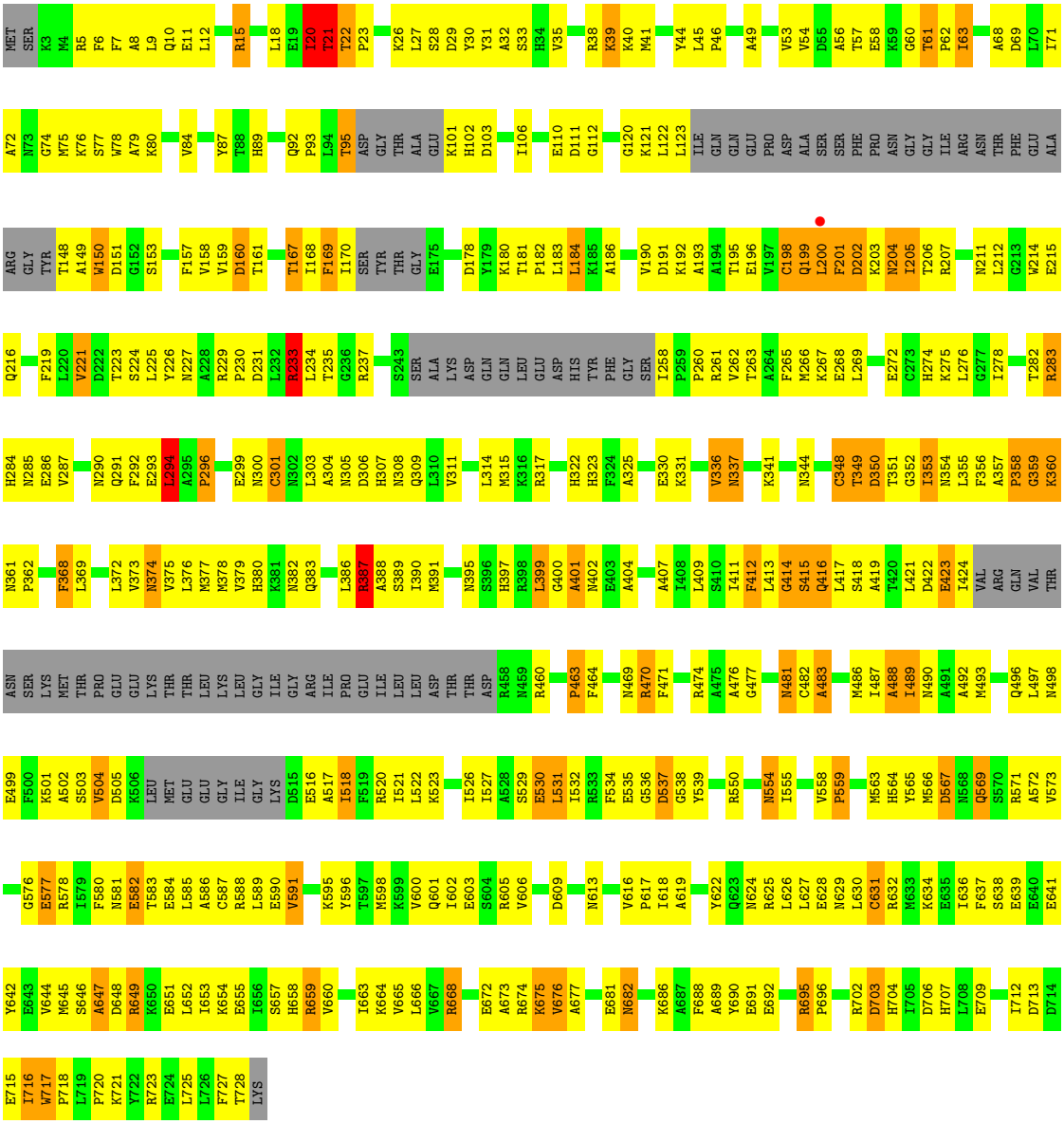
• Molecule 1: Glutamine synthetase

Chain E: 33% 45% 9% • 12%



• Molecule 1: Glutamine synthetase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	198.25Å 203.96Å 234.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.87 – 3.50 62.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.87-3.50) 100.0 (62.87-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.269 0.219 , 0.248	Depositor DCC
R_{free} test set	3016 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 70.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	30996	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: P3S, CL, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/5223	0.68	1/7048 (0.0%)
1	B	0.43	0/5223	0.63	1/7048 (0.0%)
1	C	0.43	0/5223	0.63	1/7048 (0.0%)
1	D	0.43	0/5223	0.63	1/7048 (0.0%)
1	E	0.44	0/5223	0.63	1/7048 (0.0%)
1	F	0.43	0/5223	0.63	1/7048 (0.0%)
All	All	0.44	0/31338	0.64	6/42288 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	233	ARG	N-CA-C	-5.70	95.60	111.00
1	B	233	ARG	N-CA-C	-5.68	95.67	111.00
1	E	233	ARG	N-CA-C	-5.59	95.91	111.00
1	D	233	ARG	N-CA-C	-5.57	95.97	111.00
1	F	233	ARG	N-CA-C	-5.55	96.02	111.00
1	A	233	ARG	N-CA-C	-5.55	96.03	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	TYR	Sidechain
1	B	226	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5120	0	5090	481	0
1	B	5120	0	5090	415	1
1	C	5120	0	5090	402	0
1	D	5120	0	5090	406	0
1	E	5120	0	5090	415	0
1	F	5120	0	5090	409	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	15	0	10	1	0
3	B	15	0	10	0	0
3	C	15	0	10	0	0
3	D	15	0	10	0	0
3	E	15	0	10	0	0
3	F	15	0	10	0	0
4	A	27	0	12	4	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	2	0
4	F	27	0	12	2	0
5	A	3	0	0	5	0
5	B	2	0	0	4	0
5	C	2	0	0	4	0
5	D	2	0	0	4	0
5	E	2	0	0	4	0
5	F	1	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30996	0	30672	2496	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (2496) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HD13	1:A:170:ILE:HD13	1.47	0.97
1:B:229:ARG:HD3	1:B:720:PRO:HD2	1.47	0.97
1:C:20:ILE:HG12	1:C:21:THR:H	1.31	0.96
1:F:229:ARG:HD3	1:F:720:PRO:HD2	1.46	0.96
1:F:20:ILE:HG12	1:F:21:THR:H	1.29	0.96
1:E:20:ILE:HG12	1:E:21:THR:H	1.31	0.95
1:D:20:ILE:HG12	1:D:21:THR:H	1.30	0.95
1:C:229:ARG:HD3	1:C:720:PRO:HD2	1.47	0.94
1:B:20:ILE:HG12	1:B:21:THR:H	1.29	0.94
1:E:229:ARG:HD3	1:E:720:PRO:HD2	1.49	0.94
1:D:229:ARG:HD3	1:D:720:PRO:HD2	1.47	0.94
1:D:293:GLU:HG2	1:D:294:LEU:H	1.33	0.94
1:B:293:GLU:HG2	1:B:294:LEU:H	1.34	0.93
1:F:61:THR:HB	1:F:62:PRO:HA	1.51	0.93
1:A:190:VAL:HG21	1:A:490:ASN:HB3	1.48	0.93
1:C:293:GLU:HG2	1:C:294:LEU:H	1.32	0.92
1:B:61:THR:HB	1:B:62:PRO:HA	1.52	0.92
1:D:61:THR:HB	1:D:62:PRO:HA	1.52	0.91
1:C:61:THR:HB	1:C:62:PRO:HA	1.51	0.91
1:E:61:THR:HB	1:E:62:PRO:HA	1.52	0.91
1:E:630:LEU:HD21	1:E:649:ARG:HG2	1.53	0.91
1:F:293:GLU:HG2	1:F:294:LEU:H	1.33	0.90
1:A:531:LEU:H	1:A:531:LEU:HD12	1.36	0.90
1:E:293:GLU:HG2	1:E:294:LEU:H	1.35	0.90
1:E:199:GLN:HE21	1:E:199:GLN:HA	1.36	0.90
1:C:721:LYS:NZ	5:C:5001:CL:CL	2.42	0.89
1:A:61:THR:HB	1:A:62:PRO:HA	1.54	0.89
1:A:352:GLY:O	1:A:353:ILE:HB	1.69	0.88
1:E:63:ILE:H	1:E:63:ILE:HD12	1.38	0.88
1:F:63:ILE:HD12	1:F:63:ILE:H	1.38	0.88
1:F:199:GLN:HA	1:F:199:GLN:HE21	1.38	0.88
1:B:199:GLN:HE21	1:B:199:GLN:HA	1.38	0.88
1:D:199:GLN:HA	1:D:199:GLN:HE21	1.38	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLN:HA	1:C:199:GLN:HE21	1.37	0.88
1:D:63:ILE:H	1:D:63:ILE:HD12	1.37	0.87
1:B:63:ILE:H	1:B:63:ILE:HD12	1.39	0.87
1:E:721:LYS:NZ	5:E:5001:CL:CL	2.44	0.86
1:C:63:ILE:HD12	1:C:63:ILE:H	1.38	0.85
1:A:411:ILE:HG22	1:A:412:PHE:H	1.40	0.85
1:C:20:ILE:O	1:C:21:THR:HG23	1.77	0.85
1:D:721:LYS:NZ	5:D:5001:CL:CL	2.47	0.85
1:E:554:ASN:C	1:E:554:ASN:HD22	1.80	0.85
1:B:554:ASN:HD22	1:B:554:ASN:C	1.80	0.85
1:D:20:ILE:O	1:D:21:THR:HG23	1.77	0.84
1:B:20:ILE:O	1:B:21:THR:HG23	1.76	0.84
1:A:20:ILE:O	1:A:21:THR:HG23	1.77	0.84
5:A:730:CL:CL	1:F:721:LYS:NZ	2.47	0.84
1:E:190:VAL:HG21	1:E:490:ASN:HB3	1.59	0.84
1:F:20:ILE:O	1:F:21:THR:HG23	1.76	0.84
1:E:20:ILE:O	1:E:21:THR:HG23	1.77	0.83
1:D:618:ILE:HG13	1:D:718:PRO:HD3	1.60	0.83
1:C:554:ASN:C	1:C:554:ASN:HD22	1.80	0.83
1:F:190:VAL:HG21	1:F:490:ASN:HB3	1.60	0.83
1:E:618:ILE:HG13	1:E:718:PRO:HD3	1.61	0.83
1:A:504:VAL:HG21	1:A:518:ILE:HG22	1.61	0.83
1:A:521:ILE:H	1:A:521:ILE:HD12	1.44	0.82
1:D:554:ASN:HD22	1:D:554:ASN:C	1.79	0.82
1:F:618:ILE:HG13	1:F:718:PRO:HD3	1.60	0.82
1:D:190:VAL:HG21	1:D:490:ASN:HB3	1.61	0.82
1:A:79:ALA:HB1	1:A:84:VAL:HG21	1.61	0.82
1:C:190:VAL:HG21	1:C:490:ASN:HB3	1.59	0.82
1:A:716:ILE:HG22	1:A:717:TRP:H	1.45	0.82
1:B:190:VAL:HG21	1:B:490:ASN:HB3	1.60	0.82
1:F:554:ASN:C	1:F:554:ASN:HD22	1.80	0.81
1:C:618:ILE:HG13	1:C:718:PRO:HD3	1.60	0.81
1:A:721:LYS:NZ	5:A:5001:CL:CL	2.51	0.81
1:B:721:LYS:NZ	5:B:5001:CL:CL	2.50	0.81
1:C:630:LEU:HD21	1:C:649:ARG:HG2	1.61	0.81
1:B:618:ILE:HG13	1:B:718:PRO:HD3	1.61	0.81
1:F:638:SER:OG	1:F:641:GLU:HG3	1.81	0.81
1:F:151:ASP:OD1	1:F:153:SER:HB3	1.81	0.81
1:B:638:SER:OG	1:B:641:GLU:HG3	1.80	0.80
1:B:630:LEU:HD21	1:B:649:ARG:HG2	1.61	0.80
1:F:630:LEU:HD21	1:F:649:ARG:HG2	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ARG:NH2	1:A:704:HIS:ND1	2.30	0.80
1:A:627:LEU:HD23	1:A:653:ILE:HD13	1.63	0.80
1:A:214:TRP:CE2	1:A:308:ASN:HB2	2.17	0.79
1:D:630:LEU:HD21	1:D:649:ARG:HG2	1.62	0.79
1:D:151:ASP:OD1	1:D:153:SER:HB3	1.82	0.79
1:A:20:ILE:HG12	1:A:21:THR:H	1.45	0.79
1:B:504:VAL:HG23	1:B:521:ILE:HD13	1.65	0.79
1:D:638:SER:OG	1:D:641:GLU:HG3	1.82	0.79
1:E:151:ASP:OD1	1:E:153:SER:HB3	1.83	0.79
1:B:151:ASP:OD1	1:B:153:SER:HB3	1.82	0.79
1:E:638:SER:OG	1:E:641:GLU:HG3	1.82	0.78
1:F:504:VAL:HG23	1:F:521:ILE:HD13	1.65	0.78
1:A:20:ILE:HD13	1:A:20:ILE:H	1.47	0.78
1:B:616:VAL:HB	1:B:617:PRO:HD3	1.65	0.78
1:E:616:VAL:HB	1:E:617:PRO:HD3	1.64	0.78
1:C:638:SER:OG	1:C:641:GLU:HG3	1.82	0.78
1:A:63:ILE:H	1:A:63:ILE:HD12	1.47	0.78
1:A:358:PRO:HB3	1:A:368:PHE:CE1	2.19	0.78
1:A:411:ILE:HG22	1:A:412:PHE:N	1.99	0.77
1:E:504:VAL:HG23	1:E:521:ILE:HD13	1.67	0.77
1:D:168:ILE:O	1:D:168:ILE:HG13	1.84	0.77
1:F:168:ILE:HG13	1:F:168:ILE:O	1.84	0.77
1:C:168:ILE:HG13	1:C:168:ILE:O	1.85	0.77
1:C:233:ARG:HD3	1:C:234:LEU:H	1.47	0.77
1:C:627:LEU:HD23	1:C:653:ILE:HD13	1.66	0.77
1:D:627:LEU:HD23	1:D:653:ILE:HD13	1.67	0.77
1:C:151:ASP:OD1	1:C:153:SER:HB3	1.83	0.77
1:F:233:ARG:HD3	1:F:234:LEU:H	1.48	0.77
1:A:605:ARG:NH2	5:A:6001:CL:CL	2.55	0.76
1:D:616:VAL:HB	1:D:617:PRO:HD3	1.65	0.76
1:D:54:VAL:HA	1:D:57:THR:HG22	1.67	0.76
1:E:181:THR:HB	1:E:182:PRO:HD3	1.67	0.76
1:F:349:THR:HG23	1:F:353:ILE:HB	1.67	0.76
1:A:629:ASN:ND2	1:A:649:ARG:HE	1.84	0.76
1:E:54:VAL:HA	1:E:57:THR:HG22	1.67	0.76
1:E:168:ILE:O	1:E:168:ILE:HG13	1.85	0.76
1:E:627:LEU:HD23	1:E:653:ILE:HD13	1.67	0.76
1:C:233:ARG:HD3	1:C:234:LEU:N	2.00	0.76
1:C:504:VAL:HG23	1:C:521:ILE:HD13	1.68	0.76
1:C:616:VAL:HB	1:C:617:PRO:HD3	1.66	0.76
1:C:181:THR:HB	1:C:182:PRO:HD3	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:CD2	1:A:201:PHE:N	2.52	0.76
1:D:504:VAL:HG23	1:D:521:ILE:HD13	1.67	0.76
1:E:233:ARG:HD3	1:E:234:LEU:H	1.50	0.76
1:E:233:ARG:HD3	1:E:234:LEU:N	2.00	0.76
1:E:349:THR:HG23	1:E:353:ILE:HB	1.68	0.76
1:A:616:VAL:HB	1:A:617:PRO:HD3	1.65	0.75
1:D:233:ARG:HD3	1:D:234:LEU:H	1.49	0.75
1:F:233:ARG:HD3	1:F:234:LEU:N	1.99	0.75
1:C:349:THR:HG23	1:C:353:ILE:HB	1.67	0.75
1:F:627:LEU:HD23	1:F:653:ILE:HD13	1.68	0.75
1:B:54:VAL:HA	1:B:57:THR:HG22	1.68	0.75
1:D:233:ARG:HD3	1:D:234:LEU:N	2.00	0.75
1:F:20:ILE:CG1	1:F:21:THR:H	2.00	0.75
1:A:30:TYR:O	1:A:33:SER:HB3	1.86	0.75
1:B:330:GLU:HG3	1:B:395:ASN:HA	1.69	0.75
1:D:349:THR:HG23	1:D:353:ILE:HB	1.67	0.75
1:D:376:LEU:HD23	1:D:411:ILE:HD12	1.68	0.75
1:F:181:THR:HB	1:F:182:PRO:HD3	1.69	0.75
1:F:616:VAL:HB	1:F:617:PRO:HD3	1.66	0.75
1:B:168:ILE:O	1:B:168:ILE:HG13	1.85	0.75
1:B:349:THR:HG23	1:B:353:ILE:HB	1.67	0.75
1:B:20:ILE:CG1	1:B:21:THR:H	2.00	0.75
1:E:20:ILE:CG1	1:E:21:THR:H	2.00	0.75
1:D:181:THR:HB	1:D:182:PRO:HD3	1.69	0.75
1:A:572:ALA:O	1:A:576:GLY:HA3	1.87	0.74
1:C:293:GLU:HG2	1:C:294:LEU:N	2.02	0.74
1:B:233:ARG:HD3	1:B:234:LEU:N	2.02	0.74
1:C:54:VAL:HA	1:C:57:THR:HG22	1.68	0.74
1:E:330:GLU:HG3	1:E:395:ASN:HA	1.67	0.74
1:F:716:ILE:HG22	1:F:717:TRP:H	1.52	0.74
1:A:165:ILE:O	1:A:167:THR:HG23	1.88	0.74
1:B:376:LEU:HD23	1:B:411:ILE:HD12	1.68	0.74
1:C:330:GLU:HG3	1:C:395:ASN:HA	1.69	0.74
1:F:54:VAL:HA	1:F:57:THR:HG22	1.68	0.74
1:C:79:ALA:HB1	1:C:84:VAL:HG21	1.69	0.74
1:B:181:THR:HB	1:B:182:PRO:HD3	1.69	0.74
1:C:20:ILE:CG1	1:C:21:THR:H	2.01	0.74
1:E:376:LEU:HD23	1:E:411:ILE:HD12	1.69	0.74
1:F:79:ALA:HB1	1:F:84:VAL:HG21	1.70	0.74
1:F:376:LEU:HD23	1:F:411:ILE:HD12	1.68	0.74
1:A:660:VAL:HG22	1:A:664:LYS:HE3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:CG1	1:D:21:THR:H	2.01	0.74
1:E:716:ILE:HG22	1:E:717:TRP:H	1.52	0.74
1:A:237:ARG:HB3	1:A:329:HIS:CD2	2.23	0.74
1:A:41:MET:HB3	1:A:45:LEU:HD12	1.70	0.73
1:E:79:ALA:HB1	1:E:84:VAL:HG21	1.70	0.73
1:A:181:THR:HB	1:A:182:PRO:HD3	1.68	0.73
1:C:602:ILE:HD12	1:C:602:ILE:H	1.54	0.73
1:D:293:GLU:HG2	1:D:294:LEU:N	2.03	0.73
1:D:330:GLU:HG3	1:D:395:ASN:HA	1.68	0.73
1:B:233:ARG:HD3	1:B:234:LEU:H	1.52	0.73
1:A:284:HIS:HB3	1:B:101:LYS:HA	1.68	0.73
1:A:613:ASN:ND2	5:A:730:CL:CL	2.57	0.73
1:F:605:ARG:NH2	5:F:6001:CL:CL	2.58	0.73
1:B:79:ALA:HB1	1:B:84:VAL:HG21	1.71	0.73
1:A:229:ARG:HG2	1:A:720:PRO:HD2	1.71	0.72
1:E:602:ILE:H	1:E:602:ILE:HD12	1.54	0.72
1:B:605:ARG:NH2	5:B:6001:CL:CL	2.59	0.72
1:B:716:ILE:HG22	1:B:717:TRP:H	1.53	0.72
1:D:79:ALA:HB1	1:D:84:VAL:HG21	1.70	0.72
1:C:716:ILE:HG22	1:C:717:TRP:H	1.54	0.72
1:F:330:GLU:HG3	1:F:395:ASN:HA	1.70	0.72
1:C:376:LEU:HD23	1:C:411:ILE:HD12	1.72	0.72
1:A:372:LEU:HD22	1:A:417:LEU:HD11	1.72	0.72
1:B:627:LEU:HD23	1:B:653:ILE:HD13	1.70	0.71
1:E:30:TYR:O	1:E:33:SER:HB3	1.90	0.71
1:F:387:ARG:HH11	1:F:407:ALA:HB1	1.56	0.71
1:D:237:ARG:NH2	1:D:603:GLU:OE2	2.23	0.71
1:D:716:ILE:HG22	1:D:717:TRP:H	1.56	0.71
1:A:571:ARG:O	1:A:575:ILE:HG22	1.91	0.71
1:B:30:TYR:O	1:B:33:SER:HB3	1.91	0.71
1:C:61:THR:CB	1:C:62:PRO:HA	2.21	0.71
1:E:41:MET:HB3	1:E:45:LEU:HD12	1.72	0.71
1:A:529:SER:O	1:A:531:LEU:N	2.23	0.70
1:A:20:ILE:HG12	1:A:21:THR:N	2.06	0.70
1:A:376:LEU:HD23	1:A:411:ILE:HD12	1.74	0.70
1:F:293:GLU:HG2	1:F:294:LEU:N	2.04	0.70
1:A:201:PHE:N	1:A:201:PHE:HD2	1.89	0.70
1:C:41:MET:HB3	1:C:45:LEU:HD12	1.72	0.70
1:D:41:MET:HB3	1:D:45:LEU:HD12	1.72	0.70
1:D:602:ILE:H	1:D:602:ILE:HD12	1.55	0.70
1:F:41:MET:HB3	1:F:45:LEU:HD12	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:ILE:HG22	1:F:180:LYS:HG2	1.73	0.70
1:A:230:PRO:O	1:A:233:ARG:O	2.08	0.70
1:B:61:THR:CB	1:B:62:PRO:HA	2.22	0.70
1:F:61:THR:CB	1:F:62:PRO:HA	2.21	0.70
1:A:330:GLU:HG3	1:A:395:ASN:N	2.06	0.70
1:C:168:ILE:HG22	1:C:180:LYS:HG2	1.73	0.70
1:D:30:TYR:O	1:D:33:SER:HB3	1.90	0.70
1:B:293:GLU:HG2	1:B:294:LEU:N	2.04	0.70
1:C:605:ARG:NH2	5:C:6001:CL:CL	2.62	0.70
1:A:151:ASP:OD1	1:A:153:SER:HB3	1.92	0.70
1:E:373:VAL:HA	1:E:376:LEU:HD12	1.73	0.70
1:F:207:ARG:HB2	1:F:207:ARG:HH11	1.57	0.70
1:B:207:ARG:HH11	1:B:207:ARG:HB2	1.57	0.70
1:D:168:ILE:HG22	1:D:180:LYS:HG2	1.74	0.70
1:E:168:ILE:HG22	1:E:180:LYS:HG2	1.73	0.70
1:E:387:ARG:HH11	1:E:407:ALA:HB1	1.57	0.70
1:C:521:ILE:H	1:C:521:ILE:HD12	1.54	0.70
1:C:237:ARG:NH2	1:C:603:GLU:OE2	2.26	0.69
1:D:605:ARG:NH2	5:D:6001:CL:CL	2.62	0.69
1:E:293:GLU:HG2	1:E:294:LEU:N	2.05	0.69
1:B:41:MET:HB3	1:B:45:LEU:HD12	1.75	0.69
1:D:56:ALA:HA	1:D:61:THR:HA	1.74	0.69
1:A:373:VAL:HG22	1:A:526:ILE:HD11	1.75	0.69
1:B:56:ALA:HA	1:B:61:THR:HA	1.74	0.69
1:B:373:VAL:HA	1:B:376:LEU:HD12	1.73	0.69
1:D:284:HIS:HB3	1:E:101:LYS:HA	1.74	0.69
1:D:521:ILE:H	1:D:521:ILE:HD12	1.57	0.69
1:F:233:ARG:HH11	1:F:233:ARG:HG3	1.58	0.69
1:F:373:VAL:HA	1:F:376:LEU:HD12	1.73	0.69
1:A:354:ASN:HB3	1:A:357:ALA:HB2	1.75	0.69
1:A:421:LEU:HD23	1:A:533:ARG:HH11	1.58	0.69
1:B:233:ARG:HH11	1:B:233:ARG:HG3	1.56	0.69
1:B:521:ILE:HD12	1:B:521:ILE:H	1.56	0.69
1:B:571:ARG:HH21	1:B:582:GLU:CD	1.96	0.69
1:B:602:ILE:H	1:B:602:ILE:HD12	1.58	0.69
1:C:272:GLU:O	1:C:276:LEU:HD23	1.92	0.69
1:E:56:ALA:HA	1:E:61:THR:HA	1.75	0.69
1:A:151:ASP:O	1:A:153:SER:N	2.25	0.69
1:B:168:ILE:HG22	1:B:180:LYS:HG2	1.74	0.69
1:C:207:ARG:HB2	1:C:207:ARG:HH11	1.57	0.69
1:E:233:ARG:HH11	1:E:233:ARG:HG3	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ALA:HA	1:A:550:ARG:HD3	1.74	0.69
1:D:207:ARG:HH11	1:D:207:ARG:HB2	1.56	0.69
1:B:272:GLU:O	1:B:276:LEU:HD23	1.94	0.68
1:D:61:THR:CB	1:D:62:PRO:HA	2.22	0.68
1:D:352:GLY:O	1:D:353:ILE:HB	1.93	0.68
1:D:571:ARG:HH21	1:D:582:GLU:CD	1.96	0.68
1:E:61:THR:CB	1:E:62:PRO:HA	2.22	0.68
1:F:521:ILE:H	1:F:521:ILE:HD12	1.58	0.68
1:A:46:PRO:HD2	1:A:49:ALA:HB3	1.74	0.68
1:B:387:ARG:HH11	1:B:407:ALA:HB1	1.57	0.68
1:A:469:ASN:O	1:A:470:ARG:HB3	1.92	0.68
1:C:30:TYR:O	1:C:33:SER:HB3	1.92	0.68
1:C:352:GLY:O	1:C:353:ILE:HB	1.94	0.68
1:C:387:ARG:HH11	1:C:407:ALA:HB1	1.56	0.68
1:C:571:ARG:HH21	1:C:582:GLU:CD	1.97	0.68
1:D:373:VAL:HA	1:D:376:LEU:HD12	1.75	0.68
1:F:272:GLU:O	1:F:276:LEU:HD23	1.94	0.68
1:F:571:ARG:HH21	1:F:582:GLU:CD	1.96	0.68
1:C:56:ALA:HA	1:C:61:THR:HA	1.74	0.68
1:D:272:GLU:O	1:D:276:LEU:HD23	1.93	0.68
1:A:492:ALA:HA	1:A:573:VAL:HG11	1.76	0.68
1:C:233:ARG:HH11	1:C:233:ARG:HG3	1.59	0.68
1:E:605:ARG:NH2	5:E:6001:CL:CL	2.64	0.68
4:F:4001:ADP:O2B	4:F:4001:ADP:H5'2	1.94	0.68
1:A:379:VAL:HB	1:A:411:ILE:HD11	1.75	0.68
1:D:233:ARG:HG3	1:D:233:ARG:HH11	1.58	0.68
1:F:223:THR:HG22	1:F:227:ASN:HD21	1.59	0.68
1:D:387:ARG:HH11	1:D:407:ALA:HB1	1.58	0.68
4:E:4001:ADP:O2B	4:E:4001:ADP:H5'2	1.95	0.67
1:F:602:ILE:H	1:F:602:ILE:HD12	1.58	0.67
1:C:566:MET:O	1:C:571:ARG:HD2	1.95	0.67
1:F:56:ALA:HA	1:F:61:THR:HA	1.75	0.67
1:A:674:ARG:HD2	5:A:6001:CL:CL	2.31	0.67
1:E:521:ILE:HD12	1:E:521:ILE:H	1.58	0.67
1:A:713:ASP:HB2	1:B:617:PRO:HB3	1.75	0.67
1:E:352:GLY:O	1:E:353:ILE:HB	1.94	0.67
1:F:566:MET:O	1:F:571:ARG:HD2	1.95	0.67
1:B:352:GLY:O	1:B:353:ILE:HB	1.94	0.67
1:E:272:GLU:O	1:E:276:LEU:HD23	1.94	0.67
1:E:571:ARG:HH21	1:E:582:GLU:CD	1.98	0.67
1:E:676:VAL:HG22	1:E:677:ALA:N	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:4001:ADP:O2B	4:C:4001:ADP:H5'2	1.95	0.67
1:E:355:LEU:O	1:E:356:PHE:HD1	1.78	0.67
1:D:676:VAL:HG22	1:D:677:ALA:N	2.10	0.67
1:E:214:TRP:CE2	1:E:308:ASN:HB2	2.30	0.67
1:C:223:THR:HG22	1:C:227:ASN:HD21	1.60	0.66
1:F:30:TYR:O	1:F:33:SER:HB3	1.95	0.66
1:A:53:VAL:HG22	1:A:71:ILE:CD1	2.25	0.66
4:D:4001:ADP:H5'2	4:D:4001:ADP:O2B	1.94	0.66
1:E:207:ARG:HB2	1:E:207:ARG:HH11	1.58	0.66
1:F:352:GLY:O	1:F:353:ILE:HB	1.95	0.66
1:F:637:PHE:HB3	1:F:641:GLU:HB2	1.77	0.66
1:F:676:VAL:HG22	1:F:677:ALA:N	2.08	0.66
1:B:237:ARG:NH2	1:B:603:GLU:OE2	2.28	0.66
1:A:641:GLU:O	1:A:644:VAL:HG12	1.95	0.66
1:D:223:THR:HG22	1:D:227:ASN:HD21	1.59	0.66
1:D:529:SER:O	1:D:531:LEU:N	2.29	0.66
1:D:566:MET:O	1:D:571:ARG:HD2	1.96	0.66
1:D:375:VAL:HG22	1:D:493:MET:HE2	1.77	0.66
1:F:355:LEU:O	1:F:356:PHE:HD1	1.79	0.66
1:B:566:MET:O	1:B:571:ARG:HD2	1.95	0.66
1:B:676:VAL:HG22	1:B:677:ALA:N	2.10	0.66
1:E:11:GLU:HG3	1:E:15:ARG:HH12	1.60	0.66
1:E:190:VAL:CG2	1:E:490:ASN:HB3	2.25	0.66
1:E:278:ILE:HD13	1:E:311:VAL:HG22	1.77	0.66
1:B:214:TRP:CE2	1:B:308:ASN:HB2	2.30	0.66
1:A:34:HIS:HB2	1:A:276:LEU:HD23	1.77	0.66
4:B:4001:ADP:O2B	4:B:4001:ADP:H5'2	1.95	0.66
1:C:214:TRP:CE2	1:C:308:ASN:HB2	2.30	0.66
1:C:373:VAL:HA	1:C:376:LEU:HD12	1.75	0.66
1:D:637:PHE:HB3	1:D:641:GLU:HB2	1.77	0.66
1:F:11:GLU:HG3	1:F:15:ARG:HH12	1.61	0.66
1:A:61:THR:CB	1:A:62:PRO:HA	2.26	0.66
1:B:7:PHE:O	1:B:11:GLU:HB2	1.96	0.66
1:D:214:TRP:CE2	1:D:308:ASN:HB2	2.31	0.66
1:E:237:ARG:NH2	1:E:603:GLU:OE2	2.29	0.66
1:C:7:PHE:O	1:C:11:GLU:HB2	1.96	0.65
1:C:11:GLU:HG3	1:C:15:ARG:HH12	1.61	0.65
1:C:190:VAL:CG2	1:C:490:ASN:HB3	2.26	0.65
1:F:214:TRP:CE2	1:F:308:ASN:HB2	2.30	0.65
1:D:355:LEU:O	1:D:356:PHE:HD1	1.79	0.65
1:B:411:ILE:HG22	1:B:412:PHE:N	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:H	1:A:20:ILE:CD1	2.10	0.65
1:F:469:ASN:O	1:F:470:ARG:HB3	1.97	0.65
1:A:38:ARG:HH22	1:A:54:VAL:HG13	1.60	0.65
1:B:278:ILE:HD13	1:B:311:VAL:HG22	1.77	0.65
1:C:186:ALA:O	1:C:190:VAL:HG23	1.96	0.65
1:C:637:PHE:HB3	1:C:641:GLU:HB2	1.78	0.65
1:D:11:GLU:HG3	1:D:15:ARG:HH12	1.62	0.65
1:B:190:VAL:CG2	1:B:490:ASN:HB3	2.26	0.65
1:C:521:ILE:HD12	1:C:521:ILE:N	2.12	0.65
1:E:223:THR:HG22	1:E:227:ASN:HD21	1.60	0.65
1:F:237:ARG:NH2	1:F:603:GLU:OE2	2.29	0.65
1:F:278:ILE:HD13	1:F:311:VAL:HG22	1.79	0.65
1:C:79:ALA:HB1	1:C:84:VAL:CG2	2.27	0.65
1:D:278:ILE:HD13	1:D:311:VAL:HG22	1.78	0.65
1:A:554:ASN:C	1:A:554:ASN:HD22	1.99	0.65
1:B:11:GLU:HG3	1:B:15:ARG:HH12	1.61	0.65
1:B:637:PHE:HB3	1:B:641:GLU:HB2	1.79	0.65
1:E:199:GLN:HA	1:E:199:GLN:NE2	2.11	0.65
1:E:566:MET:O	1:E:571:ARG:HD2	1.97	0.65
1:E:637:PHE:HB3	1:E:641:GLU:HB2	1.78	0.65
1:A:546:GLU:HA	1:A:549:ARG:HH12	1.62	0.64
1:C:355:LEU:O	1:C:356:PHE:HD1	1.79	0.64
1:F:190:VAL:CG2	1:F:490:ASN:HB3	2.26	0.64
1:A:190:VAL:CG2	1:A:490:ASN:HB3	2.24	0.64
1:F:529:SER:O	1:F:531:LEU:N	2.30	0.64
1:A:629:ASN:HD22	1:A:649:ARG:HE	1.46	0.64
1:A:672:GLU:O	1:A:675:LYS:HB3	1.98	0.64
1:D:413:LEU:HD13	1:D:421:LEU:HD12	1.79	0.64
1:E:412:PHE:C	1:E:412:PHE:CD2	2.71	0.64
1:A:299:GLU:OE1	1:A:307:HIS:ND1	2.28	0.64
1:B:186:ALA:O	1:B:190:VAL:HG23	1.97	0.64
1:A:278:ILE:HD12	1:A:278:ILE:N	2.13	0.64
1:C:411:ILE:HG22	1:C:412:PHE:N	2.12	0.64
1:D:695:ARG:HG2	1:D:695:ARG:HH11	1.63	0.64
1:A:354:ASN:HB3	1:A:357:ALA:CB	2.28	0.64
1:B:200:LEU:HB2	1:B:201:PHE:CE2	2.33	0.64
1:D:7:PHE:O	1:D:11:GLU:HB2	1.98	0.64
1:D:412:PHE:C	1:D:412:PHE:CD2	2.72	0.64
1:E:529:SER:O	1:E:531:LEU:N	2.30	0.64
1:B:355:LEU:O	1:B:356:PHE:HD1	1.80	0.63
1:E:330:GLU:HG3	1:E:395:ASN:CA	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:636:ILE:O	1:F:636:ILE:HG22	1.97	0.63
1:D:190:VAL:CG2	1:D:490:ASN:HB3	2.28	0.63
1:A:90:TRP:HB2	1:A:164:CYS:HB3	1.80	0.63
1:E:186:ALA:O	1:E:190:VAL:HG23	1.97	0.63
1:F:7:PHE:O	1:F:11:GLU:HB2	1.98	0.63
1:F:659:ARG:NH2	1:F:704:HIS:ND1	2.47	0.63
1:B:413:LEU:HD13	1:B:421:LEU:HD12	1.79	0.63
1:B:521:ILE:HD12	1:B:521:ILE:N	2.14	0.63
1:C:284:HIS:HB3	1:D:101:LYS:HA	1.80	0.63
1:D:199:GLN:HA	1:D:199:GLN:NE2	2.13	0.63
1:A:352:GLY:O	1:A:353:ILE:CB	2.46	0.63
1:A:503:SER:O	1:A:505:ASP:N	2.32	0.63
1:D:79:ALA:HB1	1:D:84:VAL:CG2	2.27	0.63
1:E:79:ALA:HB1	1:E:84:VAL:CG2	2.28	0.63
1:E:695:ARG:HG2	1:E:695:ARG:HH11	1.63	0.63
1:F:186:ALA:O	1:F:190:VAL:HG23	1.98	0.63
1:A:554:ASN:C	1:A:554:ASN:ND2	2.51	0.63
1:C:278:ILE:HD13	1:C:311:VAL:HG22	1.80	0.63
1:C:676:VAL:HG22	1:C:677:ALA:N	2.13	0.63
1:E:7:PHE:O	1:E:11:GLU:HB2	1.99	0.63
1:E:469:ASN:O	1:E:470:ARG:HB3	1.98	0.63
1:A:261:ARG:HH11	1:A:261:ARG:HG3	1.63	0.63
1:B:330:GLU:HG3	1:B:395:ASN:CA	2.29	0.63
1:C:330:GLU:HG3	1:C:395:ASN:CA	2.27	0.63
1:D:200:LEU:HB2	1:D:201:PHE:CE2	2.34	0.63
4:A:4001:ADP:H5'2	4:A:4001:ADP:O2B	1.99	0.63
1:B:223:THR:HG22	1:B:227:ASN:HD21	1.62	0.63
1:E:413:LEU:HD13	1:E:421:LEU:HD12	1.79	0.63
1:A:534:PHE:CD2	1:A:535:GLU:N	2.64	0.63
1:C:469:ASN:O	1:C:470:ARG:HB3	1.98	0.63
1:D:18:LEU:HD12	1:D:322:HIS:CE1	2.34	0.63
1:F:79:ALA:HB1	1:F:84:VAL:CG2	2.28	0.63
1:B:636:ILE:HG22	1:B:636:ILE:O	1.97	0.62
1:E:411:ILE:HG22	1:E:412:PHE:N	2.14	0.62
1:F:122:LEU:O	1:F:123:LEU:HD23	1.99	0.62
1:C:529:SER:O	1:C:531:LEU:N	2.32	0.62
1:D:186:ALA:O	1:D:190:VAL:HG23	1.99	0.62
1:B:529:SER:O	1:B:531:LEU:N	2.32	0.62
1:C:413:LEU:HD13	1:C:421:LEU:HD12	1.80	0.62
1:C:659:ARG:NH2	1:C:704:HIS:ND1	2.47	0.62
1:D:330:GLU:HG3	1:D:395:ASN:CA	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:ILE:HD12	1:D:521:ILE:N	2.14	0.62
1:F:411:ILE:HG22	1:F:412:PHE:N	2.12	0.62
1:B:20:ILE:CD1	1:B:20:ILE:H	2.13	0.62
1:B:412:PHE:C	1:B:412:PHE:CD2	2.73	0.62
1:A:285:ASN:HB3	1:A:292:PHE:CD1	2.34	0.62
1:D:636:ILE:HG22	1:D:636:ILE:O	1.98	0.62
1:A:411:ILE:CG2	1:A:412:PHE:H	2.11	0.62
1:A:686:LYS:O	1:A:689:ALA:HB3	1.98	0.62
1:C:695:ARG:HG2	1:C:695:ARG:HH11	1.64	0.62
1:E:200:LEU:HB2	1:E:201:PHE:CE2	2.35	0.62
1:E:284:HIS:HB3	1:F:101:LYS:HA	1.80	0.62
1:A:79:ALA:HB1	1:A:84:VAL:CG2	2.29	0.62
1:B:79:ALA:HB1	1:B:84:VAL:CG2	2.28	0.62
1:C:261:ARG:HH11	1:C:261:ARG:HG3	1.64	0.62
1:D:122:LEU:O	1:D:123:LEU:HD23	2.00	0.62
1:D:659:ARG:NH2	1:D:704:HIS:ND1	2.47	0.62
1:A:179:TYR:O	1:A:182:PRO:HD2	2.00	0.62
1:C:651:GLU:O	1:C:654:LYS:HB2	1.99	0.62
1:E:651:GLU:O	1:E:654:LYS:HB2	2.00	0.62
1:F:413:LEU:HD13	1:F:421:LEU:HD12	1.81	0.62
1:C:200:LEU:HB2	1:C:201:PHE:CE2	2.34	0.62
1:F:285:ASN:HB3	1:F:292:PHE:CD1	2.35	0.62
1:A:233:ARG:O	1:A:234:LEU:HB2	1.99	0.61
1:C:229:ARG:NH1	1:C:231:ASP:OD1	2.33	0.61
1:E:18:LEU:HD12	1:E:322:HIS:CE1	2.35	0.61
1:E:572:ALA:O	1:E:576:GLY:HA3	2.00	0.61
1:E:636:ILE:HG22	1:E:636:ILE:O	2.00	0.61
1:A:422:ASP:O	1:A:424:ILE:N	2.31	0.61
1:C:636:ILE:O	1:C:636:ILE:HG22	1.99	0.61
1:B:375:VAL:HG22	1:B:493:MET:HE2	1.82	0.61
1:D:411:ILE:HG22	1:D:412:PHE:N	2.14	0.61
1:A:715:GLU:HA	1:A:715:GLU:OE2	2.01	0.61
1:B:695:ARG:HG2	1:B:695:ARG:HH11	1.65	0.61
1:D:169:PHE:HB3	1:D:178:ASP:HB3	1.82	0.61
1:D:469:ASN:O	1:D:470:ARG:HB3	1.99	0.61
1:B:169:PHE:HB3	1:B:178:ASP:HB3	1.82	0.61
1:F:169:PHE:HB3	1:F:178:ASP:HB3	1.83	0.61
1:A:517:ALA:O	1:A:520:ARG:N	2.30	0.61
1:B:659:ARG:NH2	1:B:704:HIS:ND1	2.48	0.61
1:F:330:GLU:HG3	1:F:395:ASN:CA	2.30	0.61
1:A:169:PHE:HB2	1:A:178:ASP:HB3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASN:HB3	1:A:614:HIS:HD2	1.64	0.61
1:C:18:LEU:HD12	1:C:322:HIS:CE1	2.35	0.61
1:B:469:ASN:O	1:B:470:ARG:HB3	2.00	0.61
1:B:645:MET:CE	1:C:654:LYS:HA	2.31	0.61
1:D:554:ASN:C	1:D:554:ASN:ND2	2.53	0.61
1:A:212:LEU:HB3	1:A:301:CYS:HA	1.83	0.61
1:A:233:ARG:O	1:A:234:LEU:CB	2.49	0.61
1:A:421:LEU:HB3	1:A:533:ARG:HH12	1.65	0.61
1:A:518:ILE:HD12	1:A:519:PHE:N	2.16	0.61
1:C:285:ASN:HB3	1:C:292:PHE:CD1	2.36	0.61
1:E:521:ILE:HD12	1:E:521:ILE:N	2.14	0.61
1:F:18:LEU:HD12	1:F:322:HIS:CE1	2.36	0.61
1:A:546:GLU:HA	1:A:549:ARG:NH1	2.16	0.60
1:C:412:PHE:C	1:C:412:PHE:CD2	2.73	0.60
1:D:20:ILE:CD1	1:D:20:ILE:H	2.14	0.60
1:F:521:ILE:HD12	1:F:521:ILE:N	2.15	0.60
1:A:527:ILE:HA	1:A:530:GLU:OE2	2.01	0.60
1:D:79:ALA:O	1:D:84:VAL:HG13	2.00	0.60
1:E:169:PHE:HB3	1:E:178:ASP:HB3	1.83	0.60
1:F:237:ARG:NH2	1:F:397:HIS:NE2	2.49	0.60
1:F:412:PHE:C	1:F:412:PHE:CD2	2.74	0.60
1:F:695:ARG:HG2	1:F:695:ARG:HH11	1.66	0.60
1:A:525:ASN:HA	1:A:528:ALA:HB3	1.83	0.60
1:A:587:CYS:O	1:A:591:VAL:HG12	2.01	0.60
1:B:5:ARG:O	1:B:8:ALA:HB3	2.01	0.60
1:B:311:VAL:O	1:B:315:MET:HG3	2.02	0.60
1:B:558:VAL:HB	1:B:559:PRO:HD3	1.83	0.60
1:D:229:ARG:NH1	1:D:231:ASP:OD1	2.34	0.60
1:E:229:ARG:NH1	1:E:231:ASP:OD1	2.34	0.60
1:E:369:LEU:O	1:E:373:VAL:HG12	2.02	0.60
1:B:18:LEU:HD12	1:B:322:HIS:CE1	2.37	0.60
1:E:122:LEU:O	1:E:123:LEU:HD23	2.02	0.60
1:E:602:ILE:HD12	1:E:602:ILE:N	2.16	0.60
1:A:503:SER:C	1:A:505:ASP:H	2.05	0.60
1:F:391:MET:HG3	1:F:558:VAL:HG22	1.84	0.60
1:A:223:THR:O	1:A:226:TYR:HB3	2.02	0.60
1:B:15:ARG:NH1	1:B:323:HIS:NE2	2.50	0.60
1:B:237:ARG:NH2	1:B:397:HIS:NE2	2.49	0.60
1:B:651:GLU:O	1:B:654:LYS:HB2	2.02	0.60
1:D:569:GLN:C	1:D:569:GLN:NE2	2.55	0.60
1:E:237:ARG:NH2	1:E:397:HIS:NE2	2.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:MET:HG3	1:E:558:VAL:HG22	1.84	0.60
1:A:190:VAL:HG21	1:A:490:ASN:CB	2.27	0.60
1:B:199:GLN:HA	1:B:199:GLN:NE2	2.13	0.60
1:C:122:LEU:O	1:C:123:LEU:HD23	2.02	0.60
1:C:422:ASP:C	1:C:424:ILE:H	2.04	0.60
1:E:5:ARG:O	1:E:8:ALA:HB3	2.02	0.60
1:B:369:LEU:O	1:B:373:VAL:HG12	2.02	0.60
1:B:673:ALA:O	1:B:676:VAL:HG13	2.01	0.60
1:C:169:PHE:HB3	1:C:178:ASP:HB3	1.83	0.60
1:E:72:ALA:HB2	1:E:120:GLY:HA2	1.83	0.60
1:F:229:ARG:NH1	1:F:231:ASP:OD1	2.35	0.60
1:F:572:ALA:O	1:F:576:GLY:HA3	2.01	0.60
1:C:369:LEU:O	1:C:373:VAL:HG12	2.02	0.60
1:D:15:ARG:NH1	1:D:323:HIS:NE2	2.50	0.60
1:F:120:GLY:C	1:F:122:LEU:H	2.05	0.60
1:F:605:ARG:NH1	5:F:6001:CL:CL	2.71	0.60
1:F:651:GLU:O	1:F:654:LYS:HB2	2.02	0.60
1:B:569:GLN:NE2	1:B:569:GLN:C	2.55	0.60
1:D:285:ASN:HB3	1:D:292:PHE:CD1	2.37	0.60
1:F:311:VAL:O	1:F:315:MET:HG3	2.02	0.60
1:F:354:ASN:OD1	1:F:356:PHE:HB2	2.02	0.60
1:F:375:VAL:HG22	1:F:493:MET:HE2	1.84	0.60
1:F:567:ASP:C	1:F:567:ASP:OD2	2.41	0.60
1:A:634:LYS:HA	1:A:642:TYR:CD1	2.37	0.59
1:A:682:ASN:HB3	1:A:685:GLU:HG3	1.82	0.59
1:B:229:ARG:NH1	1:B:231:ASP:OD1	2.35	0.59
1:C:199:GLN:HA	1:C:199:GLN:NE2	2.12	0.59
1:D:72:ALA:HB2	1:D:120:GLY:HA2	1.84	0.59
1:F:20:ILE:HG12	1:F:21:THR:N	2.11	0.59
1:F:200:LEU:HB2	1:F:201:PHE:CE2	2.36	0.59
1:F:369:LEU:O	1:F:373:VAL:HG12	2.02	0.59
1:D:572:ALA:O	1:D:576:GLY:HA3	2.02	0.59
1:E:567:ASP:OD2	1:E:567:ASP:C	2.41	0.59
1:B:122:LEU:O	1:B:123:LEU:HD23	2.02	0.59
1:B:569:GLN:C	1:B:569:GLN:HE21	2.06	0.59
1:F:422:ASP:C	1:F:424:ILE:H	2.04	0.59
1:A:6:PHE:C	1:A:8:ALA:N	2.53	0.59
1:A:537:ASP:O	1:A:540:SER:HB3	2.01	0.59
1:A:558:VAL:HB	1:A:559:PRO:HD3	1.83	0.59
1:E:20:ILE:CD1	1:E:20:ILE:H	2.14	0.59
1:A:596:TYR:O	1:A:600:VAL:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:HG22	1:A:619:ALA:N	2.16	0.59
1:A:676:VAL:O	1:A:679:HIS:N	2.32	0.59
1:E:15:ARG:NH1	1:E:323:HIS:NE2	2.51	0.59
1:E:120:GLY:C	1:E:122:LEU:H	2.04	0.59
1:E:375:VAL:HG22	1:E:493:MET:HE2	1.84	0.59
1:A:157:PHE:CE2	1:A:164:CYS:HB2	2.37	0.59
1:B:554:ASN:C	1:B:554:ASN:ND2	2.54	0.59
1:D:5:ARG:O	1:D:8:ALA:HB3	2.01	0.59
1:B:422:ASP:C	1:B:424:ILE:H	2.04	0.59
1:C:311:VAL:O	1:C:315:MET:HG3	2.03	0.59
1:C:354:ASN:OD1	1:C:356:PHE:HB2	2.03	0.59
1:D:120:GLY:C	1:D:122:LEU:H	2.06	0.59
1:D:422:ASP:C	1:D:424:ILE:H	2.06	0.59
1:D:567:ASP:C	1:D:567:ASP:OD2	2.41	0.59
1:D:569:GLN:C	1:D:569:GLN:HE21	2.06	0.59
1:A:6:PHE:C	1:A:8:ALA:H	2.05	0.59
1:A:575:ILE:O	1:A:575:ILE:HD13	2.02	0.59
1:A:695:ARG:HG2	1:A:695:ARG:HH11	1.67	0.59
1:C:120:GLY:C	1:C:122:LEU:H	2.06	0.59
1:A:372:LEU:CD2	1:A:417:LEU:HD11	2.32	0.59
1:B:72:ALA:HB2	1:B:120:GLY:HA2	1.85	0.59
1:B:278:ILE:HD13	1:B:311:VAL:CG2	2.33	0.59
1:C:15:ARG:NH1	1:C:323:HIS:NE2	2.50	0.59
1:C:20:ILE:CD1	1:C:20:ILE:H	2.16	0.59
1:C:602:ILE:HD12	1:C:602:ILE:N	2.17	0.59
1:D:391:MET:HG3	1:D:558:VAL:HG22	1.85	0.59
1:E:422:ASP:C	1:E:424:ILE:H	2.05	0.59
1:E:659:ARG:NH2	1:E:704:HIS:ND1	2.51	0.59
1:F:380:HIS:HA	1:F:532:ILE:HD13	1.85	0.59
1:B:79:ALA:O	1:B:84:VAL:HG13	2.03	0.59
1:A:53:VAL:HG22	1:A:71:ILE:HD11	1.86	0.58
1:B:567:ASP:OD2	1:B:567:ASP:C	2.40	0.58
1:E:278:ILE:HD13	1:E:311:VAL:CG2	2.33	0.58
1:E:285:ASN:HB3	1:E:292:PHE:CD1	2.38	0.58
1:F:20:ILE:CD1	1:F:20:ILE:H	2.14	0.58
1:F:605:ARG:CZ	5:F:6001:CL:CL	2.88	0.58
1:A:344:ASN:ND2	4:A:4001:ADP:H4'	2.18	0.58
1:A:558:VAL:O	1:A:559:PRO:C	2.41	0.58
1:D:278:ILE:HD13	1:D:311:VAL:CG2	2.32	0.58
1:F:199:GLN:HA	1:F:199:GLN:NE2	2.12	0.58
1:F:278:ILE:HD13	1:F:311:VAL:CG2	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:H	1:A:531:LEU:CD1	2.14	0.58
1:B:572:ALA:O	1:B:576:GLY:HA3	2.02	0.58
1:C:79:ALA:O	1:C:84:VAL:HG13	2.04	0.58
1:E:354:ASN:OD1	1:E:356:PHE:HB2	2.03	0.58
1:F:569:GLN:O	1:F:572:ALA:HB3	2.02	0.58
1:B:285:ASN:HB3	1:B:292:PHE:CD1	2.38	0.58
1:B:602:ILE:HD12	1:B:602:ILE:N	2.18	0.58
1:D:56:ALA:HA	1:D:61:THR:CA	2.32	0.58
1:F:5:ARG:O	1:F:8:ALA:HB3	2.02	0.58
1:A:373:VAL:HA	1:A:376:LEU:HD12	1.86	0.58
1:A:502:ALA:O	1:A:505:ASP:HB2	2.03	0.58
1:C:56:ALA:HA	1:C:61:THR:CA	2.33	0.58
1:C:237:ARG:NH2	1:C:397:HIS:NE2	2.51	0.58
1:C:386:LEU:O	1:C:388:ALA:N	2.36	0.58
1:D:354:ASN:OD1	1:D:356:PHE:HB2	2.03	0.58
1:F:15:ARG:NH1	1:F:323:HIS:NE2	2.51	0.58
1:F:56:ALA:HA	1:F:61:THR:CA	2.33	0.58
1:B:56:ALA:HA	1:B:61:THR:CA	2.32	0.58
1:D:299:GLU:OE1	1:D:307:HIS:ND1	2.36	0.58
1:F:46:PRO:HD2	1:F:49:ALA:HB3	1.85	0.58
1:A:383:GLN:HE22	1:A:552:LEU:HA	1.68	0.58
1:C:645:MET:CE	1:D:654:LYS:HA	2.32	0.58
1:D:569:GLN:O	1:D:572:ALA:HB3	2.04	0.58
1:A:38:ARG:O	1:A:40:LYS:N	2.37	0.58
1:C:72:ALA:HB2	1:C:120:GLY:HA2	1.85	0.58
1:D:20:ILE:CG1	1:D:21:THR:N	2.67	0.58
1:D:651:GLU:O	1:D:654:LYS:HB2	2.03	0.58
1:E:569:GLN:NE2	1:E:569:GLN:C	2.57	0.58
1:E:716:ILE:O	1:E:717:TRP:HB3	2.04	0.58
1:A:387:ARG:HH11	1:A:387:ARG:HG3	1.68	0.58
1:D:372:LEU:HD22	1:D:417:LEU:HD21	1.86	0.58
1:D:716:ILE:O	1:D:717:TRP:HB3	2.04	0.58
1:E:20:ILE:CG1	1:E:21:THR:N	2.67	0.58
1:E:56:ALA:HA	1:E:61:THR:CA	2.33	0.58
1:E:311:VAL:O	1:E:315:MET:HG3	2.04	0.58
1:E:673:ALA:O	1:E:676:VAL:HG13	2.03	0.58
1:A:726:LEU:HB2	1:A:727:PHE:CE2	2.38	0.58
1:B:120:GLY:C	1:B:122:LEU:H	2.07	0.58
1:F:372:LEU:HD22	1:F:417:LEU:HD21	1.86	0.58
1:C:20:ILE:CG1	1:C:21:THR:N	2.67	0.57
1:D:492:ALA:HA	1:D:573:VAL:HG11	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:ARG:HG3	1:E:261:ARG:HH11	1.68	0.57
1:E:602:ILE:H	1:E:602:ILE:CD1	2.17	0.57
1:D:602:ILE:HD12	1:D:602:ILE:N	2.19	0.57
1:F:261:ARG:HH11	1:F:261:ARG:HG3	1.68	0.57
1:A:38:ARG:O	1:A:39:LYS:C	2.43	0.57
1:A:716:ILE:O	1:A:717:TRP:CB	2.52	0.57
1:B:481:ASN:HD22	1:B:482:CYS:N	2.03	0.57
1:C:534:PHE:CD2	1:C:535:GLU:N	2.71	0.57
1:C:558:VAL:HB	1:C:559:PRO:HD3	1.86	0.57
1:F:72:ALA:HB2	1:F:120:GLY:HA2	1.85	0.57
1:A:235:THR:CG2	1:A:603:GLU:HG2	2.33	0.57
1:A:422:ASP:C	1:A:424:ILE:H	2.07	0.57
1:A:674:ARG:HG2	1:A:690:TYR:OH	2.03	0.57
1:B:587:CYS:O	1:B:590:GLU:N	2.38	0.57
1:D:358:PRO:HD3	1:D:368:PHE:HE2	1.70	0.57
1:D:387:ARG:HH11	1:D:387:ARG:HG3	1.69	0.57
1:E:79:ALA:O	1:E:84:VAL:HG13	2.04	0.57
1:E:569:GLN:O	1:E:572:ALA:HB3	2.04	0.57
1:C:572:ALA:O	1:C:576:GLY:HA3	2.05	0.57
1:C:583:THR:O	1:C:586:ALA:HB3	2.04	0.57
1:D:369:LEU:O	1:D:373:VAL:HG12	2.04	0.57
1:E:372:LEU:HD22	1:E:417:LEU:HD21	1.87	0.57
1:F:20:ILE:CG1	1:F:21:THR:N	2.66	0.57
1:F:79:ALA:O	1:F:84:VAL:HG13	2.04	0.57
1:F:673:ALA:O	1:F:676:VAL:HG13	2.05	0.57
1:A:72:ALA:HB2	1:A:120:GLY:HA2	1.87	0.57
1:A:563:MET:O	1:A:566:MET:HG2	2.04	0.57
1:B:20:ILE:CG1	1:B:21:THR:N	2.66	0.57
1:B:583:THR:O	1:B:586:ALA:HB3	2.04	0.57
1:D:534:PHE:CD2	1:D:535:GLU:N	2.71	0.57
1:D:691:GLU:OE1	1:D:695:ARG:HD3	2.05	0.57
1:E:380:HIS:HA	1:E:532:ILE:HD13	1.86	0.57
1:F:583:THR:O	1:F:586:ALA:HB3	2.04	0.57
1:A:231:ASP:O	1:A:235:THR:HB	2.05	0.57
1:A:387:ARG:NH1	1:A:407:ALA:HB1	2.19	0.57
1:A:196:GLU:HG2	1:A:501:LYS:HE3	1.87	0.57
1:B:372:LEU:HD22	1:B:417:LEU:HD21	1.87	0.57
1:C:569:GLN:NE2	1:C:569:GLN:C	2.58	0.57
1:E:502:ALA:O	1:E:505:ASP:HB2	2.05	0.57
1:E:605:ARG:NH1	5:E:6001:CL:CL	2.74	0.57
1:F:299:GLU:OE1	1:F:307:HIS:ND1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:TRP:NE1	1:A:308:ASN:HB2	2.19	0.57
1:B:20:ILE:H	1:B:20:ILE:HD13	1.70	0.57
1:D:349:THR:CG2	1:D:353:ILE:HB	2.35	0.57
1:D:502:ALA:O	1:D:505:ASP:HB2	2.04	0.57
1:E:201:PHE:N	1:E:201:PHE:CD2	2.72	0.57
1:A:18:LEU:HD12	1:A:322:HIS:CD2	2.40	0.57
1:B:502:ALA:O	1:B:505:ASP:HB2	2.05	0.57
1:B:587:CYS:O	1:B:588:ARG:C	2.42	0.57
1:F:502:ALA:O	1:F:505:ASP:HB2	2.05	0.57
1:B:89:HIS:HB3	1:B:167:THR:HG21	1.87	0.56
1:D:481:ASN:HD22	1:D:482:CYS:N	2.03	0.56
1:E:358:PRO:HD3	1:E:368:PHE:HE2	1.70	0.56
1:E:582:GLU:OE1	1:E:582:GLU:HA	2.05	0.56
1:E:583:THR:O	1:E:586:ALA:HB3	2.04	0.56
1:F:358:PRO:HD3	1:F:368:PHE:HE2	1.70	0.56
1:A:79:ALA:O	1:A:84:VAL:HG13	2.04	0.56
1:A:716:ILE:HG22	1:A:717:TRP:N	2.19	0.56
1:B:691:GLU:OE1	1:B:695:ARG:HD3	2.05	0.56
1:C:391:MET:HG3	1:C:558:VAL:HG22	1.87	0.56
1:E:373:VAL:O	1:E:376:LEU:HB2	2.05	0.56
1:A:235:THR:HG23	1:A:603:GLU:HG2	1.86	0.56
1:A:636:ILE:HD11	1:B:631:CYS:HA	1.88	0.56
1:B:46:PRO:HD2	1:B:49:ALA:HB3	1.87	0.56
1:B:354:ASN:OD1	1:B:356:PHE:HB2	2.05	0.56
1:B:358:PRO:HD3	1:B:368:PHE:HE2	1.71	0.56
1:B:373:VAL:O	1:B:376:LEU:HB2	2.05	0.56
1:B:569:GLN:O	1:B:572:ALA:HB3	2.05	0.56
1:C:46:PRO:HD2	1:C:49:ALA:HB3	1.87	0.56
1:C:190:VAL:HG21	1:C:490:ASN:CB	2.34	0.56
1:C:201:PHE:CD2	1:C:201:PHE:N	2.73	0.56
1:C:567:ASP:C	1:C:567:ASP:OD2	2.42	0.56
1:C:720:PRO:HB2	1:C:725:LEU:HD21	1.86	0.56
1:D:237:ARG:NH2	1:D:397:HIS:NE2	2.53	0.56
1:D:282:THR:HG22	1:E:103:ASP:OD2	2.06	0.56
1:D:673:ALA:O	1:D:676:VAL:HG13	2.05	0.56
1:D:720:PRO:HB2	1:D:725:LEU:HD21	1.86	0.56
1:E:38:ARG:O	1:E:40:LYS:N	2.38	0.56
1:F:558:VAL:HB	1:F:559:PRO:HD3	1.87	0.56
1:F:569:GLN:NE2	1:F:569:GLN:C	2.59	0.56
1:F:602:ILE:HD12	1:F:602:ILE:N	2.19	0.56
1:A:201:PHE:O	1:A:202:ASP:C	2.43	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:HD23	1:A:522:LEU:C	2.26	0.56
1:A:660:VAL:O	1:A:664:LYS:HG3	2.05	0.56
1:B:201:PHE:N	1:B:201:PHE:CD2	2.72	0.56
1:C:372:LEU:HD22	1:C:417:LEU:HD21	1.87	0.56
1:C:569:GLN:O	1:C:572:ALA:HB3	2.05	0.56
1:C:691:GLU:OE1	1:C:695:ARG:HD3	2.05	0.56
1:E:587:CYS:O	1:E:588:ARG:C	2.44	0.56
1:A:50:TYR:O	1:A:54:VAL:HG23	2.05	0.56
1:B:230:PRO:O	1:B:233:ARG:O	2.24	0.56
1:E:720:PRO:HB2	1:E:725:LEU:HD21	1.88	0.56
1:F:349:THR:CG2	1:F:353:ILE:HB	2.35	0.56
1:A:411:ILE:CG2	1:A:412:PHE:N	2.69	0.56
1:A:412:PHE:CE1	1:A:535:GLU:HG3	2.41	0.56
1:C:5:ARG:O	1:C:8:ALA:HB3	2.05	0.56
1:D:311:VAL:O	1:D:315:MET:HG3	2.05	0.56
1:E:534:PHE:CD2	1:E:535:GLU:N	2.72	0.56
1:F:691:GLU:OE1	1:F:695:ARG:HD3	2.05	0.56
1:A:168:ILE:C	1:A:168:ILE:HD12	2.26	0.56
1:A:169:PHE:CB	1:A:178:ASP:HB3	2.35	0.56
1:B:261:ARG:HH11	1:B:261:ARG:HG3	1.70	0.56
1:B:375:VAL:HG22	1:B:493:MET:CE	2.35	0.56
1:B:386:LEU:O	1:B:388:ALA:N	2.39	0.56
1:B:481:ASN:HD22	1:B:481:ASN:C	2.08	0.56
1:B:720:PRO:HB2	1:B:725:LEU:HD21	1.87	0.56
1:C:380:HIS:HA	1:C:532:ILE:HD13	1.88	0.56
1:C:481:ASN:HD22	1:C:481:ASN:C	2.09	0.56
1:D:261:ARG:HH11	1:D:261:ARG:HG3	1.71	0.56
1:A:419:ALA:O	1:A:422:ASP:HB2	2.06	0.56
1:C:517:ALA:O	1:C:520:ARG:N	2.39	0.56
1:D:587:CYS:O	1:D:588:ARG:C	2.44	0.56
1:B:299:GLU:OE1	1:B:307:HIS:ND1	2.37	0.56
1:C:349:THR:CG2	1:C:353:ILE:HB	2.35	0.56
1:D:583:THR:O	1:D:586:ALA:HB3	2.06	0.56
1:F:720:PRO:HB2	1:F:725:LEU:HD21	1.87	0.56
1:A:716:ILE:O	1:A:717:TRP:HB3	2.05	0.56
1:C:673:ALA:O	1:C:676:VAL:HG13	2.05	0.56
1:D:380:HIS:HA	1:D:532:ILE:HD13	1.87	0.56
1:D:587:CYS:O	1:D:590:GLU:N	2.39	0.56
1:E:630:LEU:CD2	1:E:649:ARG:HG2	2.33	0.56
1:F:38:ARG:O	1:F:40:LYS:N	2.38	0.56
1:F:492:ALA:HA	1:F:573:VAL:HG11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:587:CYS:O	1:F:591:VAL:HG12	2.06	0.56
1:C:38:ARG:O	1:C:40:LYS:N	2.39	0.55
1:C:183:LEU:O	1:C:184:LEU:C	2.44	0.55
1:D:201:PHE:CD2	1:D:201:PHE:N	2.73	0.55
1:E:492:ALA:HA	1:E:573:VAL:HG11	1.88	0.55
1:F:534:PHE:CD2	1:F:535:GLU:N	2.72	0.55
1:B:380:HIS:HA	1:B:532:ILE:HD13	1.87	0.55
1:E:349:THR:CG2	1:E:353:ILE:HB	2.35	0.55
1:E:481:ASN:C	1:E:481:ASN:HD22	2.09	0.55
1:E:558:VAL:HB	1:E:559:PRO:HD3	1.88	0.55
1:F:201:PHE:CD2	1:F:201:PHE:N	2.74	0.55
1:A:230:PRO:O	1:A:231:ASP:C	2.44	0.55
1:C:554:ASN:C	1:C:554:ASN:ND2	2.54	0.55
1:D:558:VAL:HB	1:D:559:PRO:HD3	1.87	0.55
1:E:20:ILE:HG12	1:E:21:THR:N	2.13	0.55
1:A:709:GLU:HG3	1:A:717:TRP:CE2	2.40	0.55
1:B:602:ILE:H	1:B:602:ILE:CD1	2.19	0.55
1:C:379:VAL:HG21	1:C:411:ILE:HD11	1.88	0.55
1:C:569:GLN:C	1:C:569:GLN:HE21	2.08	0.55
1:D:286:GLU:HG3	1:D:287:VAL:H	1.70	0.55
1:E:569:GLN:C	1:E:569:GLN:HE21	2.10	0.55
1:F:190:VAL:HG21	1:F:490:ASN:CB	2.35	0.55
1:A:413:LEU:HD12	1:A:533:ARG:HD2	1.88	0.55
1:C:587:CYS:O	1:C:588:ARG:C	2.44	0.55
1:A:368:PHE:CE2	1:A:372:LEU:HB2	2.41	0.55
1:A:368:PHE:O	1:A:369:LEU:C	2.44	0.55
1:A:583:THR:OG1	1:A:584:GLU:N	2.39	0.55
1:C:481:ASN:HD22	1:C:482:CYS:N	2.04	0.55
1:D:20:ILE:H	1:D:20:ILE:HD13	1.71	0.55
1:F:387:ARG:NH1	1:F:407:ALA:HB1	2.22	0.55
1:A:294:LEU:HG	1:A:294:LEU:O	2.05	0.55
1:B:411:ILE:CG2	1:B:412:PHE:N	2.70	0.55
1:C:695:ARG:HB3	1:C:696:PRO:HD3	1.89	0.55
1:E:20:ILE:H	1:E:20:ILE:HD13	1.72	0.55
1:E:375:VAL:HG22	1:E:493:MET:CE	2.37	0.55
1:A:676:VAL:O	1:A:677:ALA:C	2.44	0.55
1:C:502:ALA:O	1:C:505:ASP:HB2	2.06	0.55
1:C:587:CYS:O	1:C:590:GLU:N	2.40	0.55
1:D:89:HIS:HB3	1:D:167:THR:HG21	1.88	0.55
1:D:645:MET:CE	1:E:654:LYS:HA	2.36	0.55
1:D:695:ARG:HB3	1:D:696:PRO:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:ILE:H	1:F:20:ILE:HD13	1.71	0.55
1:F:716:ILE:O	1:F:717:TRP:HB3	2.06	0.55
1:A:15:ARG:NH1	1:A:323:HIS:NE2	2.55	0.55
1:B:233:ARG:HH11	1:B:233:ARG:CG	2.20	0.55
1:C:358:PRO:HD3	1:C:368:PHE:HE2	1.72	0.55
1:C:411:ILE:CG2	1:C:412:PHE:N	2.69	0.55
1:C:605:ARG:NH1	5:C:6001:CL:CL	2.76	0.55
1:E:46:PRO:HD2	1:E:49:ALA:HB3	1.87	0.55
1:A:179:TYR:C	1:A:182:PRO:HD2	2.27	0.55
1:B:201:PHE:O	1:B:202:ASP:C	2.45	0.55
1:B:605:ARG:CZ	5:B:6001:CL:CL	2.92	0.55
1:C:352:GLY:O	1:C:353:ILE:CB	2.55	0.55
1:D:38:ARG:O	1:D:40:LYS:N	2.39	0.55
1:F:517:ALA:O	1:F:520:ARG:N	2.40	0.55
1:F:587:CYS:O	1:F:588:ARG:C	2.46	0.55
1:A:369:LEU:O	1:A:373:VAL:HG23	2.07	0.54
1:C:278:ILE:HD13	1:C:311:VAL:CG2	2.37	0.54
1:C:373:VAL:O	1:C:376:LEU:HB2	2.07	0.54
1:D:46:PRO:HD2	1:D:49:ALA:HB3	1.88	0.54
1:D:382:ASN:HD21	1:D:573:VAL:HG21	1.72	0.54
1:D:386:LEU:O	1:D:388:ALA:N	2.40	0.54
1:D:481:ASN:HD22	1:D:481:ASN:C	2.09	0.54
1:E:587:CYS:O	1:E:591:VAL:HG12	2.06	0.54
1:A:215:GLU:OE1	4:A:4001:ADP:O3A	2.26	0.54
1:A:636:ILE:O	1:A:636:ILE:HG22	2.07	0.54
1:C:299:GLU:OE1	1:C:307:HIS:ND1	2.37	0.54
1:C:492:ALA:HA	1:C:573:VAL:HG11	1.88	0.54
1:E:89:HIS:HB3	1:E:167:THR:HG21	1.88	0.54
1:E:299:GLU:OE1	1:E:307:HIS:ND1	2.38	0.54
1:F:554:ASN:C	1:F:554:ASN:ND2	2.54	0.54
1:F:569:GLN:C	1:F:569:GLN:HE21	2.10	0.54
1:A:404:ALA:O	1:A:539:TYR:HE1	1.90	0.54
1:B:492:ALA:HA	1:B:573:VAL:HG11	1.88	0.54
1:E:517:ALA:O	1:E:520:ARG:N	2.39	0.54
1:E:691:GLU:OE1	1:E:695:ARG:HD3	2.07	0.54
1:F:341:LYS:O	1:F:476:ALA:HB3	2.07	0.54
1:F:483:ALA:O	1:F:487:ILE:HG13	2.07	0.54
1:A:150:TRP:CD1	1:A:151:ASP:N	2.76	0.54
1:A:293:GLU:O	1:A:294:LEU:HB3	2.06	0.54
1:A:330:GLU:HG3	1:A:395:ASN:CA	2.38	0.54
1:B:27:LEU:O	1:B:29:ASP:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:O	1:B:184:LEU:C	2.45	0.54
1:C:375:VAL:HG22	1:C:493:MET:HE2	1.89	0.54
1:C:387:ARG:HH11	1:C:387:ARG:HG3	1.72	0.54
1:C:716:ILE:O	1:C:717:TRP:HB3	2.05	0.54
1:D:605:ARG:NH1	5:D:6001:CL:CL	2.77	0.54
1:E:196:GLU:O	1:E:199:GLN:HG2	2.08	0.54
1:F:702:ARG:HG2	1:F:706:ASP:OD2	2.08	0.54
1:A:625:ARG:HB2	1:A:625:ARG:HH11	1.73	0.54
1:C:382:ASN:ND2	1:C:573:VAL:HG21	2.23	0.54
1:D:352:GLY:O	1:D:353:ILE:CB	2.55	0.54
1:D:375:VAL:HG22	1:D:493:MET:CE	2.37	0.54
1:D:582:GLU:HA	1:D:582:GLU:OE1	2.08	0.54
1:E:183:LEU:O	1:E:184:LEU:C	2.44	0.54
1:E:286:GLU:HB2	1:E:291:GLN:HG2	1.90	0.54
1:E:336:VAL:O	1:E:337:ASN:C	2.46	0.54
1:A:27:LEU:O	1:A:29:ASP:N	2.40	0.54
1:A:609:ASP:N	1:A:609:ASP:OD2	2.41	0.54
1:B:221:VAL:HG23	1:B:325:ALA:HB3	1.89	0.54
1:B:695:ARG:HB3	1:B:696:PRO:HD3	1.90	0.54
1:B:716:ILE:O	1:B:717:TRP:HB3	2.07	0.54
1:C:582:GLU:OE1	1:C:582:GLU:HA	2.08	0.54
1:E:716:ILE:HG22	1:E:717:TRP:N	2.22	0.54
1:F:183:LEU:O	1:F:184:LEU:C	2.44	0.54
1:F:375:VAL:HG22	1:F:493:MET:CE	2.38	0.54
1:A:233:ARG:HD3	1:A:233:ARG:C	2.28	0.54
1:A:261:ARG:HG3	1:A:261:ARG:NH1	2.22	0.54
1:A:320:ARG:HB3	1:A:320:ARG:HH11	1.72	0.54
1:A:543:TRP:C	1:A:545:GLN:N	2.61	0.54
1:A:651:GLU:O	1:A:654:LYS:HB2	2.07	0.54
1:A:678:ASN:ND2	1:A:690:TYR:OH	2.41	0.54
1:B:605:ARG:NH1	5:B:6001:CL:CL	2.78	0.54
1:C:605:ARG:CZ	5:C:6001:CL:CL	2.93	0.54
1:C:702:ARG:HG2	1:C:706:ASP:OD2	2.08	0.54
1:E:201:PHE:O	1:E:202:ASP:C	2.46	0.54
1:F:582:GLU:OE1	1:F:582:GLU:HA	2.08	0.54
1:A:157:PHE:CD2	1:A:157:PHE:N	2.75	0.54
1:A:229:ARG:NH1	1:A:231:ASP:OD1	2.41	0.54
1:C:602:ILE:H	1:C:602:ILE:CD1	2.17	0.54
1:D:260:PRO:O	1:D:261:ARG:C	2.46	0.54
1:F:344:ASN:HB3	1:F:470:ARG:HD2	1.90	0.54
1:F:373:VAL:O	1:F:376:LEU:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:ARG:HH11	1:F:387:ARG:HG3	1.71	0.54
1:F:411:ILE:CG2	1:F:412:PHE:N	2.70	0.54
1:F:602:ILE:H	1:F:602:ILE:CD1	2.21	0.54
1:A:421:LEU:HD23	1:A:533:ARG:NH1	2.21	0.54
1:B:702:ARG:HG2	1:B:706:ASP:OD2	2.08	0.54
1:C:375:VAL:HG22	1:C:493:MET:CE	2.38	0.54
1:C:382:ASN:HD21	1:C:573:VAL:HG21	1.73	0.54
1:D:183:LEU:O	1:D:184:LEU:C	2.46	0.54
1:F:358:PRO:HG2	1:F:359:GLY:H	1.73	0.54
1:F:587:CYS:O	1:F:590:GLU:N	2.40	0.54
1:B:38:ARG:O	1:B:40:LYS:N	2.40	0.54
1:B:84:VAL:HA	1:B:161:THR:HA	1.90	0.54
1:B:587:CYS:O	1:B:591:VAL:HG12	2.07	0.54
1:C:89:HIS:HB3	1:C:167:THR:HG21	1.90	0.54
1:C:282:THR:HG22	1:D:103:ASP:OD2	2.08	0.54
1:E:387:ARG:NH1	1:E:407:ALA:HB1	2.23	0.54
1:F:89:HIS:HB3	1:F:167:THR:HG21	1.89	0.54
1:A:373:VAL:O	1:A:376:LEU:HB2	2.07	0.53
1:A:470:ARG:HD3	4:A:4001:ADP:C5	2.43	0.53
1:C:20:ILE:H	1:C:20:ILE:HD13	1.73	0.53
1:D:84:VAL:HA	1:D:161:THR:HA	1.91	0.53
1:D:201:PHE:O	1:D:202:ASP:C	2.46	0.53
1:D:602:ILE:H	1:D:602:ILE:CD1	2.19	0.53
1:E:344:ASN:HB3	1:E:470:ARG:HD2	1.89	0.53
1:E:481:ASN:HD22	1:E:482:CYS:N	2.05	0.53
1:B:344:ASN:HB3	1:B:470:ARG:HD2	1.90	0.53
1:B:534:PHE:CD2	1:B:535:GLU:N	2.71	0.53
1:D:69:ASP:OD1	1:D:120:GLY:N	2.41	0.53
1:D:379:VAL:HG21	1:D:411:ILE:HD11	1.91	0.53
1:D:627:LEU:CD2	1:D:653:ILE:HD13	2.38	0.53
1:E:27:LEU:O	1:E:29:ASP:N	2.41	0.53
1:E:387:ARG:HH11	1:E:387:ARG:HG3	1.72	0.53
1:A:571:ARG:NH2	1:A:582:GLU:OE1	2.42	0.53
1:B:352:GLY:O	1:B:353:ILE:CB	2.56	0.53
1:C:386:LEU:O	1:C:389:SER:N	2.41	0.53
1:D:221:VAL:HG23	1:D:325:ALA:HB3	1.90	0.53
1:D:373:VAL:O	1:D:376:LEU:HB2	2.08	0.53
1:D:386:LEU:O	1:D:389:SER:N	2.41	0.53
1:D:387:ARG:NH1	1:D:407:ALA:HB1	2.23	0.53
1:D:587:CYS:O	1:D:591:VAL:HG12	2.08	0.53
1:E:190:VAL:HG21	1:E:490:ASN:CB	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:VAL:HA	1:F:161:THR:HA	1.90	0.53
1:F:196:GLU:O	1:F:199:GLN:HG2	2.09	0.53
1:F:379:VAL:HG21	1:F:411:ILE:HD11	1.90	0.53
1:A:194:ALA:HA	1:A:497:LEU:HD13	1.89	0.53
1:A:630:LEU:HG	1:A:649:ARG:HG2	1.91	0.53
1:C:483:ALA:O	1:C:487:ILE:HG13	2.08	0.53
1:C:521:ILE:H	1:C:521:ILE:CD1	2.21	0.53
1:D:11:GLU:HA	1:D:11:GLU:OE2	2.08	0.53
1:D:44:TYR:CE1	1:D:78:TRP:HA	2.44	0.53
1:D:286:GLU:HB2	1:D:291:GLN:HG2	1.90	0.53
1:D:558:VAL:O	1:D:559:PRO:C	2.46	0.53
1:D:595:LYS:O	1:D:596:TYR:C	2.47	0.53
1:F:27:LEU:O	1:F:29:ASP:N	2.41	0.53
1:F:481:ASN:HD22	1:F:482:CYS:N	2.05	0.53
1:A:504:VAL:HG23	1:A:521:ILE:HD13	1.91	0.53
1:B:387:ARG:NH1	1:B:407:ALA:HB1	2.23	0.53
1:C:221:VAL:HG23	1:C:325:ALA:HB3	1.89	0.53
1:C:260:PRO:O	1:C:261:ARG:C	2.47	0.53
1:C:587:CYS:O	1:C:591:VAL:HG12	2.09	0.53
1:D:605:ARG:CZ	5:D:6001:CL:CL	2.94	0.53
1:E:260:PRO:O	1:E:261:ARG:C	2.47	0.53
1:E:379:VAL:HG21	1:E:411:ILE:HD11	1.91	0.53
1:E:411:ILE:CG2	1:E:412:PHE:N	2.72	0.53
1:F:11:GLU:HA	1:F:11:GLU:OE2	2.09	0.53
1:F:352:GLY:O	1:F:353:ILE:CB	2.56	0.53
1:B:582:GLU:OE1	1:B:582:GLU:HA	2.08	0.53
1:C:286:GLU:HG3	1:C:287:VAL:H	1.73	0.53
1:C:358:PRO:HG2	1:C:359:GLY:H	1.74	0.53
1:D:382:ASN:ND2	1:D:573:VAL:HG21	2.23	0.53
1:D:554:ASN:HD22	1:D:555:ILE:N	2.06	0.53
1:E:69:ASP:OD1	1:E:120:GLY:N	2.42	0.53
1:E:695:ARG:HB3	1:E:696:PRO:HD3	1.90	0.53
1:F:44:TYR:CE1	1:F:78:TRP:HA	2.44	0.53
1:A:488:ALA:O	1:A:489:ILE:C	2.46	0.53
1:A:613:ASN:ND2	1:F:721:LYS:NZ	2.56	0.53
1:E:386:LEU:O	1:E:388:ALA:N	2.42	0.53
1:E:587:CYS:O	1:E:590:GLU:N	2.41	0.53
1:E:605:ARG:CZ	5:E:6001:CL:CL	2.93	0.53
1:C:627:LEU:CD2	1:C:653:ILE:HD13	2.38	0.53
1:C:716:ILE:HG22	1:C:717:TRP:N	2.23	0.53
1:D:207:ARG:HH11	1:D:207:ARG:CB	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:ILE:CG2	1:D:412:PHE:N	2.71	0.53
1:F:201:PHE:O	1:F:202:ASP:C	2.46	0.53
1:F:642:TYR:CE1	1:F:646:SER:HB3	2.44	0.53
1:A:285:ASN:HA	1:A:292:PHE:HA	1.91	0.53
1:B:260:PRO:O	1:B:261:ARG:C	2.48	0.53
1:B:341:LYS:O	1:B:476:ALA:HB3	2.08	0.53
1:B:382:ASN:ND2	1:B:573:VAL:HG21	2.24	0.53
1:B:517:ALA:O	1:B:520:ARG:N	2.39	0.53
1:C:387:ARG:NH1	1:C:407:ALA:HB1	2.22	0.53
1:E:382:ASN:ND2	1:E:573:VAL:HG21	2.23	0.53
1:A:645:MET:CE	1:B:654:LYS:HG2	2.38	0.53
1:B:391:MET:HG3	1:B:558:VAL:HG22	1.91	0.53
1:B:483:ALA:O	1:B:487:ILE:HG13	2.08	0.53
1:B:595:LYS:O	1:B:596:TYR:C	2.48	0.53
1:C:84:VAL:HA	1:C:161:THR:HA	1.91	0.53
1:D:27:LEU:O	1:D:29:ASP:N	2.42	0.53
1:E:358:PRO:HG2	1:E:359:GLY:H	1.73	0.53
1:E:382:ASN:HD21	1:E:573:VAL:HG21	1.73	0.53
1:E:702:ARG:HG2	1:E:706:ASP:OD2	2.09	0.53
1:F:386:LEU:O	1:F:388:ALA:N	2.41	0.53
1:E:352:GLY:O	1:E:353:ILE:CB	2.56	0.52
1:F:260:PRO:O	1:F:261:ARG:C	2.46	0.52
1:F:286:GLU:HB2	1:F:291:GLN:HG2	1.91	0.52
1:F:286:GLU:HG3	1:F:287:VAL:H	1.73	0.52
1:A:197:VAL:HG11	1:A:497:LEU:HD22	1.91	0.52
1:B:386:LEU:O	1:B:389:SER:N	2.42	0.52
1:D:517:ALA:O	1:D:520:ARG:N	2.40	0.52
1:E:54:VAL:O	1:E:58:GLU:N	2.41	0.52
1:E:286:GLU:HG3	1:E:287:VAL:H	1.74	0.52
1:F:336:VAL:O	1:F:337:ASN:C	2.48	0.52
1:A:230:PRO:O	1:A:232:LEU:N	2.43	0.52
3:A:3001:P3S:O2A	3:A:3001:P3S:OE	2.28	0.52
1:B:382:ASN:HD21	1:B:573:VAL:HG21	1.74	0.52
1:B:558:VAL:O	1:B:559:PRO:C	2.48	0.52
1:E:221:VAL:HG23	1:E:325:ALA:HB3	1.91	0.52
1:E:230:PRO:O	1:E:233:ARG:O	2.27	0.52
1:E:558:VAL:O	1:E:559:PRO:C	2.48	0.52
1:B:349:THR:CG2	1:B:353:ILE:HB	2.36	0.52
1:B:387:ARG:NH1	1:B:555:ILE:H	2.07	0.52
1:B:630:LEU:O	1:B:631:CYS:C	2.48	0.52
1:C:201:PHE:O	1:C:202:ASP:C	2.47	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:VAL:HG21	1:D:490:ASN:CB	2.36	0.52
1:E:595:LYS:O	1:E:596:TYR:C	2.47	0.52
1:A:311:VAL:O	1:A:315:MET:HG3	2.09	0.52
1:C:44:TYR:CE1	1:C:78:TRP:HA	2.44	0.52
1:A:294:LEU:C	1:A:294:LEU:HD12	2.29	0.52
1:B:207:ARG:HH11	1:B:207:ARG:CB	2.23	0.52
1:B:229:ARG:HG3	1:B:231:ASP:OD2	2.10	0.52
1:C:196:GLU:O	1:C:199:GLN:HG2	2.09	0.52
1:C:344:ASN:HB3	1:C:470:ARG:HD2	1.90	0.52
1:A:423:GLU:C	1:A:424:ILE:HD12	2.29	0.52
1:A:624:ASN:O	1:A:625:ARG:C	2.46	0.52
1:B:314:LEU:O	1:B:317:ARG:HG2	2.10	0.52
1:E:404:ALA:O	1:E:539:TYR:HE1	1.93	0.52
1:E:627:LEU:HD21	1:E:653:ILE:HG21	1.91	0.52
1:E:702:ARG:O	1:E:703:ASP:C	2.48	0.52
1:F:674:ARG:HG3	1:F:690:TYR:OH	2.10	0.52
1:A:286:GLU:HB3	1:A:291:GLN:HB3	1.92	0.52
1:A:618:ILE:HG13	1:A:716:ILE:HG21	1.92	0.52
1:A:626:LEU:O	1:A:629:ASN:HB3	2.09	0.52
1:B:63:ILE:HD12	1:B:63:ILE:N	2.19	0.52
1:E:627:LEU:CD2	1:E:653:ILE:HD13	2.39	0.52
1:F:221:VAL:HG23	1:F:325:ALA:HB3	1.91	0.52
1:F:382:ASN:ND2	1:F:573:VAL:HG21	2.25	0.52
1:F:382:ASN:HD21	1:F:573:VAL:HG21	1.74	0.52
1:A:26:LYS:O	1:A:29:ASP:HB2	2.09	0.52
1:A:559:PRO:HG2	1:A:691:GLU:HB2	1.91	0.52
1:D:54:VAL:O	1:D:58:GLU:N	2.42	0.52
1:E:483:ALA:O	1:E:487:ILE:HG13	2.10	0.52
1:F:69:ASP:OD1	1:F:120:GLY:N	2.43	0.52
1:F:554:ASN:HD22	1:F:555:ILE:N	2.08	0.52
1:F:558:VAL:O	1:F:559:PRO:C	2.47	0.52
1:A:574:LEU:O	1:A:579:ILE:HB	2.10	0.52
1:B:379:VAL:HG21	1:B:411:ILE:HD11	1.92	0.52
1:E:387:ARG:NH1	1:E:555:ILE:H	2.07	0.52
1:A:20:ILE:HD13	1:A:20:ILE:N	2.21	0.51
1:A:401:ALA:O	1:A:403:GLU:N	2.42	0.51
1:B:646:SER:O	1:B:647:ALA:C	2.48	0.51
1:C:627:LEU:HD21	1:C:653:ILE:HG21	1.92	0.51
1:D:233:ARG:HH11	1:D:233:ARG:CG	2.23	0.51
1:D:235:THR:HG23	1:D:603:GLU:HG2	1.91	0.51
1:E:341:LYS:O	1:E:476:ALA:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:HH11	1:A:407:ALA:HB1	1.75	0.51
1:A:613:ASN:ND2	1:F:721:LYS:HZ1	2.08	0.51
1:A:662:ALA:O	1:A:666:LEU:HD13	2.10	0.51
1:B:286:GLU:HB2	1:B:291:GLN:HG2	1.91	0.51
1:B:358:PRO:HG2	1:B:359:GLY:H	1.76	0.51
1:C:387:ARG:NH1	1:C:555:ILE:H	2.07	0.51
1:D:344:ASN:HB3	1:D:470:ARG:HD2	1.91	0.51
1:D:358:PRO:HG2	1:D:359:GLY:H	1.75	0.51
1:F:481:ASN:HD22	1:F:481:ASN:C	2.12	0.51
1:A:151:ASP:C	1:A:153:SER:N	2.63	0.51
1:A:222:ASP:OD1	1:A:224:SER:HB2	2.10	0.51
1:A:278:ILE:HD12	1:A:278:ILE:H	1.74	0.51
1:B:262:VAL:O	1:B:263:THR:C	2.49	0.51
1:D:159:VAL:O	1:D:160:ASP:C	2.49	0.51
1:D:627:LEU:HD21	1:D:653:ILE:HG21	1.92	0.51
1:E:645:MET:CE	1:F:654:LYS:HA	2.39	0.51
1:A:606:VAL:O	1:A:609:ASP:N	2.43	0.51
1:B:190:VAL:HG21	1:B:490:ASN:CB	2.35	0.51
1:B:613:ASN:O	1:B:617:PRO:HG2	2.11	0.51
1:C:330:GLU:HG3	1:C:395:ASN:N	2.26	0.51
1:D:69:ASP:N	1:D:120:GLY:HA3	2.25	0.51
1:D:341:LYS:O	1:D:476:ALA:HB3	2.10	0.51
1:A:94:LEU:HD23	1:A:177:LEU:O	2.11	0.51
1:A:204:ASN:O	1:A:205:ILE:HB	2.11	0.51
1:C:554:ASN:HD22	1:C:555:ILE:N	2.09	0.51
1:D:314:LEU:O	1:D:317:ARG:HG2	2.11	0.51
1:D:642:TYR:CE1	1:D:646:SER:HB3	2.46	0.51
1:E:38:ARG:O	1:E:39:LYS:C	2.48	0.51
1:E:522:LEU:C	1:E:522:LEU:HD23	2.31	0.51
1:E:642:TYR:CE1	1:E:646:SER:HB3	2.46	0.51
1:F:230:PRO:O	1:F:233:ARG:O	2.28	0.51
1:A:293:GLU:HG2	1:A:294:LEU:H	1.76	0.51
1:B:702:ARG:O	1:B:703:ASP:C	2.48	0.51
1:C:595:LYS:O	1:C:596:TYR:C	2.47	0.51
1:A:625:ARG:HH11	1:A:625:ARG:CG	2.24	0.51
1:C:11:GLU:HA	1:C:11:GLU:OE2	2.11	0.51
1:C:61:THR:CB	1:C:62:PRO:CA	2.89	0.51
1:C:336:VAL:O	1:C:337:ASN:C	2.49	0.51
1:D:702:ARG:HG2	1:D:706:ASP:OD2	2.11	0.51
1:F:61:THR:CB	1:F:62:PRO:CA	2.88	0.51
1:F:69:ASP:N	1:F:120:GLY:HA3	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:HG22	1:A:712:ILE:HD13	1.91	0.51
1:A:646:SER:O	1:A:647:ALA:C	2.48	0.51
1:B:11:GLU:HA	1:B:11:GLU:OE2	2.10	0.51
1:B:69:ASP:N	1:B:120:GLY:HA3	2.25	0.51
1:B:387:ARG:HH11	1:B:387:ARG:HG3	1.74	0.51
1:B:554:ASN:HD22	1:B:555:ILE:N	2.08	0.51
1:D:483:ALA:O	1:D:487:ILE:HG13	2.10	0.51
1:D:646:SER:O	1:D:647:ALA:C	2.49	0.51
1:E:646:SER:O	1:E:647:ALA:C	2.48	0.51
1:F:38:ARG:O	1:F:39:LYS:C	2.50	0.51
1:F:638:SER:O	1:F:641:GLU:N	2.44	0.51
1:A:233:ARG:HD3	1:A:234:LEU:N	2.26	0.51
1:B:61:THR:CB	1:B:62:PRO:CA	2.89	0.51
1:E:26:LYS:O	1:E:29:ASP:HB2	2.11	0.51
1:E:84:VAL:HA	1:E:161:THR:HA	1.91	0.51
1:E:207:ARG:HH11	1:E:207:ARG:CB	2.23	0.51
1:E:305:ASN:O	1:E:306:ASP:C	2.50	0.51
1:E:412:PHE:C	1:E:412:PHE:HD2	2.14	0.51
1:E:716:ILE:O	1:E:717:TRP:CB	2.58	0.51
1:F:646:SER:O	1:F:647:ALA:C	2.49	0.51
1:B:54:VAL:O	1:B:58:GLU:N	2.42	0.51
1:B:504:VAL:O	1:B:504:VAL:HG22	2.11	0.51
1:B:642:TYR:CE1	1:B:646:SER:HB3	2.46	0.51
1:D:230:PRO:O	1:D:233:ARG:O	2.29	0.51
1:D:231:ASP:O	1:D:235:THR:HB	2.11	0.51
1:F:386:LEU:O	1:F:389:SER:N	2.43	0.51
1:F:702:ARG:O	1:F:703:ASP:C	2.50	0.51
1:A:399:LEU:HA	1:A:404:ALA:HB1	1.93	0.50
1:A:547:ALA:HB1	1:A:552:LEU:HB2	1.93	0.50
1:A:666:LEU:CD1	1:A:666:LEU:H	2.24	0.50
1:B:626:LEU:O	1:B:629:ASN:HB3	2.12	0.50
1:C:69:ASP:N	1:C:120:GLY:HA3	2.25	0.50
1:C:69:ASP:OD1	1:C:120:GLY:N	2.42	0.50
1:C:702:ARG:O	1:C:703:ASP:C	2.49	0.50
1:E:229:ARG:HG3	1:E:231:ASP:OD2	2.11	0.50
1:E:262:VAL:O	1:E:265:PHE:HB3	2.11	0.50
1:F:536:GLY:O	1:F:538:GLY:N	2.44	0.50
1:A:645:MET:HE1	1:B:654:LYS:HG2	1.94	0.50
1:B:235:THR:HG23	1:B:603:GLU:HG2	1.93	0.50
1:C:261:ARG:HG3	1:C:261:ARG:NH1	2.25	0.50
1:E:554:ASN:HD22	1:E:555:ILE:N	2.08	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:CD2	1:F:10:GLN:HG2	2.46	0.50
1:A:82:LEU:O	1:A:83:ASN:HB2	2.12	0.50
1:B:38:ARG:O	1:B:39:LYS:C	2.50	0.50
1:B:286:GLU:HG3	1:B:287:VAL:H	1.75	0.50
1:B:336:VAL:O	1:B:337:ASN:C	2.47	0.50
1:C:404:ALA:O	1:C:539:TYR:HE1	1.93	0.50
1:D:223:THR:HG22	1:D:227:ASN:ND2	2.26	0.50
1:A:702:ARG:O	1:A:703:ASP:C	2.50	0.50
1:B:196:GLU:O	1:B:199:GLN:HG2	2.12	0.50
1:C:207:ARG:HH11	1:C:207:ARG:CB	2.23	0.50
1:C:419:ALA:HA	1:C:422:ASP:OD2	2.12	0.50
1:D:56:ALA:HA	1:D:61:THR:N	2.26	0.50
1:D:522:LEU:HD23	1:D:522:LEU:C	2.32	0.50
1:E:231:ASP:O	1:E:235:THR:HB	2.12	0.50
1:F:521:ILE:H	1:F:521:ILE:CD1	2.24	0.50
1:F:638:SER:O	1:F:639:GLU:C	2.50	0.50
1:F:716:ILE:HG22	1:F:717:TRP:N	2.22	0.50
1:B:668:ARG:HH11	1:B:668:ARG:HG3	1.77	0.50
1:C:229:ARG:HG3	1:C:231:ASP:OD2	2.12	0.50
1:D:61:THR:HB	1:D:62:PRO:CA	2.35	0.50
1:D:196:GLU:O	1:D:199:GLN:HG2	2.11	0.50
1:E:668:ARG:HH11	1:E:668:ARG:HG3	1.77	0.50
1:F:387:ARG:NH1	1:F:555:ILE:H	2.09	0.50
1:F:627:LEU:HD21	1:F:653:ILE:HG21	1.94	0.50
1:A:11:GLU:OE1	1:A:11:GLU:HA	2.12	0.50
1:A:390:ILE:C	1:A:390:ILE:HD12	2.31	0.50
1:B:303:LEU:O	1:B:304:ALA:C	2.48	0.50
1:B:638:SER:O	1:B:639:GLU:C	2.50	0.50
1:C:8:ALA:O	1:C:11:GLU:HB3	2.12	0.50
1:C:642:TYR:CE1	1:C:646:SER:HB3	2.46	0.50
1:D:212:LEU:HB3	1:D:301:CYS:HA	1.93	0.50
1:D:536:GLY:O	1:D:538:GLY:N	2.45	0.50
1:E:372:LEU:CD2	1:E:417:LEU:HD21	2.42	0.50
1:E:630:LEU:O	1:E:631:CYS:C	2.50	0.50
1:F:8:ALA:O	1:F:11:GLU:HB3	2.12	0.50
1:F:231:ASP:OD2	1:F:231:ASP:N	2.45	0.50
1:A:7:PHE:O	1:A:11:GLU:HB2	2.11	0.50
1:A:89:HIS:ND1	1:A:167:THR:HG21	2.26	0.50
1:A:354:ASN:C	1:A:356:PHE:H	2.14	0.50
1:B:44:TYR:CE1	1:B:78:TRP:HA	2.46	0.50
1:C:11:GLU:HG2	1:C:224:SER:OG	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ARG:O	1:C:39:LYS:C	2.49	0.50
1:C:233:ARG:HH11	1:C:233:ARG:CG	2.24	0.50
1:D:38:ARG:O	1:D:39:LYS:C	2.49	0.50
1:E:354:ASN:HB3	1:E:357:ALA:CB	2.42	0.50
1:F:93:PRO:C	1:F:95:THR:H	2.15	0.50
1:C:27:LEU:O	1:C:29:ASP:N	2.44	0.50
1:D:61:THR:CB	1:D:62:PRO:CA	2.89	0.50
1:D:349:THR:HG23	1:D:352:GLY:O	2.12	0.50
1:D:521:ILE:H	1:D:521:ILE:CD1	2.23	0.50
1:D:676:VAL:O	1:D:677:ALA:C	2.50	0.50
1:D:716:ILE:O	1:D:717:TRP:CB	2.59	0.50
1:F:626:LEU:O	1:F:629:ASN:HB3	2.11	0.50
1:F:702:ARG:O	1:F:704:HIS:N	2.45	0.50
1:A:659:ARG:NH1	1:A:707:HIS:CD2	2.80	0.50
1:B:11:GLU:HG2	1:B:224:SER:OG	2.11	0.50
1:B:56:ALA:HA	1:B:61:THR:N	2.27	0.50
1:B:331:LYS:HG3	1:B:397:HIS:O	2.11	0.50
1:B:655:GLU:O	1:B:658:HIS:HB3	2.12	0.50
1:C:159:VAL:O	1:C:160:ASP:C	2.51	0.50
1:C:262:VAL:O	1:C:265:PHE:HB3	2.11	0.50
1:C:286:GLU:HB2	1:C:291:GLN:HG2	1.94	0.50
1:E:223:THR:HG22	1:E:227:ASN:ND2	2.27	0.50
1:E:386:LEU:O	1:E:389:SER:N	2.44	0.50
1:F:212:LEU:HB3	1:F:301:CYS:HA	1.94	0.50
1:F:229:ARG:HG3	1:F:231:ASP:OD2	2.12	0.50
1:F:233:ARG:HH11	1:F:233:ARG:CG	2.23	0.50
1:F:331:LYS:HG3	1:F:397:HIS:O	2.12	0.50
1:A:15:ARG:NH1	1:A:323:HIS:CE1	2.80	0.49
1:A:159:VAL:HG12	1:A:317:ARG:HH12	1.77	0.49
1:A:200:LEU:HB2	1:A:201:PHE:CE2	2.46	0.49
1:A:235:THR:O	1:A:235:THR:HG22	2.11	0.49
1:B:354:ASN:HB3	1:B:357:ALA:CB	2.42	0.49
1:B:522:LEU:C	1:B:522:LEU:HD23	2.32	0.49
1:C:372:LEU:CD2	1:C:417:LEU:HD21	2.42	0.49
1:C:681:GLU:O	1:C:682:ASN:HB2	2.12	0.49
1:D:262:VAL:O	1:D:263:THR:C	2.50	0.49
1:D:702:ARG:O	1:D:703:ASP:C	2.49	0.49
1:E:44:TYR:CE1	1:E:78:TRP:HA	2.47	0.49
1:E:56:ALA:HA	1:E:61:THR:N	2.26	0.49
1:F:120:GLY:C	1:F:122:LEU:N	2.66	0.49
1:F:522:LEU:HD23	1:F:522:LEU:C	2.32	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:O	1:A:229:ARG:HB2	2.12	0.49
1:A:282:THR:O	1:A:294:LEU:HA	2.11	0.49
1:A:286:GLU:CB	1:A:291:GLN:HG2	2.42	0.49
1:A:605:ARG:HH11	1:A:605:ARG:HG3	1.77	0.49
1:B:641:GLU:O	1:B:644:VAL:HG12	2.11	0.49
1:C:303:LEU:O	1:C:304:ALA:C	2.50	0.49
1:C:341:LYS:O	1:C:476:ALA:HB3	2.11	0.49
1:C:504:VAL:HG22	1:C:504:VAL:O	2.12	0.49
1:C:716:ILE:O	1:C:717:TRP:CB	2.60	0.49
1:D:387:ARG:HG3	1:D:387:ARG:NH1	2.27	0.49
1:E:11:GLU:HA	1:E:11:GLU:OE2	2.12	0.49
1:E:536:GLY:O	1:E:538:GLY:N	2.45	0.49
1:F:235:THR:HG22	1:F:237:ARG:HG2	1.95	0.49
1:F:305:ASN:O	1:F:306:ASP:C	2.49	0.49
1:F:627:LEU:CD2	1:F:653:ILE:HD13	2.40	0.49
1:F:695:ARG:HB3	1:F:696:PRO:HD3	1.93	0.49
1:A:386:LEU:O	1:A:389:SER:N	2.40	0.49
1:A:583:THR:O	1:A:586:ALA:HB3	2.12	0.49
1:B:212:LEU:HB3	1:B:301:CYS:HA	1.94	0.49
1:C:212:LEU:HB3	1:C:301:CYS:HA	1.95	0.49
1:C:626:LEU:O	1:C:629:ASN:HB3	2.12	0.49
1:C:668:ARG:HH11	1:C:668:ARG:HG3	1.77	0.49
1:D:336:VAL:O	1:D:337:ASN:C	2.49	0.49
1:D:419:ALA:HA	1:D:422:ASP:OD2	2.12	0.49
1:E:613:ASN:O	1:E:617:PRO:HG2	2.13	0.49
1:E:676:VAL:O	1:E:677:ALA:C	2.49	0.49
1:A:421:LEU:HB3	1:A:533:ARG:NH1	2.27	0.49
1:A:481:ASN:O	1:A:482:CYS:C	2.50	0.49
1:B:31:TYR:O	1:B:32:ALA:HB3	2.12	0.49
1:C:56:ALA:HA	1:C:61:THR:N	2.27	0.49
1:C:235:THR:HG22	1:C:237:ARG:HG2	1.93	0.49
1:C:314:LEU:O	1:C:317:ARG:HG2	2.12	0.49
1:D:686:LYS:O	1:D:689:ALA:HB3	2.13	0.49
1:E:69:ASP:N	1:E:120:GLY:HA3	2.26	0.49
1:E:481:ASN:O	1:E:482:CYS:C	2.51	0.49
1:E:624:ASN:O	1:E:625:ARG:C	2.51	0.49
1:F:504:VAL:O	1:F:504:VAL:HG22	2.13	0.49
1:A:320:ARG:HB3	1:A:320:ARG:NH1	2.26	0.49
1:A:331:LYS:HG3	1:A:397:HIS:O	2.11	0.49
1:A:529:SER:OG	1:A:530:GLU:N	2.46	0.49
1:B:330:GLU:HG3	1:B:395:ASN:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASP:OD2	1:C:231:ASP:N	2.44	0.49
1:D:504:VAL:O	1:D:504:VAL:HG22	2.13	0.49
1:D:529:SER:O	1:D:530:GLU:C	2.51	0.49
1:D:655:GLU:O	1:D:658:HIS:HB3	2.12	0.49
1:D:668:ARG:HH11	1:D:668:ARG:HG3	1.78	0.49
1:E:638:SER:O	1:E:639:GLU:C	2.50	0.49
1:F:56:ALA:HA	1:F:61:THR:N	2.27	0.49
1:F:314:LEU:O	1:F:317:ARG:HG2	2.13	0.49
1:F:404:ALA:O	1:F:539:TYR:HE1	1.96	0.49
1:F:409:LEU:N	1:F:409:LEU:HD12	2.28	0.49
1:F:630:LEU:O	1:F:631:CYS:C	2.50	0.49
1:A:659:ARG:HH12	1:A:707:HIS:CD2	2.30	0.49
1:B:627:LEU:HD21	1:B:653:ILE:HG21	1.93	0.49
1:C:20:ILE:HG12	1:C:21:THR:N	2.12	0.49
1:C:522:LEU:O	1:C:526:ILE:HG13	2.13	0.49
1:C:630:LEU:O	1:C:631:CYS:C	2.48	0.49
1:D:522:LEU:O	1:D:526:ILE:HG13	2.13	0.49
1:F:207:ARG:HH11	1:F:207:ARG:CB	2.22	0.49
1:A:286:GLU:HB2	1:A:291:GLN:HG2	1.94	0.49
1:A:606:VAL:O	1:A:607:LEU:C	2.50	0.49
1:C:26:LYS:O	1:C:29:ASP:HB2	2.13	0.49
1:C:31:TYR:O	1:C:32:ALA:HB3	2.13	0.49
1:C:522:LEU:HD23	1:C:522:LEU:C	2.33	0.49
1:C:702:ARG:O	1:C:704:HIS:N	2.46	0.49
1:D:93:PRO:C	1:D:95:THR:H	2.15	0.49
1:D:235:THR:HG22	1:D:237:ARG:HG2	1.95	0.49
1:D:409:LEU:HD12	1:D:409:LEU:N	2.28	0.49
1:D:531:LEU:HD22	1:D:550:ARG:HB3	1.95	0.49
1:E:282:THR:HG22	1:F:103:ASP:OD2	2.13	0.49
1:F:354:ASN:HB3	1:F:357:ALA:CB	2.43	0.49
1:A:486:MET:O	1:A:487:ILE:C	2.51	0.49
1:C:223:THR:HG22	1:C:227:ASN:ND2	2.27	0.49
1:C:354:ASN:HB3	1:C:357:ALA:CB	2.43	0.49
1:C:517:ALA:O	1:C:518:ILE:C	2.51	0.49
1:C:558:VAL:O	1:C:559:PRO:C	2.50	0.49
1:D:354:ASN:HB3	1:D:357:ALA:CB	2.42	0.49
1:D:624:ASN:O	1:D:625:ARG:C	2.51	0.49
1:E:235:THR:HG23	1:E:603:GLU:HG2	1.94	0.49
1:E:412:PHE:HD2	1:E:412:PHE:O	1.96	0.49
1:E:681:GLU:O	1:E:682:ASN:HB2	2.13	0.49
1:E:686:LYS:O	1:E:689:ALA:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ASP:O	1:F:192:LYS:C	2.51	0.49
1:F:262:VAL:O	1:F:265:PHE:HB3	2.11	0.49
1:F:349:THR:HG23	1:F:352:GLY:O	2.12	0.49
1:A:219:PHE:HA	1:A:290:ASN:O	2.12	0.49
1:A:282:THR:HG23	1:A:283:ARG:N	2.28	0.49
1:A:682:ASN:HB3	1:A:685:GLU:CG	2.43	0.49
1:B:536:GLY:O	1:B:538:GLY:N	2.46	0.49
1:C:652:LEU:O	1:C:655:GLU:HB3	2.13	0.49
1:D:26:LYS:O	1:D:29:ASP:HB2	2.12	0.49
1:D:613:ASN:O	1:D:617:PRO:HG2	2.12	0.49
1:E:199:GLN:NE2	1:E:199:GLN:CA	2.75	0.49
1:E:554:ASN:C	1:E:554:ASN:ND2	2.54	0.49
1:E:616:VAL:HB	1:E:617:PRO:CD	2.41	0.49
1:E:672:GLU:O	1:E:673:ALA:C	2.51	0.49
1:F:715:GLU:OE1	1:F:715:GLU:HA	2.13	0.49
1:A:38:ARG:C	1:A:40:LYS:N	2.63	0.49
1:A:237:ARG:HG3	1:A:237:ARG:O	2.13	0.49
1:A:240:MET:HA	1:A:702:ARG:NE	2.28	0.49
1:B:235:THR:HG22	1:B:237:ARG:HG2	1.94	0.49
1:B:409:LEU:HD12	1:B:409:LEU:N	2.28	0.49
1:C:191:ASP:O	1:C:192:LYS:C	2.51	0.49
1:C:231:ASP:O	1:C:235:THR:HB	2.13	0.49
1:C:374:ASN:O	1:C:375:VAL:C	2.52	0.49
1:D:120:GLY:C	1:D:122:LEU:N	2.66	0.49
1:D:191:ASP:O	1:D:192:LYS:C	2.51	0.49
1:D:404:ALA:O	1:D:539:TYR:HE1	1.95	0.49
1:D:412:PHE:C	1:D:412:PHE:HD2	2.14	0.49
1:E:231:ASP:OD2	1:E:231:ASP:N	2.46	0.49
1:E:596:TYR:O	1:E:600:VAL:HG23	2.13	0.49
1:E:638:SER:O	1:E:641:GLU:N	2.46	0.49
1:F:26:LYS:O	1:F:29:ASP:HB2	2.12	0.49
1:F:54:VAL:O	1:F:58:GLU:N	2.44	0.49
1:F:303:LEU:O	1:F:304:ALA:C	2.51	0.49
1:A:186:ALA:HA	1:A:579:ILE:HD11	1.94	0.48
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.13	0.48
1:A:358:PRO:HA	1:A:368:PHE:CD1	2.47	0.48
1:A:543:TRP:C	1:A:545:GLN:H	2.16	0.48
1:B:120:GLY:C	1:B:122:LEU:N	2.67	0.48
1:B:521:ILE:H	1:B:521:ILE:CD1	2.22	0.48
1:C:349:THR:HG23	1:C:352:GLY:O	2.12	0.48
1:D:665:VAL:O	1:D:666:LEU:C	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:702:ARG:O	1:D:704:HIS:N	2.45	0.48
1:D:715:GLU:OE1	1:D:715:GLU:HA	2.12	0.48
1:F:262:VAL:O	1:F:263:THR:C	2.52	0.48
1:F:415:SER:O	1:F:416:GLN:C	2.52	0.48
1:F:716:ILE:O	1:F:717:TRP:CB	2.61	0.48
1:B:652:LEU:O	1:B:655:GLU:HB3	2.13	0.48
1:C:150:TRP:CD1	1:C:151:ASP:N	2.81	0.48
1:C:522:LEU:CD2	1:C:526:ILE:HD11	2.44	0.48
1:C:646:SER:O	1:C:647:ALA:C	2.50	0.48
1:D:84:VAL:HG11	1:D:158:VAL:HG21	1.95	0.48
1:D:638:SER:O	1:D:639:GLU:C	2.50	0.48
1:E:212:LEU:HB3	1:E:301:CYS:HA	1.94	0.48
1:E:235:THR:HG22	1:E:237:ARG:HG2	1.95	0.48
1:E:641:GLU:O	1:E:644:VAL:HG12	2.13	0.48
1:F:223:THR:HG22	1:F:227:ASN:ND2	2.27	0.48
1:A:50:TYR:C	1:A:52:ALA:N	2.66	0.48
1:A:638:SER:O	1:A:639:GLU:C	2.52	0.48
1:A:695:ARG:HH11	1:A:695:ARG:CG	2.27	0.48
1:B:26:LYS:O	1:B:29:ASP:HB2	2.14	0.48
1:C:235:THR:HG23	1:C:603:GLU:HG2	1.95	0.48
1:D:305:ASN:O	1:D:306:ASP:C	2.51	0.48
1:E:20:ILE:CD1	1:E:20:ILE:N	2.76	0.48
1:E:61:THR:HB	1:E:62:PRO:CA	2.36	0.48
1:E:626:LEU:O	1:E:629:ASN:HB3	2.12	0.48
1:F:613:ASN:O	1:F:617:PRO:HG2	2.13	0.48
1:F:686:LYS:O	1:F:689:ALA:HB3	2.14	0.48
1:A:91:PHE:HE2	1:A:93:PRO:HB3	1.78	0.48
1:A:367:LEU:O	1:A:370:THR:HB	2.13	0.48
1:A:666:LEU:N	1:A:666:LEU:HD12	2.27	0.48
1:B:522:LEU:O	1:B:526:ILE:HG13	2.13	0.48
1:C:54:VAL:O	1:C:58:GLU:N	2.44	0.48
1:C:390:ILE:C	1:C:390:ILE:HD12	2.33	0.48
1:C:415:SER:O	1:C:416:GLN:C	2.51	0.48
1:C:481:ASN:O	1:C:482:CYS:C	2.51	0.48
1:D:415:SER:O	1:D:416:GLN:C	2.51	0.48
1:F:11:GLU:HG2	1:F:224:SER:OG	2.13	0.48
1:F:419:ALA:HA	1:F:422:ASP:OD2	2.13	0.48
1:A:609:ASP:O	1:A:610:LEU:C	2.51	0.48
1:A:660:VAL:CG2	1:A:664:LYS:HE3	2.39	0.48
1:B:415:SER:O	1:B:416:GLN:C	2.52	0.48
1:B:481:ASN:O	1:B:482:CYS:C	2.52	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:HB	1:C:62:PRO:CA	2.35	0.48
1:C:536:GLY:O	1:C:538:GLY:N	2.47	0.48
1:D:11:GLU:HG2	1:D:224:SER:OG	2.13	0.48
1:D:20:ILE:CD1	1:D:20:ILE:N	2.76	0.48
1:D:672:GLU:O	1:D:673:ALA:C	2.52	0.48
1:E:262:VAL:O	1:E:263:THR:C	2.50	0.48
1:E:314:LEU:O	1:E:317:ARG:HG2	2.13	0.48
1:E:415:SER:O	1:E:416:GLN:C	2.51	0.48
1:F:372:LEU:CD2	1:F:417:LEU:HD21	2.42	0.48
1:F:531:LEU:HD22	1:F:550:ARG:HB3	1.96	0.48
1:A:231:ASP:OD2	1:A:231:ASP:N	2.47	0.48
1:B:159:VAL:O	1:B:160:ASP:C	2.51	0.48
1:B:488:ALA:O	1:B:489:ILE:C	2.51	0.48
1:C:120:GLY:C	1:C:122:LEU:N	2.67	0.48
1:C:305:ASN:O	1:C:306:ASP:C	2.52	0.48
1:C:655:GLU:O	1:C:658:HIS:HB3	2.13	0.48
1:D:368:PHE:C	1:D:368:PHE:CD1	2.86	0.48
1:D:630:LEU:O	1:D:631:CYS:C	2.50	0.48
1:D:638:SER:O	1:D:641:GLU:N	2.46	0.48
1:E:159:VAL:O	1:E:160:ASP:C	2.50	0.48
1:E:409:LEU:HD12	1:E:409:LEU:N	2.28	0.48
1:E:517:ALA:O	1:E:518:ILE:C	2.52	0.48
1:E:715:GLU:OE1	1:E:715:GLU:HA	2.12	0.48
1:F:20:ILE:CD1	1:F:20:ILE:N	2.76	0.48
1:F:529:SER:O	1:F:530:GLU:C	2.52	0.48
1:F:641:GLU:O	1:F:644:VAL:HG12	2.13	0.48
1:A:6:PHE:HA	1:A:9:LEU:HD22	1.95	0.48
1:A:584:GLU:O	1:A:588:ARG:HG2	2.14	0.48
1:B:6:PHE:C	1:B:8:ALA:N	2.66	0.48
1:B:529:SER:O	1:B:530:GLU:C	2.52	0.48
1:C:638:SER:O	1:C:639:GLU:C	2.51	0.48
1:C:672:GLU:O	1:C:673:ALA:C	2.51	0.48
1:E:11:GLU:HG2	1:E:224:SER:OG	2.13	0.48
1:E:53:VAL:HG22	1:E:71:ILE:CD1	2.43	0.48
1:E:93:PRO:C	1:E:95:THR:H	2.16	0.48
1:E:330:GLU:HG3	1:E:395:ASN:N	2.29	0.48
1:E:521:ILE:H	1:E:521:ILE:CD1	2.24	0.48
1:E:522:LEU:CD2	1:E:526:ILE:HD11	2.44	0.48
1:E:529:SER:O	1:E:530:GLU:C	2.51	0.48
1:E:702:ARG:O	1:E:704:HIS:N	2.46	0.48
1:A:674:ARG:O	1:A:675:LYS:C	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ALA:O	1:B:11:GLU:HB3	2.14	0.48
1:B:69:ASP:OD1	1:B:120:GLY:N	2.45	0.48
1:C:412:PHE:C	1:C:412:PHE:HD2	2.17	0.48
1:D:8:ALA:O	1:D:11:GLU:HB3	2.14	0.48
1:D:207:ARG:CB	1:D:207:ARG:NH1	2.77	0.48
1:D:331:LYS:HG3	1:D:397:HIS:O	2.13	0.48
1:D:387:ARG:NH1	1:D:555:ILE:H	2.12	0.48
1:E:368:PHE:CD1	1:E:368:PHE:C	2.87	0.48
1:B:399:LEU:HA	1:B:404:ALA:HB1	1.96	0.48
1:B:419:ALA:HA	1:B:422:ASP:OD2	2.13	0.48
1:B:716:ILE:HG22	1:B:717:TRP:N	2.23	0.48
1:C:93:PRO:C	1:C:95:THR:H	2.17	0.48
1:C:368:PHE:CD1	1:C:368:PHE:C	2.86	0.48
1:C:379:VAL:CG2	1:C:411:ILE:HD11	2.44	0.48
1:D:262:VAL:O	1:D:265:PHE:HB3	2.13	0.48
1:D:517:ALA:O	1:D:518:ILE:C	2.52	0.48
1:E:303:LEU:O	1:E:304:ALA:C	2.52	0.48
1:E:652:LEU:O	1:E:655:GLU:HB3	2.13	0.48
1:E:655:GLU:O	1:E:658:HIS:HB3	2.13	0.48
1:E:674:ARG:HG3	1:E:690:TYR:OH	2.14	0.48
1:F:53:VAL:HG22	1:F:71:ILE:CD1	2.43	0.48
1:F:63:ILE:H	1:F:63:ILE:CD1	2.12	0.48
1:F:668:ARG:HG3	1:F:668:ARG:HH11	1.77	0.48
1:A:341:LYS:O	1:A:476:ALA:HB3	2.14	0.48
1:A:412:PHE:HB3	1:A:465:ALA:HA	1.96	0.48
1:B:84:VAL:HG11	1:B:158:VAL:HG21	1.96	0.48
1:B:368:PHE:CD1	1:B:368:PHE:C	2.87	0.48
1:D:231:ASP:OD2	1:D:231:ASP:N	2.46	0.48
1:E:63:ILE:HD12	1:E:63:ILE:N	2.18	0.48
1:E:191:ASP:O	1:E:192:LYS:C	2.52	0.48
1:F:159:VAL:O	1:F:160:ASP:C	2.51	0.48
1:F:522:LEU:O	1:F:526:ILE:HG13	2.14	0.48
1:F:596:TYR:O	1:F:600:VAL:HG23	2.14	0.48
1:A:9:LEU:O	1:A:12:LEU:HD12	2.14	0.47
1:A:231:ASP:H	1:A:610:LEU:HD11	1.78	0.47
1:B:93:PRO:C	1:B:95:THR:H	2.17	0.47
1:C:409:LEU:N	1:C:409:LEU:HD12	2.29	0.47
1:E:61:THR:CB	1:E:62:PRO:CA	2.90	0.47
1:E:522:LEU:O	1:E:526:ILE:HG13	2.13	0.47
1:F:84:VAL:HG11	1:F:158:VAL:HG21	1.95	0.47
1:F:207:ARG:CB	1:F:207:ARG:NH1	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:THR:HG23	1:F:603:GLU:HG2	1.96	0.47
1:F:638:SER:HG	1:F:641:GLU:HG3	1.79	0.47
1:A:517:ALA:O	1:A:518:ILE:C	2.52	0.47
1:A:602:ILE:H	1:A:602:ILE:HD12	1.79	0.47
1:A:663:ILE:O	1:A:664:LYS:C	2.51	0.47
1:B:262:VAL:O	1:B:265:PHE:HB3	2.14	0.47
1:B:702:ARG:O	1:B:704:HIS:N	2.47	0.47
1:D:372:LEU:CD2	1:D:417:LEU:HD21	2.43	0.47
1:D:482:CYS:O	1:D:483:ALA:C	2.52	0.47
1:E:233:ARG:HH11	1:E:233:ARG:CG	2.22	0.47
1:E:488:ALA:O	1:E:489:ILE:C	2.52	0.47
1:F:199:GLN:HE21	1:F:199:GLN:CA	2.08	0.47
1:F:517:ALA:O	1:F:518:ILE:C	2.52	0.47
1:A:266:MET:HE2	1:A:283:ARG:HH21	1.79	0.47
1:A:695:ARG:HB3	1:A:696:PRO:HD3	1.96	0.47
1:B:522:LEU:CD2	1:B:526:ILE:HD11	2.44	0.47
1:C:199:GLN:NE2	1:C:199:GLN:CA	2.76	0.47
1:C:488:ALA:O	1:C:489:ILE:C	2.52	0.47
1:C:531:LEU:HD22	1:C:550:ARG:HB3	1.96	0.47
1:E:262:VAL:O	1:E:265:PHE:N	2.47	0.47
1:F:150:TRP:CD1	1:F:151:ASP:N	2.82	0.47
1:A:120:GLY:C	1:A:122:LEU:N	2.68	0.47
1:A:504:VAL:HG21	1:A:518:ILE:CG2	2.39	0.47
1:D:681:GLU:O	1:D:682:ASN:HB2	2.13	0.47
1:E:419:ALA:HA	1:E:422:ASP:OD2	2.13	0.47
1:F:390:ILE:C	1:F:390:ILE:HD12	2.35	0.47
1:F:681:GLU:O	1:F:682:ASN:HB2	2.12	0.47
1:A:120:GLY:C	1:A:122:LEU:H	2.17	0.47
1:B:231:ASP:O	1:B:235:THR:HB	2.13	0.47
1:B:481:ASN:C	1:B:481:ASN:ND2	2.67	0.47
1:C:641:GLU:O	1:C:644:VAL:HG12	2.14	0.47
1:D:31:TYR:O	1:D:32:ALA:HB3	2.14	0.47
1:E:349:THR:HG23	1:E:352:GLY:O	2.13	0.47
1:E:716:ILE:CG2	1:E:717:TRP:H	2.19	0.47
1:F:41:MET:O	1:F:45:LEU:HB2	2.13	0.47
1:F:368:PHE:CD1	1:F:368:PHE:C	2.87	0.47
1:F:652:LEU:O	1:F:655:GLU:HB3	2.14	0.47
1:A:269:LEU:HA	1:A:318:ILE:CD1	2.45	0.47
1:A:301:CYS:SG	1:A:486:MET:HG3	2.55	0.47
1:B:207:ARG:CB	1:B:207:ARG:NH1	2.77	0.47
1:D:565:TYR:HB2	1:D:589:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:641:GLU:O	1:D:644:VAL:HG12	2.14	0.47
1:F:330:GLU:HG3	1:F:395:ASN:N	2.30	0.47
1:F:595:LYS:O	1:F:596:TYR:C	2.50	0.47
1:F:634:LYS:HA	1:F:642:TYR:CD1	2.50	0.47
1:F:655:GLU:O	1:F:658:HIS:HB3	2.15	0.47
1:A:11:GLU:HG2	1:A:224:SER:OG	2.14	0.47
1:A:84:VAL:HA	1:A:161:THR:HA	1.97	0.47
1:A:87:TYR:CZ	1:A:103:ASP:HB2	2.50	0.47
1:A:149:ALA:HB3	1:A:168:ILE:HD11	1.96	0.47
1:A:180:LYS:O	1:A:181:THR:C	2.53	0.47
1:A:329:HIS:ND1	1:A:330:GLU:N	2.62	0.47
1:A:350:ASP:OD2	1:A:351:THR:HG23	2.15	0.47
1:A:421:LEU:HG	1:A:526:ILE:HD12	1.95	0.47
1:A:534:PHE:CG	1:A:535:GLU:N	2.83	0.47
1:A:583:THR:O	1:A:584:GLU:C	2.52	0.47
1:A:702:ARG:O	1:A:704:HIS:N	2.48	0.47
1:B:20:ILE:O	1:B:21:THR:CG2	2.56	0.47
1:B:223:THR:HG22	1:B:227:ASN:ND2	2.28	0.47
1:B:305:ASN:O	1:B:306:ASP:C	2.51	0.47
1:B:377:MET:HE2	1:B:377:MET:HA	1.96	0.47
1:B:482:CYS:O	1:B:483:ALA:C	2.53	0.47
1:B:581:ASN:O	1:B:582:GLU:C	2.52	0.47
1:B:596:TYR:CZ	1:B:600:VAL:HG21	2.49	0.47
1:B:638:SER:O	1:B:641:GLU:N	2.48	0.47
1:B:681:GLU:O	1:B:682:ASN:HB2	2.14	0.47
1:B:715:GLU:OE1	1:B:715:GLU:HA	2.14	0.47
1:C:20:ILE:CD1	1:C:20:ILE:N	2.78	0.47
1:C:299:GLU:O	1:C:300:ASN:C	2.53	0.47
1:C:596:TYR:CZ	1:C:600:VAL:HG21	2.50	0.47
1:C:686:LYS:O	1:C:689:ALA:HB3	2.14	0.47
1:D:330:GLU:HG3	1:D:395:ASN:N	2.30	0.47
1:D:688:PHE:O	1:D:689:ALA:C	2.53	0.47
1:E:31:TYR:O	1:E:32:ALA:HB3	2.15	0.47
1:E:387:ARG:NH1	1:E:387:ARG:HG3	2.30	0.47
1:E:481:ASN:C	1:E:481:ASN:ND2	2.68	0.47
1:E:504:VAL:HG22	1:E:504:VAL:O	2.14	0.47
1:F:38:ARG:C	1:F:40:LYS:N	2.68	0.47
1:A:625:ARG:HH11	1:A:625:ARG:CB	2.28	0.47
1:B:150:TRP:CD1	1:B:151:ASP:N	2.83	0.47
1:B:349:THR:HG23	1:B:352:GLY:O	2.14	0.47
1:B:404:ALA:O	1:B:539:TYR:HE1	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:PHE:HD2	1:B:412:PHE:O	1.98	0.47
1:C:414:GLY:O	1:C:415:SER:C	2.53	0.47
1:C:529:SER:O	1:C:530:GLU:C	2.53	0.47
1:D:522:LEU:CD2	1:D:526:ILE:HD11	2.45	0.47
1:D:634:LYS:HA	1:D:642:TYR:CD1	2.50	0.47
1:E:368:PHE:HD1	1:E:369:LEU:N	2.12	0.47
1:A:5:ARG:O	1:A:9:LEU:HD22	2.15	0.47
1:A:286:GLU:HG3	1:A:287:VAL:H	1.78	0.47
1:B:299:GLU:O	1:B:300:ASN:C	2.53	0.47
1:B:372:LEU:CD2	1:B:417:LEU:HD21	2.44	0.47
1:B:517:ALA:O	1:B:518:ILE:C	2.53	0.47
1:C:207:ARG:CB	1:C:207:ARG:NH1	2.78	0.47
1:C:368:PHE:HD1	1:C:369:LEU:N	2.13	0.47
1:C:412:PHE:HD2	1:C:412:PHE:O	1.98	0.47
1:D:20:ILE:O	1:D:21:THR:CG2	2.58	0.47
1:E:150:TRP:CD1	1:E:151:ASP:N	2.83	0.47
1:E:261:ARG:HG3	1:E:261:ARG:NH1	2.29	0.47
1:E:482:CYS:O	1:E:483:ALA:C	2.53	0.47
1:F:71:ILE:O	1:F:74:GLY:N	2.47	0.47
1:F:565:TYR:HB2	1:F:589:LEU:HD13	1.97	0.47
1:A:355:LEU:HD21	1:A:371:PHE:CZ	2.50	0.47
1:A:595:LYS:O	1:A:596:TYR:C	2.52	0.47
1:A:695:ARG:N	1:A:696:PRO:CD	2.78	0.47
1:B:368:PHE:HD1	1:B:369:LEU:N	2.12	0.47
1:B:390:ILE:C	1:B:390:ILE:HD12	2.35	0.47
1:C:68:ALA:O	1:C:71:ILE:N	2.47	0.47
1:C:202:ASP:C	1:C:202:ASP:OD2	2.54	0.47
1:C:716:ILE:CG2	1:C:717:TRP:H	2.20	0.47
1:D:53:VAL:HG22	1:D:71:ILE:CD1	2.45	0.47
1:D:266:MET:O	1:D:267:LYS:C	2.53	0.47
1:D:368:PHE:HD1	1:D:369:LEU:N	2.12	0.47
1:E:120:GLY:C	1:E:122:LEU:N	2.65	0.47
1:E:207:ARG:CB	1:E:207:ARG:NH1	2.78	0.47
1:E:634:LYS:HA	1:E:642:TYR:CD1	2.50	0.47
1:F:231:ASP:O	1:F:235:THR:HB	2.14	0.47
1:B:199:GLN:NE2	1:B:199:GLN:CA	2.76	0.46
1:B:676:VAL:O	1:B:677:ALA:C	2.53	0.46
1:B:686:LYS:O	1:B:689:ALA:HB3	2.14	0.46
1:C:53:VAL:HG22	1:C:71:ILE:CD1	2.45	0.46
1:C:84:VAL:HG11	1:C:158:VAL:HG21	1.96	0.46
1:C:399:LEU:HA	1:C:404:ALA:HB1	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:ASN:C	1:C:481:ASN:ND2	2.69	0.46
1:C:634:LYS:HA	1:C:642:TYR:CD1	2.49	0.46
1:C:665:VAL:O	1:C:666:LEU:C	2.54	0.46
1:D:412:PHE:HD2	1:D:412:PHE:O	1.98	0.46
1:D:504:VAL:O	1:D:504:VAL:HG13	2.15	0.46
1:E:414:GLY:O	1:E:415:SER:C	2.54	0.46
1:E:727:PHE:O	1:E:728:THR:O	2.33	0.46
1:F:53:VAL:HG22	1:F:71:ILE:HD11	1.97	0.46
1:A:601:GLN:HG3	1:A:674:ARG:HD3	1.97	0.46
1:A:665:VAL:O	1:A:668:ARG:N	2.49	0.46
1:B:262:VAL:O	1:B:265:PHE:N	2.48	0.46
1:C:387:ARG:HG3	1:C:387:ARG:NH1	2.30	0.46
1:C:482:CYS:O	1:C:483:ALA:C	2.54	0.46
1:D:303:LEU:O	1:D:304:ALA:C	2.54	0.46
1:D:652:LEU:O	1:D:655:GLU:HB3	2.15	0.46
1:E:8:ALA:O	1:E:11:GLU:HB3	2.15	0.46
1:E:530:GLU:O	1:E:531:LEU:C	2.54	0.46
1:F:261:ARG:HG3	1:F:261:ARG:NH1	2.28	0.46
1:F:387:ARG:NH1	1:F:387:ARG:HG3	2.30	0.46
1:A:61:THR:CB	1:A:62:PRO:CA	2.93	0.46
1:A:638:SER:O	1:A:641:GLU:N	2.48	0.46
1:A:697:TYR:O	1:A:698:LEU:C	2.51	0.46
1:B:71:ILE:O	1:B:72:ALA:C	2.54	0.46
1:C:331:LYS:HG3	1:C:397:HIS:O	2.14	0.46
1:C:715:GLU:OE1	1:C:715:GLU:HA	2.15	0.46
1:D:199:GLN:NE2	1:D:199:GLN:CA	2.77	0.46
1:D:481:ASN:O	1:D:482:CYS:C	2.53	0.46
1:E:182:PRO:HB2	1:E:487:ILE:HD13	1.98	0.46
1:F:522:LEU:CD2	1:F:526:ILE:HD11	2.46	0.46
1:A:199:GLN:OE1	1:A:199:GLN:HA	2.15	0.46
1:B:68:ALA:O	1:B:71:ILE:N	2.49	0.46
1:B:233:ARG:CG	1:B:233:ARG:NH1	2.78	0.46
1:B:634:LYS:HA	1:B:642:TYR:CD1	2.50	0.46
1:C:262:VAL:O	1:C:263:THR:C	2.52	0.46
1:D:581:ASN:O	1:D:582:GLU:C	2.53	0.46
1:F:6:PHE:C	1:F:8:ALA:N	2.68	0.46
1:F:374:ASN:O	1:F:375:VAL:C	2.53	0.46
1:F:676:VAL:O	1:F:677:ALA:C	2.53	0.46
1:A:63:ILE:H	1:A:63:ILE:CD1	2.13	0.46
1:A:65:ARG:HG2	1:A:65:ARG:HH11	1.80	0.46
1:B:422:ASP:O	1:B:424:ILE:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ILE:O	1:D:74:GLY:N	2.48	0.46
1:D:399:LEU:HA	1:D:404:ALA:HB1	1.97	0.46
1:E:695:ARG:HG2	1:E:695:ARG:NH1	2.29	0.46
1:F:11:GLU:HG3	1:F:15:ARG:NH1	2.29	0.46
1:A:122:LEU:O	1:A:123:LEU:HD23	2.15	0.46
1:A:266:MET:HE2	1:A:283:ARG:HD2	1.98	0.46
1:A:318:ILE:O	1:A:321:LYS:HB3	2.16	0.46
1:A:521:ILE:HD12	1:A:521:ILE:N	2.23	0.46
1:A:575:ILE:HA	1:A:580:PHE:O	2.16	0.46
1:A:602:ILE:O	1:A:606:VAL:HG23	2.16	0.46
1:B:41:MET:SD	1:B:53:VAL:HG11	2.56	0.46
1:B:41:MET:O	1:B:45:LEU:HB2	2.16	0.46
1:B:716:ILE:O	1:B:717:TRP:CB	2.62	0.46
1:C:20:ILE:O	1:C:21:THR:CG2	2.57	0.46
1:C:230:PRO:O	1:C:233:ARG:O	2.32	0.46
1:E:11:GLU:HG3	1:E:15:ARG:NH1	2.28	0.46
1:E:120:GLY:O	1:E:122:LEU:N	2.48	0.46
1:E:709:GLU:HG3	1:E:717:TRP:CE2	2.51	0.46
1:F:422:ASP:O	1:F:424:ILE:N	2.49	0.46
1:F:665:VAL:O	1:F:666:LEU:C	2.52	0.46
1:A:354:ASN:O	1:A:356:PHE:N	2.49	0.46
1:A:492:ALA:HA	1:A:573:VAL:CG1	2.44	0.46
1:A:583:THR:O	1:A:586:ALA:N	2.49	0.46
1:A:587:CYS:O	1:A:590:GLU:HB3	2.16	0.46
1:B:672:GLU:O	1:B:673:ALA:C	2.53	0.46
1:D:229:ARG:HG3	1:D:231:ASP:OD2	2.15	0.46
1:E:10:GLN:HG2	1:F:7:PHE:CG	2.50	0.46
1:E:202:ASP:C	1:E:202:ASP:OD2	2.54	0.46
1:F:31:TYR:O	1:F:32:ALA:HB3	2.14	0.46
1:F:616:VAL:HB	1:F:617:PRO:CD	2.42	0.46
1:A:349:THR:O	1:A:350:ASP:C	2.53	0.46
1:A:349:THR:O	1:A:352:GLY:N	2.48	0.46
1:A:380:HIS:HA	1:A:532:ILE:HD13	1.97	0.46
1:A:716:ILE:CG2	1:A:717:TRP:H	2.15	0.46
1:B:412:PHE:C	1:B:412:PHE:HD2	2.16	0.46
1:B:414:GLY:O	1:B:415:SER:C	2.54	0.46
1:C:530:GLU:O	1:C:531:LEU:C	2.54	0.46
1:D:68:ALA:O	1:D:71:ILE:N	2.48	0.46
1:D:377:MET:HA	1:D:377:MET:HE2	1.97	0.46
1:D:481:ASN:C	1:D:481:ASN:ND2	2.69	0.46
1:D:716:ILE:HG22	1:D:717:TRP:N	2.25	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:VAL:HG11	1:E:158:VAL:HG21	1.97	0.46
1:E:565:TYR:HB2	1:E:589:LEU:HD13	1.97	0.46
1:E:598:MET:O	1:E:602:ILE:HD13	2.16	0.46
1:F:309:GLN:OE1	1:F:309:GLN:HA	2.16	0.46
1:F:368:PHE:HD1	1:F:369:LEU:N	2.12	0.46
1:A:186:ALA:O	1:A:190:VAL:HG23	2.16	0.46
1:A:222:ASP:O	1:A:223:THR:C	2.53	0.46
1:A:278:ILE:N	1:A:278:ILE:CD1	2.78	0.46
1:A:278:ILE:H	1:A:278:ILE:CD1	2.29	0.46
1:B:624:ASN:O	1:B:625:ARG:C	2.55	0.46
1:C:674:ARG:HG3	1:C:690:TYR:OH	2.15	0.46
1:D:299:GLU:O	1:D:300:ASN:C	2.54	0.46
1:E:71:ILE:O	1:E:74:GLY:N	2.49	0.46
1:E:331:LYS:HG3	1:E:397:HIS:O	2.15	0.46
1:E:659:ARG:NH1	1:E:707:HIS:CG	2.84	0.46
1:F:63:ILE:CD1	1:F:63:ILE:N	2.79	0.46
1:A:353:ILE:HG22	1:A:353:ILE:O	2.14	0.46
1:B:261:ARG:HG3	1:B:261:ARG:NH1	2.31	0.46
1:B:284:HIS:HB3	1:C:101:LYS:HA	1.98	0.46
1:B:596:TYR:O	1:B:600:VAL:HG23	2.16	0.46
1:B:609:ASP:OD2	1:B:609:ASP:N	2.48	0.46
1:D:674:ARG:HG3	1:D:690:TYR:OH	2.15	0.46
1:E:41:MET:O	1:E:45:LEU:HB2	2.15	0.46
1:E:157:PHE:N	1:E:157:PHE:CD2	2.84	0.46
1:E:199:GLN:HE21	1:E:199:GLN:CA	2.07	0.46
1:E:531:LEU:HD22	1:E:550:ARG:HB3	1.97	0.46
1:F:268:GLU:OE1	1:F:322:HIS:HE1	2.00	0.46
1:F:379:VAL:CG2	1:F:411:ILE:HD11	2.45	0.46
1:F:399:LEU:HA	1:F:404:ALA:HB1	1.97	0.46
1:F:423:GLU:C	1:F:424:ILE:HD12	2.37	0.46
1:A:6:PHE:O	1:A:8:ALA:N	2.49	0.45
1:A:399:LEU:HB2	1:A:405:PRO:O	2.16	0.45
1:B:20:ILE:CD1	1:B:20:ILE:N	2.75	0.45
1:C:581:ASN:O	1:C:582:GLU:C	2.54	0.45
1:D:71:ILE:O	1:D:72:ALA:C	2.53	0.45
1:D:151:ASP:O	1:D:153:SER:N	2.49	0.45
1:E:374:ASN:O	1:E:375:VAL:C	2.53	0.45
1:E:399:LEU:HA	1:E:404:ALA:HB1	1.98	0.45
1:F:262:VAL:O	1:F:265:PHE:N	2.49	0.45
1:F:482:CYS:O	1:F:483:ALA:C	2.53	0.45
1:F:695:ARG:HG2	1:F:695:ARG:NH1	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD22	1:A:417:LEU:HD23	1.99	0.45
1:B:201:PHE:CZ	1:B:518:ILE:HD13	2.51	0.45
1:B:229:ARG:HG3	1:B:229:ARG:HH11	1.82	0.45
1:B:266:MET:O	1:B:267:LYS:C	2.54	0.45
1:B:486:MET:O	1:B:487:ILE:C	2.55	0.45
1:D:379:VAL:CG2	1:D:411:ILE:HD11	2.47	0.45
1:E:665:VAL:O	1:E:666:LEU:C	2.53	0.45
1:F:120:GLY:O	1:F:122:LEU:N	2.49	0.45
1:F:378:MET:HG3	1:F:493:MET:HA	1.99	0.45
1:F:481:ASN:O	1:F:482:CYS:C	2.54	0.45
1:A:21:THR:O	1:A:22:THR:CB	2.65	0.45
1:A:230:PRO:O	1:A:233:ARG:N	2.49	0.45
1:A:529:SER:O	1:A:530:GLU:C	2.54	0.45
1:B:191:ASP:O	1:B:192:LYS:C	2.54	0.45
1:B:268:GLU:OE1	1:B:322:HIS:HE1	1.99	0.45
1:B:379:VAL:CG2	1:B:411:ILE:HD11	2.47	0.45
1:D:285:ASN:HA	1:D:292:PHE:HA	1.98	0.45
1:D:488:ALA:O	1:D:489:ILE:C	2.54	0.45
1:E:68:ALA:O	1:E:71:ILE:N	2.49	0.45
1:E:72:ALA:CB	1:E:120:GLY:HA2	2.46	0.45
1:E:504:VAL:O	1:E:504:VAL:HG13	2.16	0.45
1:E:688:PHE:O	1:E:689:ALA:C	2.55	0.45
1:F:659:ARG:HG3	1:F:659:ARG:HH21	1.81	0.45
1:A:200:LEU:C	1:A:201:PHE:CD2	2.90	0.45
1:A:303:LEU:O	1:A:304:ALA:C	2.55	0.45
1:A:336:VAL:O	1:A:337:ASN:C	2.55	0.45
1:B:53:VAL:HG22	1:B:71:ILE:CD1	2.46	0.45
1:B:665:VAL:O	1:B:666:LEU:C	2.54	0.45
1:C:581:ASN:OD1	1:C:584:GLU:HG3	2.17	0.45
1:C:624:ASN:O	1:C:625:ARG:C	2.53	0.45
1:C:630:LEU:CD2	1:C:649:ARG:HG2	2.40	0.45
1:D:596:TYR:CZ	1:D:600:VAL:HG21	2.52	0.45
1:E:38:ARG:C	1:E:40:LYS:N	2.69	0.45
1:A:704:HIS:O	1:A:707:HIS:N	2.49	0.45
1:C:110:GLU:C	1:C:112:GLY:H	2.20	0.45
1:C:565:TYR:HB2	1:C:589:LEU:HD13	1.98	0.45
1:C:688:PHE:O	1:C:689:ALA:C	2.55	0.45
1:C:727:PHE:O	1:C:728:THR:O	2.33	0.45
1:D:150:TRP:CD1	1:D:151:ASP:N	2.84	0.45
1:D:261:ARG:HG3	1:D:261:ARG:NH1	2.31	0.45
1:E:422:ASP:C	1:E:424:ILE:N	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:GLN:C	1:F:201:PHE:H	2.20	0.45
1:A:38:ARG:HA	1:A:41:MET:HB2	1.98	0.45
1:A:182:PRO:O	1:A:183:LEU:C	2.54	0.45
1:A:284:HIS:CB	1:B:101:LYS:HA	2.43	0.45
1:A:408:ILE:HG12	1:A:554:ASN:HB2	1.99	0.45
1:A:459:ASN:O	1:A:460:ARG:O	2.35	0.45
1:B:207:ARG:HB2	1:B:207:ARG:NH1	2.30	0.45
1:C:199:GLN:C	1:C:201:PHE:H	2.20	0.45
1:C:422:ASP:O	1:C:424:ILE:N	2.49	0.45
1:D:10:GLN:HG2	1:E:7:PHE:CD2	2.51	0.45
1:D:503:SER:C	1:D:505:ASP:H	2.20	0.45
1:D:695:ARG:HG2	1:D:695:ARG:NH1	2.29	0.45
1:E:409:LEU:HA	1:E:463:PRO:HG2	1.99	0.45
1:E:584:GLU:O	1:E:587:CYS:N	2.50	0.45
1:F:422:ASP:C	1:F:424:ILE:N	2.69	0.45
1:A:21:THR:O	1:A:22:THR:HB	2.17	0.45
1:A:330:GLU:HG3	1:A:395:ASN:HA	1.99	0.45
1:B:38:ARG:C	1:B:40:LYS:N	2.69	0.45
1:B:231:ASP:OD2	1:B:231:ASP:N	2.48	0.45
1:C:201:PHE:CZ	1:C:518:ILE:HD13	2.51	0.45
1:C:676:VAL:O	1:C:677:ALA:C	2.54	0.45
1:D:41:MET:O	1:D:45:LEU:HB2	2.17	0.45
1:D:72:ALA:CB	1:D:120:GLY:HA2	2.46	0.45
1:D:183:LEU:HA	1:D:487:ILE:HG12	1.99	0.45
1:D:497:LEU:C	1:D:499:GLU:N	2.70	0.45
1:E:53:VAL:HG22	1:E:71:ILE:HD11	1.98	0.45
1:E:58:GLU:C	1:E:60:GLY:H	2.20	0.45
1:E:183:LEU:HA	1:E:487:ILE:HG12	1.98	0.45
1:E:341:LYS:HB3	1:E:477:GLY:O	2.17	0.45
1:E:378:MET:HG3	1:E:493:MET:HA	1.99	0.45
1:E:379:VAL:CG2	1:E:411:ILE:HD11	2.46	0.45
1:F:71:ILE:O	1:F:72:ALA:C	2.55	0.45
1:F:110:GLU:C	1:F:112:GLY:H	2.20	0.45
1:A:58:GLU:C	1:A:60:GLY:H	2.20	0.45
1:A:181:THR:O	1:A:182:PRO:C	2.55	0.45
1:A:354:ASN:CB	1:A:357:ALA:HB2	2.46	0.45
1:A:726:LEU:HB2	1:A:727:PHE:CD2	2.52	0.45
1:B:374:ASN:O	1:B:375:VAL:C	2.54	0.45
1:B:727:PHE:O	1:B:728:THR:O	2.35	0.45
1:C:169:PHE:O	1:C:170:ILE:HD13	2.17	0.45
1:C:386:LEU:C	1:C:388:ALA:N	2.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:584:GLU:O	1:C:587:CYS:N	2.50	0.45
1:D:201:PHE:CZ	1:D:518:ILE:HD13	2.51	0.45
1:D:414:GLY:O	1:D:415:SER:C	2.54	0.45
1:E:309:GLN:OE1	1:E:309:GLN:HA	2.17	0.45
1:E:359:GLY:O	1:E:360:LYS:O	2.35	0.45
1:A:53:VAL:HG22	1:A:71:ILE:HD13	1.99	0.45
1:A:373:VAL:HG22	1:A:526:ILE:CD1	2.46	0.45
1:A:387:ARG:HG2	1:A:391:MET:CE	2.47	0.45
1:A:412:PHE:CD2	1:A:412:PHE:C	2.90	0.45
1:A:616:VAL:HG13	1:A:660:VAL:HG23	1.98	0.45
1:B:151:ASP:O	1:B:153:SER:N	2.50	0.45
1:B:581:ASN:OD1	1:B:584:GLU:HG3	2.16	0.45
1:C:71:ILE:O	1:C:72:ALA:C	2.55	0.45
1:C:71:ILE:O	1:C:74:GLY:N	2.50	0.45
1:C:182:PRO:HB2	1:C:487:ILE:HD13	1.99	0.45
1:C:227:ASN:C	1:C:229:ARG:H	2.21	0.45
1:D:151:ASP:C	1:D:153:SER:N	2.70	0.45
1:D:199:GLN:C	1:D:201:PHE:H	2.21	0.45
1:E:266:MET:O	1:E:267:LYS:C	2.56	0.45
1:E:286:GLU:CB	1:E:291:GLN:HG2	2.46	0.45
1:E:497:LEU:C	1:E:499:GLU:N	2.70	0.45
1:F:359:GLY:O	1:F:360:LYS:O	2.35	0.45
1:A:27:LEU:O	1:A:28:SER:C	2.55	0.45
1:B:358:PRO:HD3	1:B:368:PHE:CE2	2.52	0.45
1:D:202:ASP:C	1:D:202:ASP:OD2	2.55	0.45
1:D:530:GLU:O	1:D:531:LEU:C	2.56	0.45
1:E:6:PHE:C	1:E:8:ALA:N	2.69	0.45
1:E:110:GLU:C	1:E:112:GLY:H	2.21	0.45
1:E:229:ARG:HG3	1:E:229:ARG:HH11	1.82	0.45
1:E:390:ILE:C	1:E:390:ILE:HD12	2.38	0.45
1:F:488:ALA:O	1:F:489:ILE:C	2.55	0.45
1:A:36:PHE:HB2	1:A:78:TRP:CZ3	2.52	0.44
1:A:50:TYR:O	1:A:52:ALA:N	2.50	0.44
1:A:382:ASN:ND2	1:A:492:ALA:HB1	2.32	0.44
1:A:562:LEU:O	1:A:563:MET:C	2.54	0.44
1:B:415:SER:O	1:B:418:SER:HB3	2.16	0.44
1:B:422:ASP:C	1:B:424:ILE:N	2.70	0.44
1:B:530:GLU:O	1:B:531:LEU:C	2.55	0.44
1:C:183:LEU:HA	1:C:487:ILE:HG12	1.99	0.44
1:C:285:ASN:HA	1:C:292:PHE:HA	2.00	0.44
1:C:341:LYS:HB3	1:C:477:GLY:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:GLY:O	1:C:360:LYS:O	2.35	0.44
1:D:182:PRO:HB2	1:D:487:ILE:HD13	1.99	0.44
1:D:400:GLY:O	1:D:401:ALA:HB2	2.17	0.44
1:E:201:PHE:CZ	1:E:518:ILE:HD13	2.52	0.44
1:F:72:ALA:CB	1:F:120:GLY:HA2	2.48	0.44
1:F:202:ASP:C	1:F:202:ASP:OD2	2.55	0.44
1:F:341:LYS:HB3	1:F:477:GLY:O	2.16	0.44
1:F:672:GLU:O	1:F:673:ALA:C	2.55	0.44
1:A:382:ASN:HD22	1:A:492:ALA:HB1	1.82	0.44
1:A:504:VAL:O	1:A:504:VAL:HG22	2.17	0.44
1:A:567:ASP:O	1:A:567:ASP:OD1	2.35	0.44
1:B:11:GLU:HG3	1:B:15:ARG:NH1	2.30	0.44
1:B:531:LEU:HD22	1:B:550:ARG:HB3	1.98	0.44
1:B:584:GLU:O	1:B:585:LEU:C	2.56	0.44
1:B:695:ARG:HG2	1:B:695:ARG:NH1	2.31	0.44
1:C:309:GLN:OE1	1:C:309:GLN:HA	2.16	0.44
1:C:620:VAL:O	1:C:621:SER:C	2.55	0.44
1:D:169:PHE:CB	1:D:178:ASP:HB3	2.48	0.44
1:D:626:LEU:O	1:D:629:ASN:HB3	2.16	0.44
1:E:202:ASP:OD2	1:E:204:ASN:HB2	2.17	0.44
1:E:237:ARG:HD3	1:E:603:GLU:OE1	2.17	0.44
1:E:285:ASN:HA	1:E:292:PHE:HA	1.99	0.44
1:E:423:GLU:C	1:E:424:ILE:HD12	2.38	0.44
1:F:92:GLN:HG2	1:F:92:GLN:O	2.18	0.44
1:F:227:ASN:C	1:F:229:ARG:H	2.21	0.44
1:A:8:ALA:HB1	1:A:225:LEU:HD23	1.99	0.44
1:A:297:ILE:O	1:A:298:PHE:C	2.55	0.44
1:B:237:ARG:HD3	1:B:603:GLU:OE1	2.17	0.44
1:C:41:MET:O	1:C:45:LEU:HB2	2.17	0.44
1:C:215:GLU:OE1	4:C:4001:ADP:O3A	2.36	0.44
1:C:695:ARG:HG2	1:C:695:ARG:NH1	2.29	0.44
1:D:534:PHE:CG	1:D:535:GLU:N	2.85	0.44
1:D:630:LEU:CD2	1:D:649:ARG:HG2	2.41	0.44
1:E:596:TYR:CZ	1:E:600:VAL:HG21	2.53	0.44
1:F:285:ASN:HA	1:F:292:PHE:HA	1.99	0.44
1:F:624:ASN:O	1:F:625:ARG:C	2.55	0.44
1:F:636:ILE:O	1:F:636:ILE:CG2	2.65	0.44
1:A:181:THR:HB	1:A:182:PRO:CD	2.44	0.44
1:A:219:PHE:HB2	1:A:327:LEU:HB2	2.00	0.44
1:A:269:LEU:HA	1:A:318:ILE:HD13	1.99	0.44
1:A:386:LEU:O	1:A:387:ARG:C	2.54	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:HG2	1:C:7:PHE:CG	2.52	0.44
1:B:58:GLU:C	1:B:60:GLY:H	2.21	0.44
1:B:182:PRO:HB2	1:B:487:ILE:HD13	1.98	0.44
1:B:227:ASN:C	1:B:229:ARG:H	2.21	0.44
1:C:157:PHE:CD2	1:C:157:PHE:N	2.86	0.44
1:C:486:MET:O	1:C:487:ILE:C	2.56	0.44
1:D:87:TYR:CE2	1:D:103:ASP:HB2	2.53	0.44
1:D:268:GLU:OE1	1:D:322:HIS:HE1	2.00	0.44
1:F:195:THR:HG21	1:F:206:THR:O	2.17	0.44
1:F:284:HIS:NE2	1:F:293:GLU:OE2	2.50	0.44
1:F:414:GLY:O	1:F:415:SER:C	2.55	0.44
1:F:581:ASN:O	1:F:584:GLU:N	2.50	0.44
1:F:581:ASN:O	1:F:582:GLU:C	2.56	0.44
1:A:219:PHE:HE1	1:A:291:GLN:NE2	2.16	0.44
1:A:260:PRO:O	1:A:261:ARG:C	2.55	0.44
1:A:358:PRO:HB3	1:A:368:PHE:HE1	1.75	0.44
1:B:110:GLU:C	1:B:112:GLY:H	2.21	0.44
1:B:202:ASP:C	1:B:202:ASP:OD2	2.56	0.44
1:B:285:ASN:HA	1:B:292:PHE:HA	1.99	0.44
1:C:6:PHE:C	1:C:8:ALA:N	2.68	0.44
1:C:268:GLU:OE1	1:C:322:HIS:HE1	2.01	0.44
1:D:10:GLN:HG2	1:E:7:PHE:CG	2.52	0.44
1:D:581:ASN:O	1:D:584:GLU:N	2.51	0.44
1:F:266:MET:O	1:F:267:LYS:C	2.56	0.44
1:F:415:SER:O	1:F:418:SER:HB3	2.18	0.44
1:F:530:GLU:O	1:F:531:LEU:C	2.55	0.44
1:F:584:GLU:O	1:F:585:LEU:C	2.56	0.44
1:A:22:THR:O	1:A:23:PRO:C	2.56	0.44
1:B:151:ASP:C	1:B:153:SER:N	2.71	0.44
1:B:183:LEU:HA	1:B:487:ILE:HG12	2.00	0.44
1:B:223:THR:O	1:B:226:TYR:HB3	2.18	0.44
1:C:415:SER:O	1:C:418:SER:HB3	2.17	0.44
1:D:268:GLU:O	1:D:269:LEU:C	2.56	0.44
1:D:309:GLN:OE1	1:D:309:GLN:HA	2.17	0.44
1:D:495:ASN:O	1:D:497:LEU:N	2.51	0.44
1:D:727:PHE:O	1:D:728:THR:O	2.35	0.44
1:E:15:ARG:HH21	1:E:15:ARG:HG3	1.83	0.44
1:E:581:ASN:OD1	1:E:584:GLU:HG3	2.16	0.44
1:F:87:TYR:CE2	1:F:103:ASP:HB2	2.53	0.44
1:F:581:ASN:OD1	1:F:584:GLU:HG3	2.18	0.44
1:A:27:LEU:C	1:A:29:ASP:N	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:HIS:O	1:A:308:ASN:C	2.55	0.44
1:B:387:ARG:NH1	1:B:387:ARG:HG3	2.32	0.44
1:B:423:GLU:C	1:B:424:ILE:HD12	2.38	0.44
1:B:503:SER:C	1:B:505:ASP:H	2.20	0.44
1:B:581:ASN:O	1:B:584:GLU:N	2.51	0.44
1:C:202:ASP:OD2	1:C:204:ASN:HB2	2.18	0.44
1:C:232:LEU:HD12	1:C:232:LEU:HA	1.84	0.44
1:C:618:ILE:O	1:C:619:ALA:C	2.56	0.44
1:D:120:GLY:O	1:D:122:LEU:N	2.51	0.44
1:E:71:ILE:O	1:E:72:ALA:C	2.55	0.44
1:E:169:PHE:O	1:E:170:ILE:HD13	2.17	0.44
1:E:205:ILE:O	1:E:205:ILE:HG22	2.18	0.44
1:E:422:ASP:O	1:E:424:ILE:N	2.51	0.44
1:E:584:GLU:O	1:E:585:LEU:C	2.55	0.44
1:F:68:ALA:O	1:F:71:ILE:N	2.50	0.44
1:F:182:PRO:HB2	1:F:487:ILE:HD13	1.98	0.44
1:A:356:PHE:CE2	1:A:471:PHE:HD2	2.36	0.44
1:B:205:ILE:O	1:B:205:ILE:HG22	2.18	0.44
1:B:309:GLN:OE1	1:B:309:GLN:HA	2.18	0.44
1:B:400:GLY:O	1:B:401:ALA:HB2	2.18	0.44
1:B:676:VAL:CG2	1:B:677:ALA:N	2.80	0.44
1:C:233:ARG:CG	1:C:233:ARG:NH1	2.81	0.44
1:C:596:TYR:O	1:C:600:VAL:HG23	2.18	0.44
1:C:659:ARG:NH1	1:C:707:HIS:CG	2.85	0.44
1:D:157:PHE:N	1:D:157:PHE:CD2	2.86	0.44
1:D:199:GLN:HE21	1:D:199:GLN:CA	2.09	0.44
1:E:92:GLN:HG2	1:E:92:GLN:O	2.17	0.44
1:E:268:GLU:O	1:E:269:LEU:C	2.55	0.44
1:E:581:ASN:O	1:E:582:GLU:C	2.56	0.44
1:F:58:GLU:C	1:F:60:GLY:H	2.21	0.44
1:A:50:TYR:C	1:A:52:ALA:H	2.21	0.44
1:B:534:PHE:CG	1:B:535:GLU:N	2.86	0.44
1:C:53:VAL:HG22	1:C:71:ILE:HD11	2.00	0.44
1:C:422:ASP:C	1:C:424:ILE:N	2.69	0.44
1:C:630:LEU:O	1:C:632:ARG:N	2.51	0.44
1:D:195:THR:HG21	1:D:206:THR:O	2.18	0.44
1:D:262:VAL:O	1:D:265:PHE:N	2.51	0.44
1:D:374:ASN:O	1:D:375:VAL:C	2.56	0.44
1:D:415:SER:O	1:D:418:SER:HB3	2.17	0.44
1:E:63:ILE:H	1:E:63:ILE:CD1	2.12	0.44
1:F:286:GLU:CB	1:F:291:GLN:HG2	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:GLU:O	1:F:300:ASN:C	2.54	0.44
1:F:596:TYR:CZ	1:F:600:VAL:HG21	2.53	0.44
1:A:262:VAL:O	1:A:265:PHE:HB3	2.18	0.43
1:A:266:MET:H	1:A:266:MET:HG2	1.37	0.43
1:B:15:ARG:HG3	1:B:15:ARG:HH21	1.83	0.43
1:B:386:LEU:C	1:B:388:ALA:N	2.71	0.43
1:C:581:ASN:O	1:C:584:GLU:N	2.51	0.43
1:C:695:ARG:N	1:C:696:PRO:CD	2.81	0.43
1:D:286:GLU:CB	1:D:291:GLN:HG2	2.48	0.43
1:E:406:PRO:O	1:E:408:ILE:N	2.49	0.43
1:E:534:PHE:CG	1:E:535:GLU:N	2.86	0.43
1:E:618:ILE:O	1:E:619:ALA:C	2.56	0.43
1:E:659:ARG:HG3	1:E:659:ARG:HH21	1.83	0.43
1:F:201:PHE:CZ	1:F:518:ILE:HD13	2.52	0.43
1:F:358:PRO:HD3	1:F:368:PHE:CE2	2.52	0.43
1:F:609:ASP:OD2	1:F:609:ASP:N	2.51	0.43
1:A:262:VAL:O	1:A:263:THR:C	2.55	0.43
1:A:638:SER:C	1:A:640:GLU:N	2.71	0.43
1:A:659:ARG:NH1	1:A:707:HIS:CG	2.85	0.43
1:B:286:GLU:CB	1:B:291:GLN:HG2	2.48	0.43
1:B:616:VAL:HB	1:B:617:PRO:CD	2.42	0.43
1:C:598:MET:O	1:C:602:ILE:HD13	2.18	0.43
1:D:92:GLN:O	1:D:92:GLN:HG2	2.19	0.43
1:D:195:THR:O	1:D:198:CYS:HB2	2.18	0.43
1:D:237:ARG:HD3	1:D:603:GLU:OE1	2.17	0.43
1:E:199:GLN:C	1:E:201:PHE:H	2.21	0.43
1:F:534:PHE:CG	1:F:535:GLU:N	2.87	0.43
1:A:283:ARG:HH21	1:A:283:ARG:HG3	1.83	0.43
1:A:713:ASP:O	1:A:715:GLU:N	2.52	0.43
1:B:632:ARG:HD3	1:C:628:GLU:HA	1.99	0.43
1:B:675:LYS:O	1:B:676:VAL:C	2.57	0.43
1:C:169:PHE:CB	1:C:178:ASP:HB3	2.48	0.43
1:C:284:HIS:NE2	1:C:293:GLU:OE2	2.52	0.43
1:C:409:LEU:HA	1:C:463:PRO:HG2	2.01	0.43
1:C:609:ASP:OD2	1:C:609:ASP:N	2.50	0.43
1:D:620:VAL:O	1:D:621:SER:C	2.56	0.43
1:E:151:ASP:C	1:E:153:SER:N	2.72	0.43
1:F:9:LEU:HD23	1:F:225:LEU:HD21	2.01	0.43
1:F:223:THR:O	1:F:226:TYR:HB3	2.19	0.43
1:A:68:ALA:O	1:A:71:ILE:N	2.51	0.43
1:A:102:HIS:HB2	1:F:283:ARG:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:SER:C	1:A:505:ASP:N	2.71	0.43
1:A:652:LEU:HA	1:A:655:GLU:HB3	2.00	0.43
1:B:378:MET:HG3	1:B:493:MET:HA	2.01	0.43
1:B:497:LEU:C	1:B:499:GLU:N	2.71	0.43
1:B:565:TYR:HB2	1:B:589:LEU:HD13	1.99	0.43
1:B:620:VAL:O	1:B:621:SER:C	2.57	0.43
1:C:400:GLY:O	1:C:401:ALA:HB2	2.18	0.43
1:C:559:PRO:O	1:C:560:GLU:C	2.57	0.43
1:D:41:MET:SD	1:D:53:VAL:HG11	2.59	0.43
1:D:409:LEU:HA	1:D:463:PRO:HG2	2.01	0.43
1:E:268:GLU:OE1	1:E:322:HIS:HE1	2.01	0.43
1:F:229:ARG:HG3	1:F:229:ARG:HH11	1.84	0.43
1:F:503:SER:C	1:F:505:ASP:H	2.21	0.43
1:A:186:ALA:HA	1:A:579:ILE:CD1	2.49	0.43
1:A:385:LEU:HD21	1:A:574:LEU:HD11	2.01	0.43
1:B:75:MET:O	1:B:78:TRP:HB3	2.19	0.43
1:C:41:MET:SD	1:C:53:VAL:HG11	2.58	0.43
1:C:497:LEU:C	1:C:499:GLU:N	2.72	0.43
1:C:534:PHE:CG	1:C:535:GLU:N	2.86	0.43
1:C:584:GLU:O	1:C:585:LEU:C	2.56	0.43
1:C:638:SER:O	1:C:641:GLU:N	2.51	0.43
1:D:58:GLU:C	1:D:60:GLY:H	2.21	0.43
1:D:282:THR:HA	1:E:102:HIS:O	2.19	0.43
1:D:284:HIS:NE2	1:D:293:GLU:OE2	2.51	0.43
1:D:359:GLY:O	1:D:360:LYS:O	2.35	0.43
1:D:636:ILE:O	1:D:636:ILE:CG2	2.66	0.43
1:F:709:GLU:HG3	1:F:717:TRP:CE2	2.54	0.43
1:A:482:CYS:O	1:A:483:ALA:C	2.54	0.43
1:A:669:ASP:HB3	1:A:697:TYR:OH	2.19	0.43
1:B:92:GLN:O	1:B:92:GLN:HG2	2.19	0.43
1:B:359:GLY:O	1:B:360:LYS:O	2.35	0.43
1:B:636:ILE:O	1:B:636:ILE:CG2	2.65	0.43
1:C:652:LEU:HA	1:C:655:GLU:HB3	2.00	0.43
1:D:9:LEU:HD23	1:D:225:LEU:HD21	2.00	0.43
1:D:38:ARG:C	1:D:40:LYS:N	2.69	0.43
1:D:368:PHE:O	1:D:369:LEU:C	2.56	0.43
1:E:211:ASN:ND2	1:E:348:CYS:HB2	2.33	0.43
1:E:415:SER:O	1:E:418:SER:HB3	2.18	0.43
1:F:15:ARG:HH21	1:F:15:ARG:HG3	1.83	0.43
1:F:206:THR:N	1:F:350:ASP:OD2	2.51	0.43
1:A:387:ARG:HG3	1:A:387:ARG:NH1	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ALA:O	1:A:550:ARG:N	2.52	0.43
1:B:36:PHE:HB2	1:B:78:TRP:CZ3	2.53	0.43
1:B:284:HIS:NE2	1:B:293:GLU:OE2	2.51	0.43
1:B:504:VAL:O	1:B:504:VAL:HG13	2.17	0.43
1:B:648:ASP:O	1:B:649:ARG:C	2.57	0.43
1:C:72:ALA:CB	1:C:120:GLY:HA2	2.47	0.43
1:C:199:GLN:O	1:C:201:PHE:N	2.52	0.43
1:C:377:MET:HE2	1:C:377:MET:HA	2.00	0.43
1:D:11:GLU:HG3	1:D:15:ARG:NH1	2.29	0.43
1:D:386:LEU:C	1:D:388:ALA:N	2.71	0.43
1:D:422:ASP:C	1:D:424:ILE:N	2.71	0.43
1:D:618:ILE:O	1:D:619:ALA:C	2.57	0.43
1:E:182:PRO:HB3	1:E:580:PHE:CZ	2.54	0.43
1:E:486:MET:O	1:E:487:ILE:C	2.57	0.43
1:E:563:MET:CE	1:E:684:LYS:HD2	2.48	0.43
1:F:157:PHE:CD2	1:F:157:PHE:N	2.86	0.43
1:F:268:GLU:O	1:F:269:LEU:C	2.55	0.43
1:F:412:PHE:HD2	1:F:412:PHE:O	2.01	0.43
1:F:652:LEU:HA	1:F:655:GLU:HB3	2.01	0.43
1:B:53:VAL:HG22	1:B:71:ILE:HD11	2.01	0.43
1:B:89:HIS:CB	1:B:167:THR:HG21	2.48	0.43
1:B:199:GLN:HE21	1:B:199:GLN:CA	2.08	0.43
1:B:409:LEU:HA	1:B:463:PRO:HG2	2.01	0.43
1:B:652:LEU:HA	1:B:655:GLU:HB3	2.01	0.43
1:C:92:GLN:HG2	1:C:92:GLN:O	2.19	0.43
1:C:636:ILE:HD11	1:D:631:CYS:HB2	2.01	0.43
1:C:676:VAL:CG2	1:C:677:ALA:N	2.82	0.43
1:D:341:LYS:HB3	1:D:477:GLY:O	2.19	0.43
1:D:390:ILE:C	1:D:390:ILE:HD12	2.39	0.43
1:D:584:GLU:O	1:D:585:LEU:C	2.57	0.43
1:D:675:LYS:O	1:D:676:VAL:C	2.57	0.43
1:E:169:PHE:CB	1:E:178:ASP:HB3	2.49	0.43
1:E:652:LEU:HA	1:E:655:GLU:HB3	1.99	0.43
1:F:54:VAL:HA	1:F:57:THR:CG2	2.46	0.43
1:F:412:PHE:C	1:F:412:PHE:HD2	2.18	0.43
1:F:663:ILE:O	1:F:664:LYS:C	2.56	0.43
1:A:76:LYS:O	1:A:77:SER:C	2.57	0.43
1:A:101:LYS:O	1:A:102:HIS:CD2	2.72	0.43
1:A:648:ASP:O	1:A:649:ARG:C	2.57	0.43
1:B:157:PHE:N	1:B:157:PHE:CD2	2.87	0.43
1:B:368:PHE:O	1:B:369:LEU:C	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LYS:O	1:B:527:ILE:HG12	2.19	0.43
1:B:659:ARG:NH1	1:B:707:HIS:CG	2.86	0.43
1:C:262:VAL:O	1:C:265:PHE:N	2.51	0.43
1:D:202:ASP:OD2	1:D:204:ASN:HB2	2.19	0.43
1:D:358:PRO:HD3	1:D:368:PHE:CE2	2.52	0.43
1:D:690:TYR:O	1:D:691:GLU:C	2.57	0.43
1:E:89:HIS:CB	1:E:167:THR:HG21	2.49	0.43
1:E:206:THR:O	1:E:207:ARG:HG3	2.19	0.43
1:E:356:PHE:CE2	1:E:471:PHE:HD2	2.37	0.43
1:E:559:PRO:O	1:E:560:GLU:C	2.57	0.43
1:E:581:ASN:O	1:E:584:GLU:N	2.51	0.43
1:E:620:VAL:O	1:E:621:SER:C	2.57	0.43
1:E:695:ARG:N	1:E:696:PRO:CD	2.82	0.43
1:F:20:ILE:O	1:F:21:THR:CG2	2.57	0.43
1:F:237:ARG:HD3	1:F:603:GLU:OE1	2.19	0.43
1:F:409:LEU:HA	1:F:463:PRO:HG2	2.00	0.43
1:A:7:PHE:CG	1:F:10:GLN:HG2	2.54	0.43
1:A:414:GLY:O	1:A:415:SER:C	2.56	0.43
1:A:688:PHE:O	1:A:692:GLU:HB2	2.18	0.43
1:B:598:MET:O	1:B:602:ILE:HD13	2.19	0.43
1:B:709:GLU:HG3	1:B:717:TRP:CE2	2.54	0.43
1:C:15:ARG:HH21	1:C:15:ARG:HG3	1.83	0.43
1:C:58:GLU:C	1:C:60:GLY:H	2.22	0.43
1:C:195:THR:HG21	1:C:206:THR:O	2.19	0.43
1:C:563:MET:CE	1:C:684:LYS:HD2	2.49	0.43
1:D:89:HIS:CB	1:D:167:THR:HG21	2.49	0.43
1:D:215:GLU:OE1	4:D:4001:ADP:O3A	2.37	0.43
1:D:229:ARG:HG3	1:D:229:ARG:HH11	1.84	0.43
1:D:422:ASP:O	1:D:424:ILE:N	2.51	0.43
1:D:581:ASN:OD1	1:D:584:GLU:HG3	2.19	0.43
1:E:299:GLU:O	1:E:300:ASN:C	2.56	0.43
1:F:206:THR:O	1:F:207:ARG:HG3	2.19	0.43
1:A:151:ASP:O	1:A:152:GLY:C	2.57	0.42
1:A:495:ASN:O	1:A:497:LEU:N	2.52	0.42
1:A:606:VAL:HG12	1:A:607:LEU:N	2.33	0.42
1:A:616:VAL:CB	1:A:617:PRO:HD3	2.44	0.42
1:B:304:ALA:O	1:B:307:HIS:HB2	2.19	0.42
1:B:627:LEU:CD2	1:B:653:ILE:HD13	2.43	0.42
1:C:205:ILE:O	1:C:205:ILE:HG22	2.18	0.42
1:C:503:SER:C	1:C:505:ASP:H	2.21	0.42
1:C:613:ASN:O	1:C:617:PRO:HG2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASN:ND2	1:D:348:CYS:HB2	2.34	0.42
1:D:596:TYR:O	1:D:600:VAL:HG23	2.19	0.42
1:E:10:GLN:HG2	1:F:7:PHE:CD2	2.54	0.42
1:E:87:TYR:CE2	1:E:103:ASP:HB2	2.54	0.42
1:E:377:MET:HE2	1:E:377:MET:HA	2.00	0.42
1:E:497:LEU:O	1:E:499:GLU:N	2.52	0.42
1:E:690:TYR:O	1:E:691:GLU:C	2.58	0.42
1:F:377:MET:HE2	1:F:377:MET:HA	2.01	0.42
1:F:481:ASN:C	1:F:481:ASN:ND2	2.72	0.42
1:A:341:LYS:HB3	1:A:477:GLY:O	2.19	0.42
1:A:423:GLU:O	1:A:424:ILE:HG13	2.19	0.42
1:A:652:LEU:O	1:A:653:ILE:C	2.57	0.42
1:B:120:GLY:O	1:B:122:LEU:N	2.52	0.42
1:B:193:ALA:HA	1:B:498:ASN:HD21	1.84	0.42
1:B:199:GLN:C	1:B:201:PHE:H	2.21	0.42
1:B:237:ARG:O	1:B:237:ARG:HG3	2.18	0.42
1:B:413:LEU:HD22	1:B:417:LEU:HD23	2.00	0.42
1:B:584:GLU:O	1:B:587:CYS:N	2.52	0.42
1:B:674:ARG:HG3	1:B:690:TYR:OH	2.18	0.42
1:D:6:PHE:C	1:D:8:ALA:N	2.69	0.42
1:D:616:VAL:HB	1:D:617:PRO:CD	2.42	0.42
1:D:628:GLU:OE2	1:D:632:ARG:NE	2.49	0.42
1:D:672:GLU:O	1:D:675:LYS:N	2.52	0.42
1:D:716:ILE:CG2	1:D:717:TRP:H	2.21	0.42
1:E:227:ASN:C	1:E:229:ARG:H	2.22	0.42
1:E:413:LEU:HD22	1:E:417:LEU:HD23	2.01	0.42
1:F:193:ALA:HA	1:F:498:ASN:HD21	1.85	0.42
1:F:576:GLY:C	1:F:578:ARG:H	2.22	0.42
1:F:690:TYR:O	1:F:692:GLU:N	2.52	0.42
1:A:664:LYS:NZ	1:F:649:ARG:NH2	2.67	0.42
1:B:56:ALA:HA	1:B:61:THR:H	1.84	0.42
1:B:195:THR:HG21	1:B:206:THR:O	2.19	0.42
1:C:378:MET:HG3	1:C:493:MET:HA	2.02	0.42
1:C:576:GLY:C	1:C:578:ARG:H	2.23	0.42
1:D:53:VAL:HG22	1:D:71:ILE:HD11	2.01	0.42
1:D:486:MET:O	1:D:487:ILE:C	2.58	0.42
1:D:663:ILE:O	1:D:664:LYS:C	2.58	0.42
1:E:400:GLY:O	1:E:401:ALA:HB2	2.19	0.42
1:E:503:SER:C	1:E:505:ASP:H	2.22	0.42
1:E:609:ASP:OD2	1:E:609:ASP:N	2.52	0.42
1:E:709:GLU:HB2	1:E:717:TRP:CZ2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:PRO:HB3	1:F:580:PHE:CZ	2.55	0.42
1:F:199:GLN:O	1:F:201:PHE:N	2.52	0.42
1:F:202:ASP:OD2	1:F:204:ASN:HB2	2.19	0.42
1:F:368:PHE:O	1:F:369:LEU:C	2.58	0.42
1:A:294:LEU:O	1:A:294:LEU:CG	2.67	0.42
1:A:469:ASN:O	1:A:470:ARG:CB	2.64	0.42
1:A:543:TRP:O	1:A:545:GLN:N	2.53	0.42
1:A:666:LEU:CD1	1:A:666:LEU:N	2.82	0.42
1:B:71:ILE:O	1:B:74:GLY:N	2.52	0.42
1:B:76:LYS:O	1:B:77:SER:C	2.58	0.42
1:B:598:MET:O	1:B:601:GLN:HB3	2.20	0.42
1:B:618:ILE:O	1:B:619:ALA:C	2.57	0.42
1:C:229:ARG:HG3	1:C:229:ARG:HH11	1.84	0.42
1:D:497:LEU:O	1:D:499:GLU:N	2.53	0.42
1:E:358:PRO:HD3	1:E:368:PHE:CE2	2.52	0.42
1:F:195:THR:O	1:F:198:CYS:HB2	2.19	0.42
1:F:205:ILE:HG22	1:F:205:ILE:O	2.19	0.42
1:F:598:MET:O	1:F:601:GLN:HB3	2.20	0.42
1:A:80:LYS:C	1:A:82:LEU:N	2.73	0.42
1:A:466:PHE:CZ	1:A:468:GLY:HA2	2.54	0.42
1:A:648:ASP:O	1:A:651:GLU:N	2.53	0.42
1:B:232:LEU:HD12	1:B:232:LEU:HA	1.84	0.42
1:B:356:PHE:CE2	1:B:471:PHE:HD2	2.38	0.42
1:C:206:THR:N	1:C:350:ASP:OD2	2.52	0.42
1:D:15:ARG:HH21	1:D:15:ARG:HG3	1.84	0.42
1:D:56:ALA:HA	1:D:61:THR:H	1.84	0.42
1:D:704:HIS:O	1:D:705:ILE:C	2.58	0.42
1:E:41:MET:SD	1:E:53:VAL:HG11	2.60	0.42
1:E:151:ASP:O	1:E:153:SER:N	2.51	0.42
1:E:386:LEU:C	1:E:388:ALA:N	2.73	0.42
1:F:584:GLU:O	1:F:588:ARG:HG2	2.20	0.42
1:A:300:ASN:HD21	1:A:303:LEU:HB2	1.84	0.42
1:A:358:PRO:HG2	1:A:359:GLY:H	1.85	0.42
1:A:415:SER:O	1:A:416:GLN:C	2.58	0.42
1:A:568:ASN:O	1:A:571:ARG:HB2	2.19	0.42
1:A:571:ARG:HH11	1:A:571:ARG:HG3	1.84	0.42
1:A:666:LEU:H	1:A:666:LEU:HD12	1.82	0.42
1:B:72:ALA:CB	1:B:120:GLY:HA2	2.47	0.42
1:B:202:ASP:OD2	1:B:204:ASN:HB2	2.19	0.42
1:B:206:THR:N	1:B:350:ASP:OD2	2.53	0.42
1:B:386:LEU:O	1:B:387:ARG:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:LEU:O	1:B:632:ARG:N	2.52	0.42
1:B:688:PHE:O	1:B:689:ALA:C	2.56	0.42
1:C:151:ASP:O	1:C:153:SER:N	2.53	0.42
1:C:358:PRO:HD3	1:C:368:PHE:CE2	2.54	0.42
1:C:522:LEU:HD21	1:C:526:ILE:HD11	2.02	0.42
1:D:182:PRO:HB3	1:D:580:PHE:CZ	2.54	0.42
1:D:378:MET:HG3	1:D:493:MET:HA	2.01	0.42
1:D:659:ARG:NH1	1:D:707:HIS:CG	2.87	0.42
1:E:237:ARG:O	1:E:237:ARG:HG3	2.19	0.42
1:E:622:TYR:O	1:E:625:ARG:HB3	2.19	0.42
1:F:151:ASP:C	1:F:153:SER:N	2.72	0.42
1:A:293:GLU:O	1:A:294:LEU:CB	2.68	0.42
1:A:405:PRO:HG3	1:A:474:ARG:HB2	2.00	0.42
1:A:683:PHE:CG	1:A:684:LYS:N	2.88	0.42
1:B:211:ASN:ND2	1:B:348:CYS:HB2	2.34	0.42
1:B:215:GLU:OE1	4:B:4001:ADP:O3A	2.38	0.42
1:C:75:MET:O	1:C:78:TRP:HB3	2.20	0.42
1:C:413:LEU:HD22	1:C:417:LEU:HD23	2.01	0.42
1:C:523:LYS:O	1:C:527:ILE:HG12	2.20	0.42
1:E:45:LEU:CD2	1:E:71:ILE:HA	2.50	0.42
1:E:195:THR:O	1:E:198:CYS:HB2	2.20	0.42
1:F:183:LEU:HA	1:F:487:ILE:HG12	2.00	0.42
1:A:69:ASP:N	1:A:120:GLY:HA3	2.35	0.42
1:A:103:ASP:OD2	1:F:282:THR:HG22	2.19	0.42
1:A:220:LEU:HD12	1:A:262:VAL:HG22	2.01	0.42
1:A:493:MET:O	1:A:494:ALA:C	2.58	0.42
1:A:581:ASN:ND2	1:A:584:GLU:HG3	2.35	0.42
1:A:690:TYR:O	1:A:691:GLU:C	2.58	0.42
1:B:182:PRO:HB3	1:B:580:PHE:CZ	2.55	0.42
1:C:56:ALA:HA	1:C:61:THR:H	1.84	0.42
1:C:87:TYR:CE2	1:C:103:ASP:HB2	2.55	0.42
1:C:120:GLY:O	1:C:122:LEU:N	2.52	0.42
1:C:181:THR:O	1:C:182:PRO:C	2.58	0.42
1:C:237:ARG:O	1:C:237:ARG:HG3	2.20	0.42
1:C:423:GLU:C	1:C:424:ILE:HD12	2.39	0.42
1:D:21:THR:O	1:D:22:THR:CB	2.67	0.42
1:D:169:PHE:O	1:D:170:ILE:HD13	2.20	0.42
1:E:195:THR:HG21	1:E:206:THR:O	2.20	0.42
1:F:386:LEU:C	1:F:388:ALA:N	2.72	0.42
1:F:690:TYR:O	1:F:691:GLU:C	2.57	0.42
1:F:717:TRP:HA	1:F:718:PRO:HD2	1.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:OD1	1:A:120:GLY:N	2.44	0.42
1:A:288:ALA:CB	1:A:336:VAL:HG23	2.50	0.42
1:A:382:ASN:O	1:A:386:LEU:HD13	2.19	0.42
1:B:181:THR:O	1:B:182:PRO:C	2.57	0.42
1:C:237:ARG:HD3	1:C:603:GLU:OE1	2.20	0.42
1:C:259:PRO:HG2	1:C:262:VAL:HB	2.02	0.42
1:C:266:MET:O	1:C:267:LYS:C	2.59	0.42
1:C:663:ILE:O	1:C:664:LYS:C	2.58	0.42
1:D:193:ALA:HA	1:D:498:ASN:HD21	1.84	0.42
1:D:465:ALA:HB3	1:D:474:ARG:HH12	1.85	0.42
1:D:659:ARG:HG3	1:D:659:ARG:HH21	1.85	0.42
1:D:695:ARG:N	1:D:696:PRO:CD	2.83	0.42
1:E:717:TRP:HA	1:E:718:PRO:HD2	1.79	0.42
1:F:21:THR:O	1:F:22:THR:CB	2.68	0.42
1:F:618:ILE:O	1:F:619:ALA:C	2.56	0.42
1:F:688:PHE:O	1:F:689:ALA:C	2.58	0.42
1:A:320:ARG:NH1	1:A:320:ARG:CB	2.82	0.42
1:B:712:ILE:HG22	1:B:713:ASP:N	2.35	0.42
1:C:21:THR:O	1:C:22:THR:CB	2.68	0.42
1:C:199:GLN:C	1:C:201:PHE:N	2.74	0.42
1:C:386:LEU:O	1:C:387:ARG:C	2.58	0.42
1:C:612:ILE:HD13	1:C:667:VAL:HG21	2.02	0.42
1:C:672:GLU:O	1:C:675:LYS:N	2.53	0.42
1:C:673:ALA:O	1:C:674:ARG:C	2.56	0.42
1:D:227:ASN:C	1:D:229:ARG:H	2.21	0.42
1:D:406:PRO:O	1:D:408:ILE:N	2.50	0.42
1:D:584:GLU:O	1:D:587:CYS:N	2.52	0.42
1:E:196:GLU:HG2	1:E:501:LYS:HZ1	1.85	0.42
1:F:356:PHE:CE2	1:F:471:PHE:HD2	2.38	0.42
1:F:497:LEU:C	1:F:499:GLU:N	2.71	0.42
1:F:695:ARG:N	1:F:696:PRO:CD	2.83	0.42
1:F:712:ILE:HG22	1:F:713:ASP:N	2.35	0.42
1:F:716:ILE:CG2	1:F:717:TRP:H	2.18	0.42
1:A:385:LEU:HD13	1:A:570:SER:HB3	2.01	0.41
1:A:695:ARG:CG	1:A:695:ARG:NH1	2.83	0.41
1:B:268:GLU:O	1:B:269:LEU:C	2.58	0.41
1:B:386:LEU:CB	1:B:409:LEU:HD21	2.50	0.41
1:B:695:ARG:N	1:B:696:PRO:CD	2.82	0.41
1:C:406:PRO:O	1:C:408:ILE:N	2.53	0.41
1:D:179:TYR:C	1:D:182:PRO:HD2	2.40	0.41
1:D:199:GLN:O	1:D:201:PHE:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:ASP:N	1:D:609:ASP:OD2	2.51	0.41
1:E:75:MET:O	1:E:78:TRP:HB3	2.20	0.41
1:F:501:LYS:O	1:F:502:ALA:C	2.58	0.41
1:F:622:TYR:O	1:F:625:ARG:HB3	2.20	0.41
1:F:688:PHE:O	1:F:692:GLU:HB2	2.20	0.41
1:B:169:PHE:O	1:B:170:ILE:HD13	2.19	0.41
1:B:576:GLY:C	1:B:578:ARG:H	2.23	0.41
1:D:76:LYS:O	1:D:77:SER:C	2.58	0.41
1:D:110:GLU:C	1:D:112:GLY:H	2.22	0.41
1:D:523:LYS:O	1:D:527:ILE:HG12	2.19	0.41
1:D:563:MET:CE	1:D:684:LYS:HD2	2.50	0.41
1:E:206:THR:N	1:E:350:ASP:OD2	2.53	0.41
1:E:628:GLU:OE2	1:E:632:ARG:NE	2.51	0.41
1:E:704:HIS:O	1:E:705:ILE:C	2.59	0.41
1:F:89:HIS:CB	1:F:167:THR:HG21	2.51	0.41
1:F:215:GLU:OE1	4:F:4001:ADP:O3A	2.38	0.41
1:A:20:ILE:O	1:A:21:THR:CG2	2.60	0.41
1:A:72:ALA:CB	1:A:120:GLY:HA2	2.49	0.41
1:A:150:TRP:CD1	1:A:150:TRP:C	2.92	0.41
1:A:225:LEU:O	1:A:226:TYR:C	2.58	0.41
1:A:305:ASN:O	1:A:306:ASP:C	2.57	0.41
1:A:679:HIS:O	1:A:680:LYS:C	2.59	0.41
1:C:38:ARG:C	1:C:40:LYS:N	2.69	0.41
1:C:193:ALA:HA	1:C:498:ASN:HD21	1.84	0.41
1:C:645:MET:HE3	1:D:654:LYS:HA	2.00	0.41
1:D:206:THR:O	1:D:207:ARG:HG3	2.20	0.41
1:D:293:GLU:CG	1:D:294:LEU:N	2.78	0.41
1:D:598:MET:O	1:D:601:GLN:HB3	2.20	0.41
1:E:199:GLN:O	1:E:201:PHE:N	2.53	0.41
1:E:233:ARG:CG	1:E:233:ARG:NH1	2.80	0.41
1:E:282:THR:HA	1:F:102:HIS:O	2.19	0.41
1:E:284:HIS:NE2	1:E:293:GLU:OE2	2.53	0.41
1:E:368:PHE:O	1:E:369:LEU:C	2.57	0.41
1:E:413:LEU:CD1	1:E:421:LEU:HD12	2.50	0.41
1:E:465:ALA:HB3	1:E:474:ARG:HH12	1.86	0.41
1:F:151:ASP:O	1:F:153:SER:N	2.52	0.41
1:F:598:MET:O	1:F:602:ILE:HD13	2.21	0.41
1:A:472:GLU:OE2	1:A:474:ARG:NH1	2.53	0.41
1:B:54:VAL:HA	1:B:57:THR:CG2	2.46	0.41
1:B:543:TRP:CE2	1:B:547:ALA:HB2	2.55	0.41
1:C:188:ALA:O	1:C:189:ALA:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HG12	1:D:21:THR:N	2.12	0.41
1:D:206:THR:N	1:D:350:ASP:OD2	2.53	0.41
1:D:598:MET:O	1:D:602:ILE:HD13	2.20	0.41
1:E:56:ALA:HA	1:E:61:THR:H	1.84	0.41
1:E:333:TYR:HB3	1:E:722:TYR:CE1	2.55	0.41
1:E:648:ASP:O	1:E:649:ARG:C	2.59	0.41
1:F:169:PHE:O	1:F:170:ILE:HD13	2.19	0.41
1:F:358:PRO:N	1:F:368:PHE:CE2	2.89	0.41
1:F:584:GLU:O	1:F:587:CYS:N	2.54	0.41
1:F:727:PHE:O	1:F:728:THR:O	2.38	0.41
1:A:196:GLU:O	1:A:199:GLN:N	2.51	0.41
1:A:293:GLU:CG	1:A:294:LEU:H	2.33	0.41
1:A:386:LEU:HB2	1:A:409:LEU:HD11	2.02	0.41
1:A:386:LEU:HB2	1:A:409:LEU:CD1	2.51	0.41
1:B:559:PRO:O	1:B:560:GLU:C	2.58	0.41
1:B:659:ARG:O	1:B:660:VAL:C	2.59	0.41
1:C:11:GLU:HG3	1:C:15:ARG:NH1	2.29	0.41
1:D:91:PHE:O	1:D:91:PHE:CD2	2.73	0.41
1:D:576:GLY:C	1:D:578:ARG:H	2.24	0.41
1:D:673:ALA:O	1:D:674:ARG:C	2.58	0.41
1:E:523:LYS:O	1:E:527:ILE:HG12	2.20	0.41
1:E:563:MET:O	1:E:566:MET:HG2	2.21	0.41
1:E:602:ILE:N	1:E:602:ILE:CD1	2.82	0.41
1:F:76:LYS:O	1:F:77:SER:C	2.58	0.41
1:A:199:GLN:C	1:A:201:PHE:N	2.74	0.41
1:A:208:VAL:HG13	1:A:349:THR:HG22	2.02	0.41
1:A:304:ALA:O	1:A:307:HIS:HB2	2.20	0.41
1:B:341:LYS:HB3	1:B:477:GLY:O	2.19	0.41
1:B:372:LEU:C	1:B:372:LEU:HD12	2.41	0.41
1:C:194:ALA:HA	1:C:497:LEU:HD13	2.03	0.41
1:D:686:LYS:HE3	1:D:686:LYS:HB2	1.93	0.41
1:E:199:GLN:C	1:E:201:PHE:N	2.74	0.41
1:E:522:LEU:HD21	1:E:526:ILE:HD11	2.02	0.41
1:F:45:LEU:CD2	1:F:71:ILE:HA	2.50	0.41
1:F:56:ALA:HA	1:F:61:THR:H	1.84	0.41
1:F:199:GLN:C	1:F:201:PHE:N	2.73	0.41
1:F:304:ALA:O	1:F:307:HIS:HB2	2.20	0.41
1:A:105:PHE:O	1:A:106:ILE:C	2.58	0.41
1:A:200:LEU:HD23	1:A:518:ILE:CG2	2.51	0.41
1:A:273:CYS:SG	1:A:314:LEU:HD23	2.61	0.41
1:A:501:LYS:HA	1:A:504:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:MET:HE2	1:B:654:LYS:HG2	2.03	0.41
1:C:648:ASP:O	1:C:649:ARG:C	2.59	0.41
1:D:386:LEU:O	1:D:387:ARG:C	2.58	0.41
1:D:690:TYR:O	1:D:692:GLU:N	2.54	0.41
1:F:486:MET:O	1:F:487:ILE:C	2.59	0.41
1:F:630:LEU:CD2	1:F:649:ARG:HG2	2.41	0.41
1:A:178:ASP:OD1	1:A:178:ASP:C	2.59	0.41
1:A:461:THR:HA	1:A:539:TYR:OH	2.20	0.41
1:A:604:SER:O	1:A:605:ARG:C	2.59	0.41
1:B:259:PRO:HG2	1:B:262:VAL:HB	2.03	0.41
1:B:629:ASN:ND2	1:C:627:LEU:CD1	2.83	0.41
1:B:716:ILE:CG2	1:B:717:TRP:H	2.20	0.41
1:C:206:THR:O	1:C:207:ARG:HG3	2.20	0.41
1:C:230:PRO:HB2	1:C:610:LEU:HD21	2.03	0.41
1:C:268:GLU:O	1:C:269:LEU:C	2.57	0.41
1:D:361:ASN:N	1:D:362:PRO:HD3	2.36	0.41
1:D:652:LEU:HA	1:D:655:GLU:HB3	2.01	0.41
1:E:179:TYR:C	1:E:182:PRO:HD2	2.41	0.41
1:E:361:ASN:N	1:E:362:PRO:HD3	2.36	0.41
1:E:688:PHE:O	1:E:692:GLU:HB2	2.21	0.41
1:F:474:ARG:HH11	1:F:474:ARG:HG3	1.86	0.41
1:F:659:ARG:NH1	1:F:707:HIS:CG	2.89	0.41
1:A:41:MET:HB3	1:A:45:LEU:CD1	2.46	0.41
1:A:157:PHE:N	1:A:157:PHE:HD2	2.19	0.41
1:A:168:ILE:C	1:A:168:ILE:CD1	2.89	0.41
1:A:196:GLU:O	1:A:199:GLN:HG2	2.21	0.41
1:A:549:ARG:NH1	1:A:549:ARG:CB	2.84	0.41
1:A:634:LYS:HB2	1:A:642:TYR:CE1	2.56	0.41
1:B:195:THR:O	1:B:198:CYS:HB2	2.21	0.41
1:B:386:LEU:HB2	1:B:409:LEU:HD21	2.03	0.41
1:B:474:ARG:HH11	1:B:474:ARG:HG3	1.86	0.41
1:B:563:MET:CE	1:B:684:LYS:HD2	2.51	0.41
1:B:612:ILE:HD13	1:B:667:VAL:HG21	2.03	0.41
1:B:663:ILE:O	1:B:664:LYS:C	2.60	0.41
1:B:717:TRP:HA	1:B:718:PRO:HD2	1.78	0.41
1:C:211:ASN:ND2	1:C:348:CYS:HB2	2.36	0.41
1:C:304:ALA:O	1:C:307:HIS:HB2	2.21	0.41
1:C:622:TYR:O	1:C:625:ARG:HB3	2.21	0.41
1:C:665:VAL:O	1:C:668:ARG:N	2.54	0.41
1:C:688:PHE:O	1:C:692:GLU:HB2	2.21	0.41
1:D:219:PHE:HA	1:D:290:ASN:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ARG:CG	1:D:233:ARG:NH1	2.80	0.41
1:D:547:ALA:HB1	1:D:552:LEU:HD12	2.02	0.41
1:D:559:PRO:O	1:D:560:GLU:C	2.56	0.41
1:E:215:GLU:OE1	4:E:4001:ADP:O3A	2.39	0.41
1:E:223:THR:O	1:E:226:TYR:HB3	2.21	0.41
1:E:358:PRO:N	1:E:368:PHE:CE2	2.88	0.41
1:E:576:GLY:C	1:E:578:ARG:H	2.24	0.41
1:E:630:LEU:O	1:E:632:ARG:N	2.53	0.41
1:F:41:MET:SD	1:F:53:VAL:HG11	2.60	0.41
1:F:75:MET:O	1:F:78:TRP:HB3	2.21	0.41
1:F:168:ILE:HG22	1:F:180:LYS:CG	2.48	0.41
1:F:211:ASN:ND2	1:F:348:CYS:HB2	2.35	0.41
1:F:219:PHE:HA	1:F:290:ASN:O	2.21	0.41
1:F:413:LEU:HD22	1:F:417:LEU:HD23	2.02	0.41
1:F:504:VAL:O	1:F:504:VAL:HG13	2.19	0.41
1:F:523:LYS:O	1:F:527:ILE:HG12	2.20	0.41
1:F:672:GLU:O	1:F:675:LYS:N	2.54	0.41
1:A:38:ARG:HH12	1:A:54:VAL:HG13	1.85	0.41
1:A:468:GLY:O	1:A:469:ASN:C	2.58	0.41
1:A:726:LEU:C	1:A:727:PHE:CD2	2.94	0.41
1:B:199:GLN:C	1:B:201:PHE:N	2.74	0.41
1:B:206:THR:O	1:B:207:ARG:HG3	2.20	0.41
1:C:182:PRO:HB3	1:C:580:PHE:CZ	2.55	0.41
1:F:361:ASN:N	1:F:362:PRO:HD3	2.36	0.41
1:A:7:PHE:CE2	1:F:10:GLN:HG2	2.56	0.40
1:A:195:THR:OG1	1:A:207:ARG:HA	2.21	0.40
1:A:199:GLN:O	1:A:201:PHE:N	2.54	0.40
1:A:311:VAL:HG12	1:A:315:MET:HE2	2.03	0.40
1:A:596:TYR:CZ	1:A:600:VAL:HG21	2.57	0.40
1:A:682:ASN:O	1:A:685:GLU:N	2.54	0.40
1:B:361:ASN:N	1:B:362:PRO:HD3	2.36	0.40
1:B:704:HIS:O	1:B:705:ILE:C	2.58	0.40
1:C:195:THR:O	1:C:198:CYS:HB2	2.21	0.40
1:C:286:GLU:CB	1:C:291:GLN:HG2	2.50	0.40
1:C:293:GLU:CG	1:C:294:LEU:N	2.77	0.40
1:C:465:ALA:HB3	1:C:474:ARG:HH12	1.86	0.40
1:C:656:ILE:O	1:C:657:SER:C	2.60	0.40
1:D:223:THR:O	1:D:226:TYR:HB3	2.20	0.40
1:D:423:GLU:C	1:D:424:ILE:HD12	2.40	0.40
1:D:622:TYR:O	1:D:625:ARG:HB3	2.21	0.40
1:E:598:MET:O	1:E:601:GLN:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:ILE:HA	1:F:351:THR:HG23	2.03	0.40
1:F:709:GLU:HB2	1:F:717:TRP:CZ2	2.57	0.40
1:A:151:ASP:C	1:A:153:SER:H	2.23	0.40
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.84	0.40
1:A:380:HIS:HB2	1:A:532:ILE:HB	2.02	0.40
1:A:630:LEU:HA	1:A:633:MET:HG2	2.03	0.40
1:A:675:LYS:O	1:A:678:ASN:HB2	2.21	0.40
1:B:10:GLN:HG2	1:C:7:PHE:CD2	2.56	0.40
1:B:87:TYR:CE2	1:B:103:ASP:HB2	2.56	0.40
1:B:194:ALA:HA	1:B:497:LEU:HD13	2.02	0.40
1:B:569:GLN:HE21	1:B:570:SER:N	2.19	0.40
1:B:697:TYR:O	1:B:698:LEU:C	2.59	0.40
1:C:598:MET:O	1:C:601:GLN:HB3	2.22	0.40
1:C:636:ILE:O	1:C:636:ILE:CG2	2.68	0.40
1:D:181:THR:O	1:D:182:PRO:C	2.59	0.40
1:D:259:PRO:HG2	1:D:262:VAL:HB	2.03	0.40
1:D:536:GLY:O	1:D:537:ASP:C	2.59	0.40
1:E:21:THR:O	1:E:22:THR:CB	2.69	0.40
1:E:27:LEU:C	1:E:29:ASP:N	2.75	0.40
1:E:304:ALA:O	1:E:307:HIS:HB2	2.21	0.40
1:F:400:GLY:O	1:F:401:ALA:HB2	2.20	0.40
1:F:536:GLY:O	1:F:537:ASP:C	2.60	0.40
1:A:590:GLU:OE2	1:A:683:PHE:CE2	2.74	0.40
1:A:654:LYS:HA	1:F:645:MET:CE	2.51	0.40
1:B:199:GLN:O	1:B:201:PHE:N	2.54	0.40
1:B:205:ILE:HA	1:B:351:THR:HG23	2.03	0.40
1:B:274:HIS:O	1:B:275:LYS:C	2.58	0.40
1:B:672:GLU:O	1:B:675:LYS:N	2.54	0.40
1:C:45:LEU:CD2	1:C:71:ILE:HA	2.51	0.40
1:C:151:ASP:C	1:C:153:SER:N	2.71	0.40
1:D:270:GLU:O	1:D:271:ILE:C	2.58	0.40
1:D:630:LEU:O	1:D:632:ARG:N	2.54	0.40
1:E:76:LYS:O	1:E:77:SER:C	2.58	0.40
1:E:259:PRO:HG2	1:E:262:VAL:HB	2.02	0.40
1:E:495:ASN:O	1:E:497:LEU:N	2.53	0.40
1:E:612:ILE:HD13	1:E:667:VAL:HG21	2.02	0.40
1:F:169:PHE:CB	1:F:178:ASP:HB3	2.48	0.40
1:F:274:HIS:O	1:F:275:LYS:C	2.60	0.40
1:F:522:LEU:HD21	1:F:526:ILE:HD11	2.03	0.40
1:F:563:MET:O	1:F:566:MET:HG2	2.21	0.40
1:F:675:LYS:O	1:F:676:VAL:C	2.58	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:THR:HA	1:A:347:LEU:HD23	2.04	0.40
1:A:374:ASN:O	1:A:375:VAL:C	2.58	0.40
1:A:521:ILE:H	1:A:521:ILE:CD1	2.21	0.40
1:B:14:ASN:O	1:B:15:ARG:HG2	2.22	0.40
1:B:497:LEU:O	1:B:499:GLU:N	2.54	0.40
1:B:522:LEU:HD21	1:B:526:ILE:HD11	2.02	0.40
1:B:563:MET:O	1:B:566:MET:HG2	2.21	0.40
1:B:659:ARG:HH21	1:B:659:ARG:HG3	1.85	0.40
1:C:89:HIS:CB	1:C:167:THR:HG21	2.51	0.40
1:C:219:PHE:HA	1:C:290:ASN:O	2.21	0.40
1:C:563:MET:O	1:C:566:MET:HG2	2.22	0.40
1:C:704:HIS:O	1:C:705:ILE:C	2.58	0.40
1:D:67:MET:O	1:D:71:ILE:HG13	2.22	0.40
1:D:75:MET:O	1:D:78:TRP:HB3	2.21	0.40
1:D:354:ASN:HB3	1:D:357:ALA:HB2	2.04	0.40
1:D:358:PRO:N	1:D:368:PHE:CE2	2.89	0.40
1:D:569:GLN:HE21	1:D:570:SER:N	2.20	0.40
1:E:20:ILE:HD13	1:E:20:ILE:N	2.36	0.40
1:E:424:ILE:N	1:E:424:ILE:HD12	2.37	0.40
1:E:659:ARG:O	1:E:660:VAL:C	2.60	0.40
1:F:27:LEU:C	1:F:29:ASP:N	2.74	0.40
1:F:497:LEU:O	1:F:499:GLU:N	2.54	0.40
1:F:630:LEU:O	1:F:632:ARG:N	2.54	0.40
1:A:76:LYS:O	1:A:78:TRP:N	2.55	0.40
1:A:230:PRO:HB2	1:A:610:LEU:HD21	2.03	0.40
1:A:559:PRO:HG2	1:A:691:GLU:CB	2.52	0.40
1:B:6:PHE:C	1:B:8:ALA:H	2.24	0.40
1:B:67:MET:O	1:B:71:ILE:HG13	2.22	0.40
1:B:169:PHE:CB	1:B:178:ASP:HB3	2.48	0.40
1:B:354:ASN:HB3	1:B:357:ALA:HB2	2.03	0.40
1:C:165:ILE:O	1:C:167:THR:HG23	2.22	0.40
1:C:358:PRO:N	1:C:368:PHE:CE2	2.90	0.40
1:C:563:MET:O	1:C:565:TYR:N	2.54	0.40
1:C:659:ARG:HH21	1:C:659:ARG:HG3	1.86	0.40
1:C:712:ILE:HG22	1:C:713:ASP:N	2.36	0.40
1:D:50:TYR:C	1:D:52:ALA:N	2.75	0.40
1:D:709:GLU:HG3	1:D:717:TRP:CE2	2.56	0.40
1:E:36:PHE:HB2	1:E:78:TRP:CZ3	2.57	0.40
1:E:168:ILE:HG22	1:E:180:LYS:CG	2.48	0.40
1:E:274:HIS:O	1:E:275:LYS:C	2.58	0.40
1:E:386:LEU:CB	1:E:409:LEU:HD21	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:LEU:HB2	1:E:409:LEU:HD21	2.02	0.40
1:E:712:ILE:HG22	1:E:713:ASP:N	2.36	0.40
1:F:725:LEU:HD13	1:F:725:LEU:HA	1.93	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:GLU:OE1	1:F:423:GLU:OE2[8_457]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	624/729 (86%)	408 (65%)	148 (24%)	68 (11%)	0 6
1	B	624/729 (86%)	438 (70%)	128 (20%)	58 (9%)	0 8
1	C	624/729 (86%)	441 (71%)	124 (20%)	59 (10%)	0 8
1	D	624/729 (86%)	433 (69%)	132 (21%)	59 (10%)	0 8
1	E	624/729 (86%)	444 (71%)	121 (19%)	59 (10%)	0 8
1	F	624/729 (86%)	442 (71%)	124 (20%)	58 (9%)	0 8
All	All	3744/4374 (86%)	2606 (70%)	777 (21%)	361 (10%)	0 8

All (361) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	23	PRO
1	A	149	ALA
1	A	204	ASN
1	A	234	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	294	LEU
1	A	353	ILE
1	A	402	ASN
1	A	415	SER
1	A	416	GLN
1	A	460	ARG
1	A	470	ARG
1	A	489	ILE
1	A	504	VAL
1	A	530	GLU
1	A	606	VAL
1	A	647	ALA
1	B	21	THR
1	B	22	THR
1	B	23	PRO
1	B	204	ASN
1	B	301	CYS
1	B	358	PRO
1	B	360	LYS
1	B	415	SER
1	B	416	GLN
1	B	460	ARG
1	B	470	ARG
1	B	530	GLU
1	B	537	ASP
1	B	647	ALA
1	C	21	THR
1	C	22	THR
1	C	23	PRO
1	C	204	ASN
1	C	358	PRO
1	C	360	LYS
1	C	415	SER
1	C	416	GLN
1	C	460	ARG
1	C	470	ARG
1	C	530	GLU
1	C	537	ASP
1	C	647	ALA
1	D	21	THR
1	D	22	THR
1	D	23	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	204	ASN
1	D	358	PRO
1	D	360	LYS
1	D	402	ASN
1	D	415	SER
1	D	416	GLN
1	D	460	ARG
1	D	530	GLU
1	D	537	ASP
1	D	647	ALA
1	E	21	THR
1	E	22	THR
1	E	23	PRO
1	E	204	ASN
1	E	358	PRO
1	E	360	LYS
1	E	415	SER
1	E	416	GLN
1	E	460	ARG
1	E	530	GLU
1	E	537	ASP
1	E	647	ALA
1	F	21	THR
1	F	22	THR
1	F	23	PRO
1	F	204	ASN
1	F	358	PRO
1	F	360	LYS
1	F	415	SER
1	F	416	GLN
1	F	460	ARG
1	F	530	GLU
1	F	537	ASP
1	F	647	ALA
1	A	21	THR
1	A	28	SER
1	A	60	GLY
1	A	102	HIS
1	A	106	ILE
1	A	152	GLY
1	A	202	ASP
1	A	203	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	231	ASP
1	A	383	GLN
1	A	401	ALA
1	A	414	GLY
1	A	423	GLU
1	A	488	ALA
1	A	496	GLN
1	A	537	ASP
1	B	28	SER
1	B	39	LYS
1	B	61	THR
1	B	202	ASP
1	B	337	ASN
1	B	353	ILE
1	B	387	ARG
1	B	401	ALA
1	B	402	ASN
1	B	423	GLU
1	B	488	ALA
1	B	496	GLN
1	B	504	VAL
1	B	577	GLU
1	B	582	GLU
1	B	682	ASN
1	C	28	SER
1	C	61	THR
1	C	202	ASP
1	C	301	CYS
1	C	337	ASN
1	C	353	ILE
1	C	387	ARG
1	C	401	ALA
1	C	402	ASN
1	C	423	GLU
1	C	488	ALA
1	C	504	VAL
1	C	577	GLU
1	C	582	GLU
1	C	682	ASN
1	D	28	SER
1	D	39	LYS
1	D	61	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	202	ASP
1	D	301	CYS
1	D	337	ASN
1	D	353	ILE
1	D	387	ARG
1	D	401	ALA
1	D	423	GLU
1	D	470	ARG
1	D	488	ALA
1	D	496	GLN
1	D	504	VAL
1	D	582	GLU
1	D	682	ASN
1	E	28	SER
1	E	39	LYS
1	E	61	THR
1	E	202	ASP
1	E	301	CYS
1	E	337	ASN
1	E	353	ILE
1	E	387	ARG
1	E	401	ALA
1	E	402	ASN
1	E	423	GLU
1	E	470	ARG
1	E	496	GLN
1	E	504	VAL
1	E	577	GLU
1	E	582	GLU
1	E	682	ASN
1	F	28	SER
1	F	39	LYS
1	F	61	THR
1	F	202	ASP
1	F	301	CYS
1	F	337	ASN
1	F	353	ILE
1	F	401	ALA
1	F	402	ASN
1	F	423	GLU
1	F	470	ARG
1	F	488	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	504	VAL
1	F	577	GLU
1	F	582	GLU
1	F	682	ASN
1	A	22	THR
1	A	47	LYS
1	A	153	SER
1	A	160	ASP
1	A	226	TYR
1	A	230	PRO
1	A	309	GLN
1	A	350	ASP
1	A	355	LEU
1	A	358	PRO
1	A	531	LEU
1	A	605	ARG
1	A	703	ASP
1	B	203	LYS
1	B	383	GLN
1	B	489	ILE
1	B	518	ILE
1	B	564	HIS
1	C	39	LYS
1	C	160	ASP
1	C	203	LYS
1	C	383	GLN
1	C	489	ILE
1	C	496	GLN
1	C	518	ILE
1	C	564	HIS
1	D	160	ASP
1	D	203	LYS
1	D	383	GLN
1	D	489	ILE
1	D	518	ILE
1	D	564	HIS
1	D	577	GLU
1	E	121	LYS
1	E	160	ASP
1	E	203	LYS
1	E	383	GLN
1	E	488	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	489	ILE
1	E	518	ILE
1	E	564	HIS
1	F	121	LYS
1	F	203	LYS
1	F	383	GLN
1	F	387	ARG
1	F	483	ALA
1	F	489	ILE
1	F	496	GLN
1	F	518	ILE
1	F	564	HIS
1	A	39	LYS
1	A	61	THR
1	A	72	ALA
1	A	200	LEU
1	A	368	PHE
1	A	418	SER
1	A	584	GLU
1	A	714	ASP
1	B	111	ASP
1	B	149	ALA
1	B	160	ASP
1	B	294	LEU
1	B	483	ALA
1	B	675	LYS
1	C	111	ASP
1	C	121	LYS
1	C	149	ALA
1	C	483	ALA
1	C	631	CYS
1	C	703	ASP
1	D	111	ASP
1	D	121	LYS
1	D	149	ALA
1	D	483	ALA
1	D	703	ASP
1	E	111	ASP
1	E	149	ALA
1	E	359	GLY
1	E	483	ALA
1	E	631	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	111	ASP
1	F	149	ALA
1	F	160	ASP
1	F	294	LEU
1	F	359	GLY
1	F	703	ASP
1	A	298	PHE
1	A	495	ASN
1	A	526	ILE
1	A	559	PRO
1	A	563	MET
1	A	568	ASN
1	A	717	TRP
1	B	20	ILE
1	B	106	ILE
1	B	121	LYS
1	B	359	GLY
1	B	531	LEU
1	B	631	CYS
1	B	703	ASP
1	B	717	TRP
1	C	20	ILE
1	C	106	ILE
1	C	200	LEU
1	C	294	LEU
1	C	359	GLY
1	C	531	LEU
1	C	675	LYS
1	C	717	TRP
1	D	20	ILE
1	D	106	ILE
1	D	200	LEU
1	D	294	LEU
1	D	359	GLY
1	D	531	LEU
1	D	631	CYS
1	D	675	LYS
1	D	717	TRP
1	E	20	ILE
1	E	106	ILE
1	E	294	LEU
1	E	414	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	675	LYS
1	E	703	ASP
1	E	717	TRP
1	F	20	ILE
1	F	106	ILE
1	F	200	LEU
1	F	531	LEU
1	F	631	CYS
1	F	675	LYS
1	F	717	TRP
1	A	205	ILE
1	A	535	GLU
1	A	607	LEU
1	B	205	ILE
1	B	414	GLY
1	B	560	GLU
1	B	716	ILE
1	C	205	ILE
1	C	560	GLU
1	C	716	ILE
1	D	205	ILE
1	D	414	GLY
1	D	716	ILE
1	E	205	ILE
1	E	498	ASN
1	E	531	LEU
1	E	716	ILE
1	F	205	ILE
1	F	414	GLY
1	F	716	ILE
1	A	716	ILE
1	B	606	VAL
1	C	414	GLY
1	D	559	PRO
1	D	606	VAL
1	E	606	VAL
1	F	606	VAL
1	A	518	ILE
1	B	559	PRO
1	C	296	PRO
1	C	606	VAL
1	D	296	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	296	PRO
1	E	559	PRO
1	F	296	PRO
1	A	93	PRO
1	A	463	PRO
1	B	296	PRO
1	B	463	PRO
1	B	660	VAL
1	C	559	PRO
1	C	660	VAL
1	D	152	GLY
1	D	463	PRO
1	D	660	VAL
1	E	463	PRO
1	E	660	VAL
1	F	559	PRO
1	F	660	VAL
1	C	463	PRO
1	F	463	PRO
1	E	152	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	554/631 (88%)	496 (90%)	58 (10%)	7 31
1	B	554/631 (88%)	506 (91%)	48 (9%)	10 38
1	C	554/631 (88%)	506 (91%)	48 (9%)	10 38
1	D	554/631 (88%)	505 (91%)	49 (9%)	10 38
1	E	554/631 (88%)	508 (92%)	46 (8%)	11 40
1	F	554/631 (88%)	505 (91%)	49 (9%)	10 38
All	All	3324/3786 (88%)	3026 (91%)	298 (9%)	9 37

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	9	LEU
1	A	12	LEU
1	A	20	ILE
1	A	21	THR
1	A	33	SER
1	A	35	VAL
1	A	51	LYS
1	A	55	ASP
1	A	63	ILE
1	A	102	HIS
1	A	103	ASP
1	A	148	THR
1	A	157	PHE
1	A	169	PHE
1	A	198	CYS
1	A	201	PHE
1	A	207	ARG
1	A	216	GLN
1	A	221	VAL
1	A	229	ARG
1	A	233	ARG
1	A	237	ARG
1	A	258	ILE
1	A	266	MET
1	A	282	THR
1	A	294	LEU
1	A	296	PRO
1	A	310	LEU
1	A	312	MET
1	A	323	HIS
1	A	330	GLU
1	A	336	VAL
1	A	348	CYS
1	A	399	LEU
1	A	464	PHE
1	A	530	GLU
1	A	535	GLU
1	A	542	GLU
1	A	554	ASN
1	A	559	PRO
1	A	565	TYR
1	A	567	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	575	ILE
1	A	577	GLU
1	A	583	THR
1	A	587	CYS
1	A	591	VAL
1	A	609	ASP
1	A	618	ILE
1	A	625	ARG
1	A	633	MET
1	A	648	ASP
1	A	659	ARG
1	A	692	GLU
1	A	695	ARG
1	A	698	LEU
1	A	699	GLU
1	B	12	LEU
1	B	15	ARG
1	B	20	ILE
1	B	21	THR
1	B	33	SER
1	B	35	VAL
1	B	63	ILE
1	B	80	LYS
1	B	95	THR
1	B	148	THR
1	B	167	THR
1	B	169	PHE
1	B	184	LEU
1	B	198	CYS
1	B	199	GLN
1	B	201	PHE
1	B	216	GLN
1	B	221	VAL
1	B	233	ARG
1	B	258	ILE
1	B	283	ARG
1	B	294	LEU
1	B	296	PRO
1	B	336	VAL
1	B	348	CYS
1	B	349	THR
1	B	350	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	368	PHE
1	B	374	ASN
1	B	399	LEU
1	B	412	PHE
1	B	464	PHE
1	B	481	ASN
1	B	516	GLU
1	B	554	ASN
1	B	567	ASP
1	B	569	GLN
1	B	577	GLU
1	B	591	VAL
1	B	628	GLU
1	B	648	ASP
1	B	649	ARG
1	B	657	SER
1	B	659	ARG
1	B	668	ARG
1	B	676	VAL
1	B	695	ARG
1	B	723	ARG
1	C	12	LEU
1	C	15	ARG
1	C	20	ILE
1	C	21	THR
1	C	33	SER
1	C	35	VAL
1	C	63	ILE
1	C	80	LYS
1	C	95	THR
1	C	148	THR
1	C	150	TRP
1	C	167	THR
1	C	184	LEU
1	C	198	CYS
1	C	199	GLN
1	C	201	PHE
1	C	216	GLN
1	C	221	VAL
1	C	233	ARG
1	C	258	ILE
1	C	283	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	294	LEU
1	C	296	PRO
1	C	336	VAL
1	C	348	CYS
1	C	349	THR
1	C	350	ASP
1	C	374	ASN
1	C	387	ARG
1	C	399	LEU
1	C	412	PHE
1	C	464	PHE
1	C	481	ASN
1	C	516	GLU
1	C	554	ASN
1	C	567	ASP
1	C	569	GLN
1	C	577	GLU
1	C	591	VAL
1	C	628	GLU
1	C	648	ASP
1	C	649	ARG
1	C	657	SER
1	C	659	ARG
1	C	668	ARG
1	C	676	VAL
1	C	695	ARG
1	C	723	ARG
1	D	12	LEU
1	D	15	ARG
1	D	20	ILE
1	D	21	THR
1	D	33	SER
1	D	35	VAL
1	D	63	ILE
1	D	80	LYS
1	D	95	THR
1	D	148	THR
1	D	167	THR
1	D	169	PHE
1	D	184	LEU
1	D	198	CYS
1	D	199	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	201	PHE
1	D	216	GLN
1	D	221	VAL
1	D	233	ARG
1	D	258	ILE
1	D	283	ARG
1	D	294	LEU
1	D	296	PRO
1	D	336	VAL
1	D	348	CYS
1	D	349	THR
1	D	350	ASP
1	D	368	PHE
1	D	374	ASN
1	D	387	ARG
1	D	399	LEU
1	D	412	PHE
1	D	464	PHE
1	D	481	ASN
1	D	516	GLU
1	D	554	ASN
1	D	567	ASP
1	D	569	GLN
1	D	577	GLU
1	D	591	VAL
1	D	628	GLU
1	D	648	ASP
1	D	649	ARG
1	D	657	SER
1	D	659	ARG
1	D	668	ARG
1	D	676	VAL
1	D	695	ARG
1	D	723	ARG
1	E	12	LEU
1	E	15	ARG
1	E	20	ILE
1	E	21	THR
1	E	33	SER
1	E	35	VAL
1	E	63	ILE
1	E	80	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	95	THR
1	E	148	THR
1	E	167	THR
1	E	184	LEU
1	E	198	CYS
1	E	199	GLN
1	E	201	PHE
1	E	216	GLN
1	E	221	VAL
1	E	233	ARG
1	E	258	ILE
1	E	283	ARG
1	E	294	LEU
1	E	296	PRO
1	E	336	VAL
1	E	348	CYS
1	E	349	THR
1	E	350	ASP
1	E	374	ASN
1	E	399	LEU
1	E	412	PHE
1	E	464	PHE
1	E	481	ASN
1	E	516	GLU
1	E	554	ASN
1	E	567	ASP
1	E	569	GLN
1	E	577	GLU
1	E	591	VAL
1	E	628	GLU
1	E	648	ASP
1	E	649	ARG
1	E	657	SER
1	E	659	ARG
1	E	668	ARG
1	E	676	VAL
1	E	695	ARG
1	E	723	ARG
1	F	12	LEU
1	F	15	ARG
1	F	20	ILE
1	F	21	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	35	VAL
1	F	63	ILE
1	F	80	LYS
1	F	95	THR
1	F	148	THR
1	F	150	TRP
1	F	167	THR
1	F	169	PHE
1	F	184	LEU
1	F	198	CYS
1	F	199	GLN
1	F	201	PHE
1	F	216	GLN
1	F	221	VAL
1	F	233	ARG
1	F	258	ILE
1	F	283	ARG
1	F	294	LEU
1	F	296	PRO
1	F	336	VAL
1	F	348	CYS
1	F	349	THR
1	F	350	ASP
1	F	368	PHE
1	F	374	ASN
1	F	387	ARG
1	F	399	LEU
1	F	412	PHE
1	F	464	PHE
1	F	481	ASN
1	F	516	GLU
1	F	554	ASN
1	F	567	ASP
1	F	569	GLN
1	F	577	GLU
1	F	591	VAL
1	F	628	GLU
1	F	648	ASP
1	F	649	ARG
1	F	657	SER
1	F	659	ARG
1	F	668	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	676	VAL
1	F	695	ARG
1	F	723	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	92	GLN
1	A	285	ASN
1	A	290	ASN
1	A	302	ASN
1	A	337	ASN
1	A	382	ASN
1	A	383	GLN
1	A	525	ASN
1	A	613	ASN
1	A	629	ASN
1	A	678	ASN
1	A	707	HIS
1	B	199	GLN
1	B	211	ASN
1	B	227	ASN
1	B	285	ASN
1	B	290	ASN
1	B	305	ASN
1	B	322	HIS
1	B	382	ASN
1	B	481	ASN
1	B	498	ASN
1	B	554	ASN
1	B	569	GLN
1	B	601	GLN
1	B	614	HIS
1	B	678	ASN
1	B	682	ASN
1	B	707	HIS
1	C	199	GLN
1	C	211	ASN
1	C	227	ASN
1	C	285	ASN
1	C	290	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	305	ASN
1	C	322	HIS
1	C	343	ASN
1	C	382	ASN
1	C	481	ASN
1	C	498	ASN
1	C	554	ASN
1	C	569	GLN
1	C	601	GLN
1	C	678	ASN
1	C	682	ASN
1	C	707	HIS
1	D	199	GLN
1	D	211	ASN
1	D	227	ASN
1	D	285	ASN
1	D	290	ASN
1	D	305	ASN
1	D	322	HIS
1	D	343	ASN
1	D	382	ASN
1	D	481	ASN
1	D	498	ASN
1	D	554	ASN
1	D	569	GLN
1	D	601	GLN
1	D	678	ASN
1	D	682	ASN
1	D	707	HIS
1	E	199	GLN
1	E	211	ASN
1	E	227	ASN
1	E	285	ASN
1	E	290	ASN
1	E	305	ASN
1	E	322	HIS
1	E	343	ASN
1	E	382	ASN
1	E	481	ASN
1	E	498	ASN
1	E	554	ASN
1	E	569	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	601	GLN
1	E	614	HIS
1	E	678	ASN
1	E	682	ASN
1	E	707	HIS
1	F	199	GLN
1	F	211	ASN
1	F	227	ASN
1	F	285	ASN
1	F	290	ASN
1	F	305	ASN
1	F	322	HIS
1	F	343	ASN
1	F	382	ASN
1	F	481	ASN
1	F	498	ASN
1	F	554	ASN
1	F	569	GLN
1	F	601	GLN
1	F	678	ASN
1	F	682	ASN
1	F	707	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	ADP	C	4001	2	24,29,29	0.95	1 (4%)	29,45,45	1.92	9 (31%)
4	ADP	B	4001	2	24,29,29	0.95	1 (4%)	29,45,45	1.93	9 (31%)
3	P3S	D	3001	2	11,14,14	3.30	3 (27%)	12,21,21	4.18	5 (41%)
3	P3S	A	3001	2	11,14,14	3.29	3 (27%)	12,21,21	4.03	5 (41%)
3	P3S	F	3001	2	11,14,14	3.30	3 (27%)	12,21,21	4.18	5 (41%)
3	P3S	E	3001	2	11,14,14	3.30	3 (27%)	12,21,21	4.15	5 (41%)
4	ADP	A	4001	2	24,29,29	0.94	1 (4%)	29,45,45	1.85	8 (27%)
3	P3S	B	3001	2	11,14,14	3.31	3 (27%)	12,21,21	4.14	5 (41%)
4	ADP	E	4001	2	24,29,29	0.93	1 (4%)	29,45,45	1.93	9 (31%)
3	P3S	C	3001	2	11,14,14	3.29	3 (27%)	12,21,21	4.16	5 (41%)
4	ADP	F	4001	2	24,29,29	0.93	0	29,45,45	1.93	9 (31%)
4	ADP	D	4001	2	24,29,29	0.93	0	29,45,45	1.94	9 (31%)

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	ADP	C	4001	2	-	1/12/32/32	0/3/3/3
4	ADP	B	4001	2	-	1/12/32/32	0/3/3/3
3	P3S	D	3001	2	-	3/9/16/16	-
3	P3S	A	3001	2	-	2/9/16/16	-
3	P3S	F	3001	2	-	3/9/16/16	-
3	P3S	E	3001	2	-	3/9/16/16	-
4	ADP	A	4001	2	-	1/12/32/32	0/3/3/3
3	P3S	B	3001	2	-	3/9/16/16	-
4	ADP	E	4001	2	-	1/12/32/32	0/3/3/3
3	P3S	C	3001	2	-	3/9/16/16	-
4	ADP	F	4001	2	-	1/12/32/32	0/3/3/3
4	ADP	D	4001	2	-	1/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3001	P3S	PA-O1A	9.70	1.61	1.46
3	E	3001	P3S	PA-O1A	9.67	1.61	1.46
3	F	3001	P3S	PA-O1A	9.67	1.61	1.46
3	D	3001	P3S	PA-O1A	9.65	1.61	1.46
3	C	3001	P3S	PA-O1A	9.64	1.61	1.46
3	A	3001	P3S	PA-O1A	9.63	1.61	1.46
3	A	3001	P3S	PA-O2A	3.20	1.61	1.54
3	B	3001	P3S	PA-O2A	3.20	1.61	1.54
3	C	3001	P3S	PA-O2A	3.20	1.61	1.54
3	F	3001	P3S	PA-O2A	3.20	1.61	1.54
3	D	3001	P3S	PA-O2A	3.20	1.61	1.54
3	E	3001	P3S	PA-O2A	3.20	1.61	1.54
3	B	3001	P3S	PA-O3A	-3.12	1.48	1.54
3	A	3001	P3S	PA-O3A	-3.11	1.48	1.54
3	D	3001	P3S	PA-O3A	-3.11	1.48	1.54
3	E	3001	P3S	PA-O3A	-3.09	1.48	1.54
3	C	3001	P3S	PA-O3A	-3.08	1.48	1.54
3	F	3001	P3S	PA-O3A	-3.07	1.48	1.54
4	B	4001	ADP	O4'-C1'	2.11	1.44	1.41
4	A	4001	ADP	O4'-C1'	2.07	1.44	1.41
4	C	4001	ADP	O4'-C1'	2.03	1.43	1.41
4	E	4001	ADP	O4'-C1'	2.00	1.43	1.41

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3001	P3S	OE-SD-CG	-11.08	99.70	108.37
3	D	3001	P3S	OE-SD-CG	-11.07	99.70	108.37
3	C	3001	P3S	OE-SD-CG	-10.94	99.80	108.37
3	E	3001	P3S	OE-SD-CG	-10.94	99.81	108.37
3	B	3001	P3S	OE-SD-CG	-10.91	99.83	108.37
3	A	3001	P3S	OE-SD-CG	-10.52	100.13	108.37
3	F	3001	P3S	OE-SD-CE	6.84	120.14	109.24
3	E	3001	P3S	OE-SD-CE	6.83	120.12	109.24
3	B	3001	P3S	OE-SD-CE	6.81	120.09	109.24
3	D	3001	P3S	OE-SD-CE	6.79	120.06	109.24
3	C	3001	P3S	OE-SD-CE	6.79	120.05	109.24
3	A	3001	P3S	OE-SD-CE	6.66	119.85	109.24
4	A	4001	ADP	O4'-C1'-C2'	-5.02	99.60	106.93
4	B	4001	ADP	O4'-C1'-C2'	-4.94	99.71	106.93
4	E	4001	ADP	O4'-C1'-C2'	-4.92	99.73	106.93
4	F	4001	ADP	O4'-C1'-C2'	-4.91	99.75	106.93
4	D	4001	ADP	O4'-C1'-C2'	-4.90	99.76	106.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	4001	ADP	O4'-C1'-C2'	-4.86	99.82	106.93
4	B	4001	ADP	N3-C2-N1	-4.47	121.69	128.68
4	F	4001	ADP	N3-C2-N1	-4.43	121.76	128.68
4	D	4001	ADP	N3-C2-N1	-4.42	121.76	128.68
4	C	4001	ADP	N3-C2-N1	-4.42	121.78	128.68
4	A	4001	ADP	N3-C2-N1	-4.41	121.78	128.68
4	E	4001	ADP	N3-C2-N1	-4.40	121.80	128.68
3	D	3001	P3S	CE-SD-CG	-3.96	90.86	105.10
3	C	3001	P3S	CE-SD-CG	-3.96	90.86	105.10
3	E	3001	P3S	CE-SD-CG	-3.94	90.92	105.10
3	B	3001	P3S	CE-SD-CG	-3.93	90.95	105.10
3	F	3001	P3S	CE-SD-CG	-3.93	90.95	105.10
3	A	3001	P3S	CE-SD-CG	-3.85	91.25	105.10
3	A	3001	P3S	O2A-PA-O1A	-3.62	105.68	113.45
3	C	3001	P3S	O2A-PA-O1A	-3.55	105.85	113.45
3	E	3001	P3S	O2A-PA-O1A	-3.51	105.91	113.45
3	F	3001	P3S	O2A-PA-O1A	-3.51	105.93	113.45
3	D	3001	P3S	O2A-PA-O1A	-3.49	105.96	113.45
3	B	3001	P3S	O2A-PA-O1A	-3.48	105.99	113.45
4	F	4001	ADP	O3B-PB-O3A	-3.02	94.50	104.64
4	D	4001	ADP	O3B-PB-O3A	-3.02	94.51	104.64
4	B	4001	ADP	O3B-PB-O3A	-3.01	94.55	104.64
4	C	4001	ADP	O3B-PB-O3A	-3.00	94.58	104.64
4	D	4001	ADP	O2B-PB-O3A	-2.97	94.68	104.64
4	E	4001	ADP	O3B-PB-O3A	-2.96	94.69	104.64
4	E	4001	ADP	O2B-PB-O3A	-2.96	94.69	104.64
4	D	4001	ADP	PA-O3A-PB	-2.96	122.67	132.83
4	E	4001	ADP	PA-O3A-PB	-2.95	122.72	132.83
4	F	4001	ADP	O2B-PB-O3A	-2.94	94.76	104.64
4	B	4001	ADP	O2B-PB-O3A	-2.94	94.78	104.64
4	F	4001	ADP	PA-O3A-PB	-2.94	122.75	132.83
4	C	4001	ADP	PA-O3A-PB	-2.93	122.75	132.83
4	C	4001	ADP	O2B-PB-O3A	-2.92	94.85	104.64
4	B	4001	ADP	O3B-PB-O1B	2.91	122.08	110.68
4	B	4001	ADP	PA-O3A-PB	-2.90	122.86	132.83
4	C	4001	ADP	O3B-PB-O1B	2.88	121.96	110.68
4	D	4001	ADP	O3B-PB-O1B	2.88	121.94	110.68
4	A	4001	ADP	O3B-PB-O1B	2.87	121.93	110.68
4	E	4001	ADP	O3B-PB-O1B	2.87	121.92	110.68
4	F	4001	ADP	O3B-PB-O1B	2.86	121.89	110.68
4	E	4001	ADP	O2B-PB-O1B	2.83	121.76	110.68
4	D	4001	ADP	O2B-PB-O1B	2.81	121.69	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	4001	ADP	O2B-PB-O1B	2.80	121.66	110.68
4	C	4001	ADP	O2B-PB-O1B	2.80	121.62	110.68
4	B	4001	ADP	O2B-PB-O1B	2.77	121.54	110.68
4	A	4001	ADP	O2B-PB-O1B	2.73	121.37	110.68
4	A	4001	ADP	O3B-PB-O3A	-2.65	95.74	104.64
4	A	4001	ADP	O2B-PB-O3A	-2.61	95.89	104.64
3	C	3001	P3S	CE-SD-NE	2.50	116.23	107.48
3	E	3001	P3S	CE-SD-NE	2.47	116.13	107.48
3	B	3001	P3S	CE-SD-NE	2.46	116.09	107.48
3	F	3001	P3S	CE-SD-NE	2.46	116.06	107.48
3	D	3001	P3S	CE-SD-NE	2.45	116.06	107.48
3	A	3001	P3S	CE-SD-NE	2.35	115.69	107.48
4	A	4001	ADP	PA-O3A-PB	-2.32	124.87	132.83
4	D	4001	ADP	C3'-C2'-C1'	-2.24	97.61	100.98
4	F	4001	ADP	C3'-C2'-C1'	-2.21	97.65	100.98
4	E	4001	ADP	C3'-C2'-C1'	-2.20	97.66	100.98
4	C	4001	ADP	C3'-C2'-C1'	-2.16	97.72	100.98
4	D	4001	ADP	O3A-PB-O1B	-2.12	99.41	111.19
4	E	4001	ADP	O3A-PB-O1B	-2.11	99.48	111.19
4	B	4001	ADP	O3A-PB-O1B	-2.09	99.58	111.19
4	F	4001	ADP	O3A-PB-O1B	-2.09	99.59	111.19
4	B	4001	ADP	C3'-C2'-C1'	-2.08	97.84	100.98
4	C	4001	ADP	O3A-PB-O1B	-2.07	99.70	111.19
4	A	4001	ADP	O3A-PB-O1B	-2.07	99.70	111.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	3001	P3S	OT-C-CA-CB
3	B	3001	P3S	O-C-CA-CB
3	C	3001	P3S	OT-C-CA-CB
3	C	3001	P3S	O-C-CA-CB
3	D	3001	P3S	OT-C-CA-CB
3	D	3001	P3S	O-C-CA-CB
3	E	3001	P3S	OT-C-CA-CB
3	E	3001	P3S	O-C-CA-CB
3	F	3001	P3S	OT-C-CA-CB
3	F	3001	P3S	O-C-CA-CB
3	A	3001	P3S	OT-C-CA-CB
3	A	3001	P3S	O-C-CA-CB
3	B	3001	P3S	OT-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	3001	P3S	OT-C-CA-N
4	A	4001	ADP	O4'-C4'-C5'-O5'
4	B	4001	ADP	O4'-C4'-C5'-O5'
4	C	4001	ADP	O4'-C4'-C5'-O5'
4	D	4001	ADP	O4'-C4'-C5'-O5'
4	E	4001	ADP	O4'-C4'-C5'-O5'
4	F	4001	ADP	O4'-C4'-C5'-O5'
3	C	3001	P3S	OT-C-CA-N
3	E	3001	P3S	OT-C-CA-N
3	F	3001	P3S	OT-C-CA-N

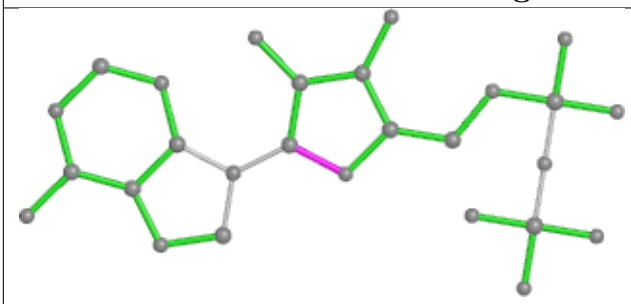
There are no ring outliers.

7 monomers are involved in 15 short contacts:

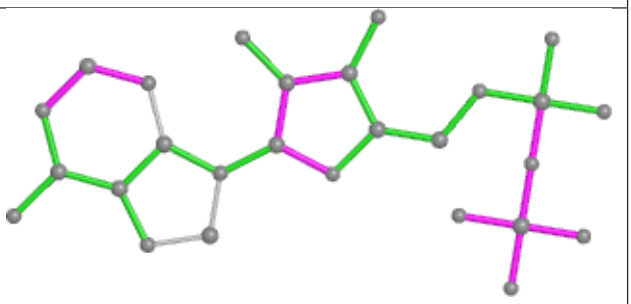
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4001	ADP	2	0
4	B	4001	ADP	2	0
3	A	3001	P3S	1	0
4	A	4001	ADP	4	0
4	E	4001	ADP	2	0
4	F	4001	ADP	2	0
4	D	4001	ADP	2	0

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

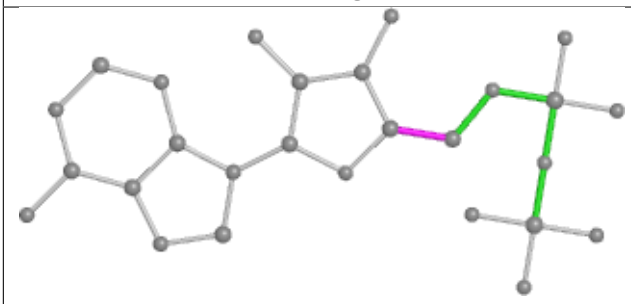
Ligand ADP C 4001



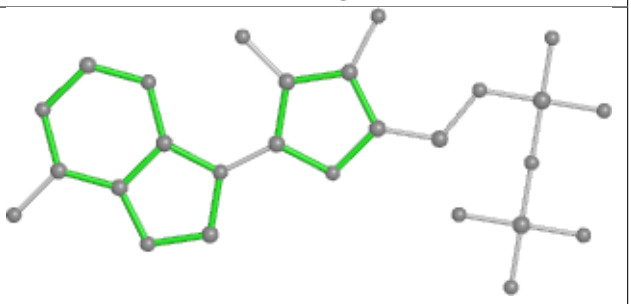
Bond lengths



Bond angles

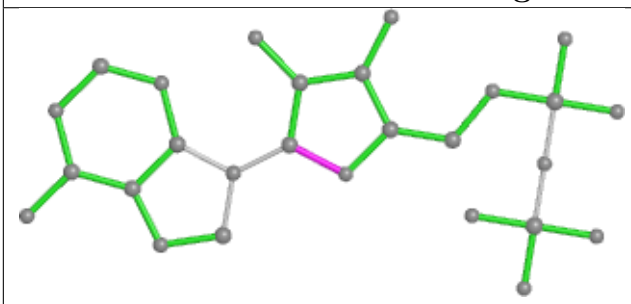


Torsions

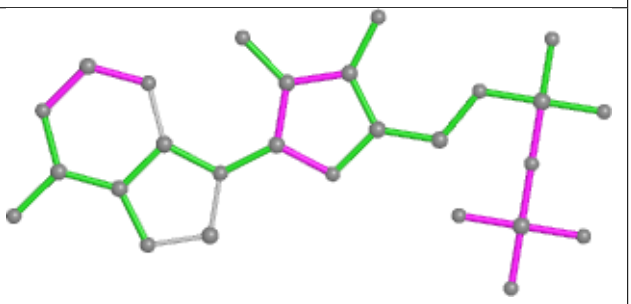


Rings

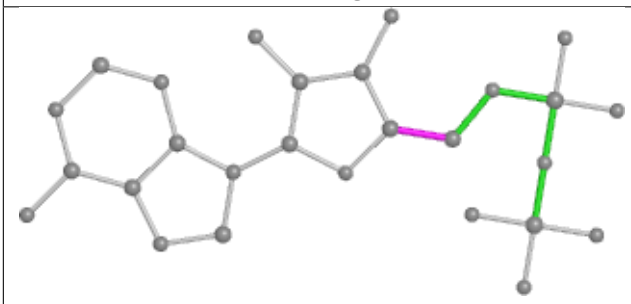
Ligand ADP B 4001



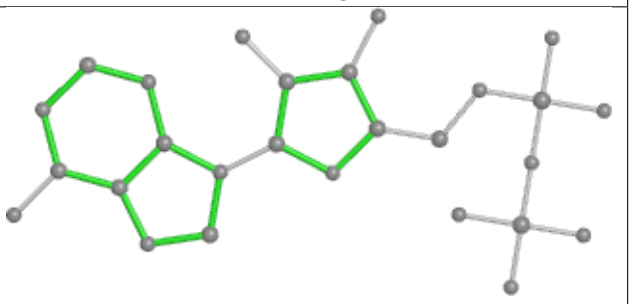
Bond lengths



Bond angles

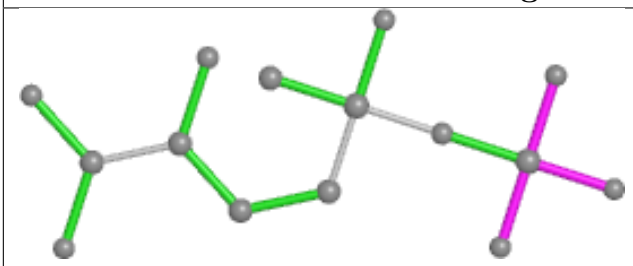


Torsions

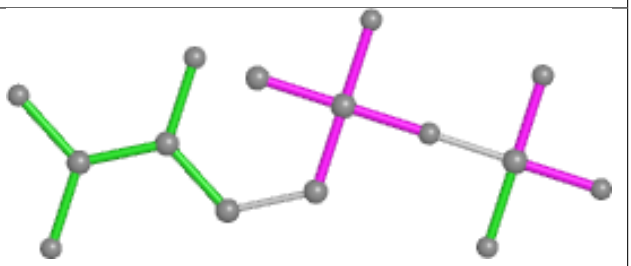


Rings

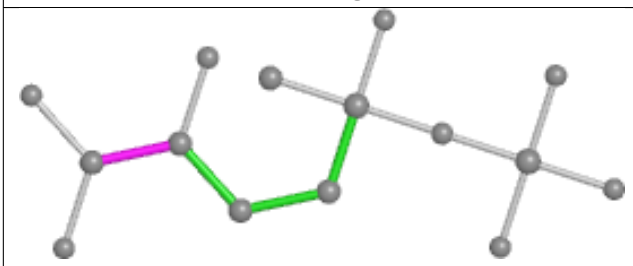
Ligand P3S D 3001



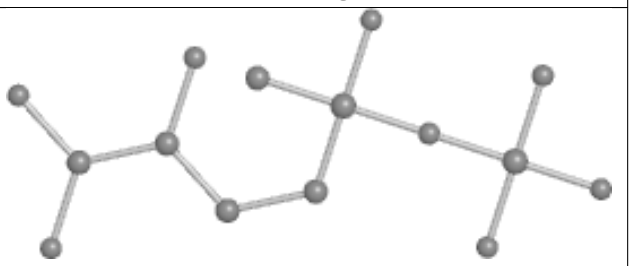
Bond lengths



Bond angles

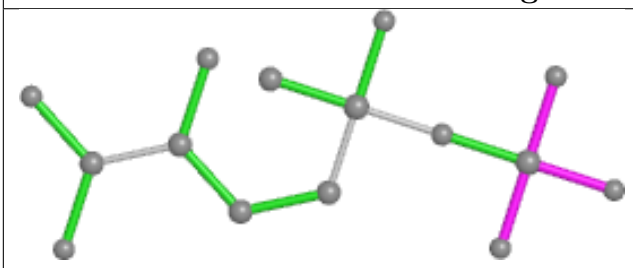


Torsions

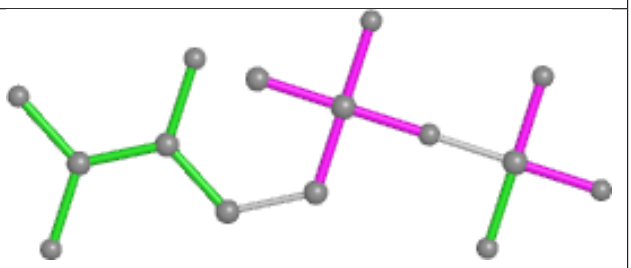


Rings

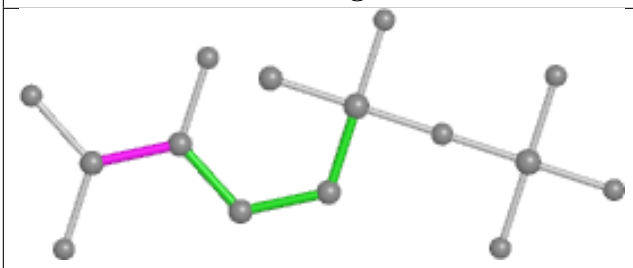
Ligand P3S A 3001



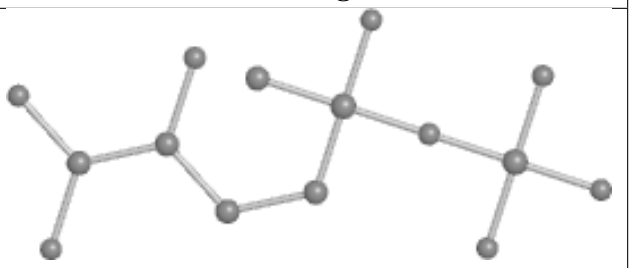
Bond lengths



Bond angles

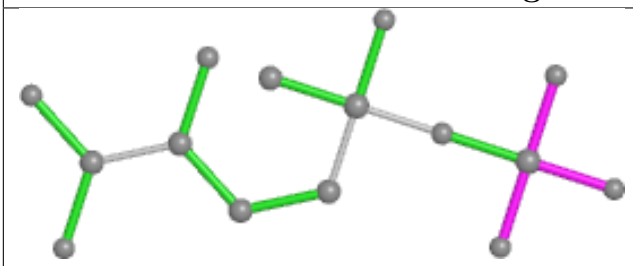


Torsions

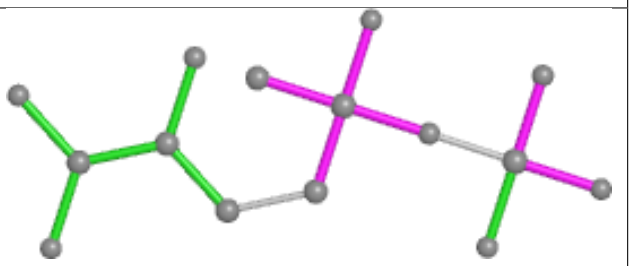


Rings

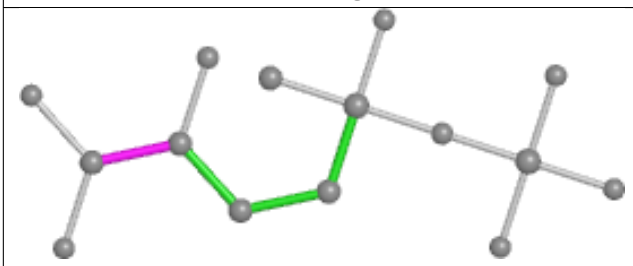
Ligand P3S F 3001



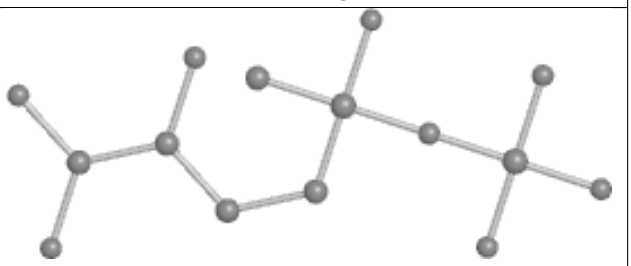
Bond lengths



Bond angles

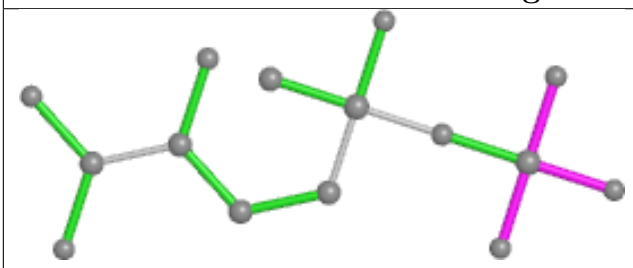


Torsions

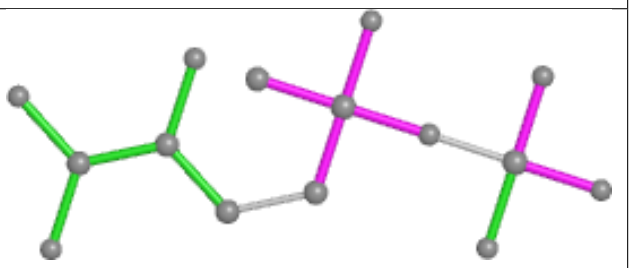


Rings

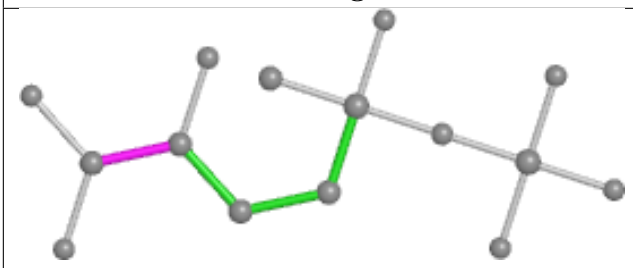
Ligand P3S E 3001



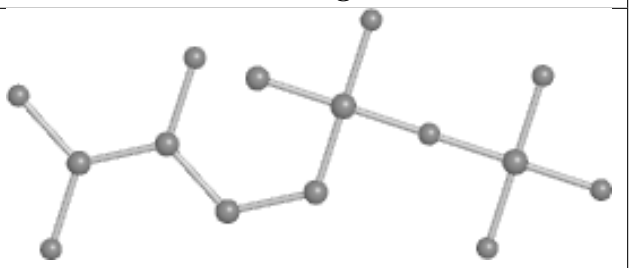
Bond lengths



Bond angles

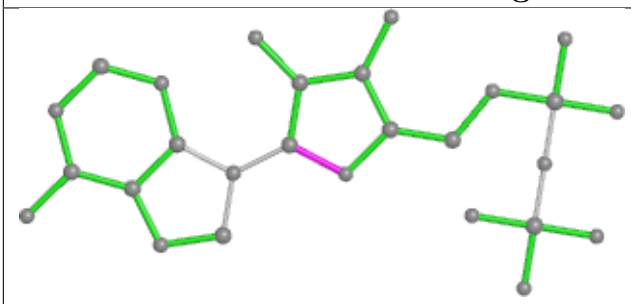


Torsions

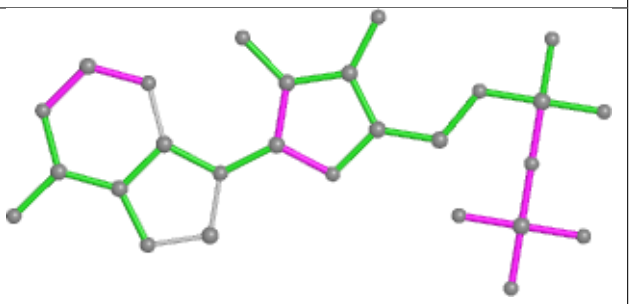


Rings

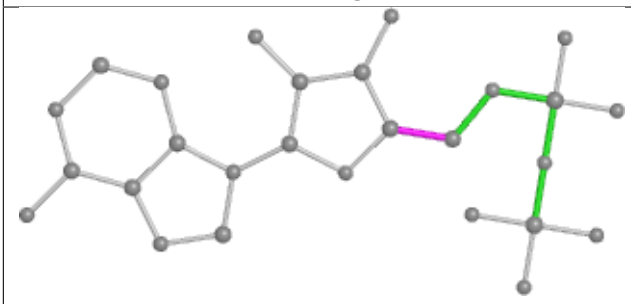
Ligand ADP A 4001



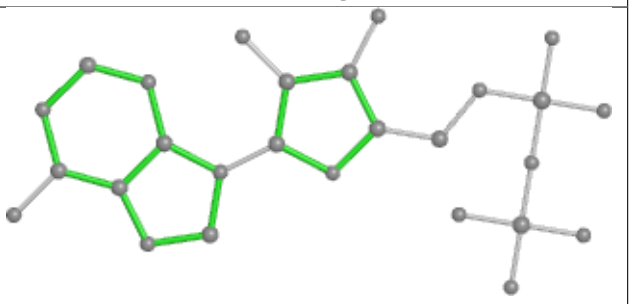
Bond lengths



Bond angles

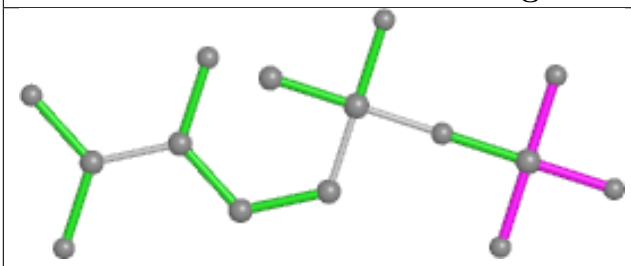


Torsions

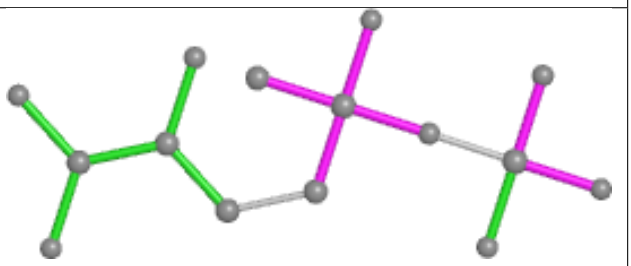


Rings

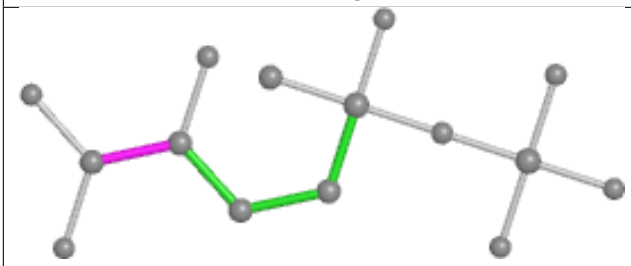
Ligand P3S B 3001



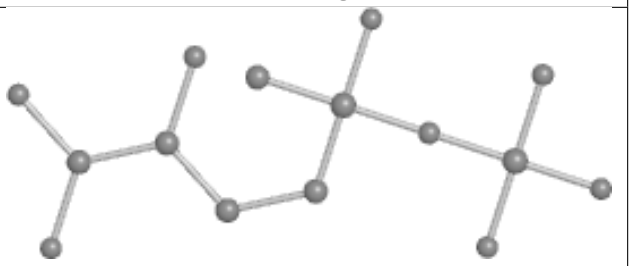
Bond lengths



Bond angles

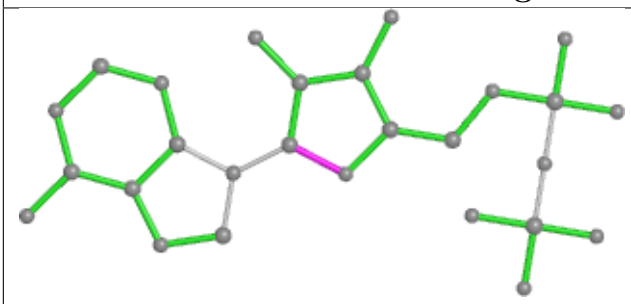


Torsions

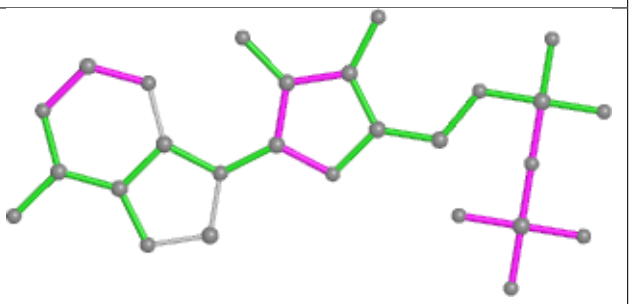


Rings

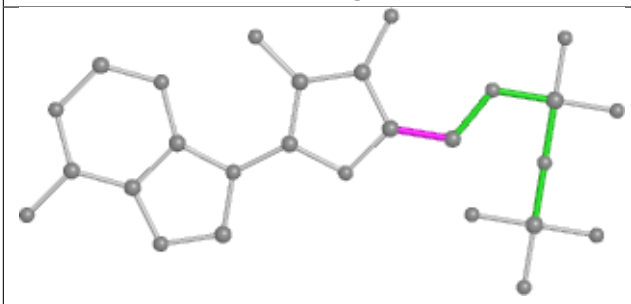
Ligand ADP E 4001



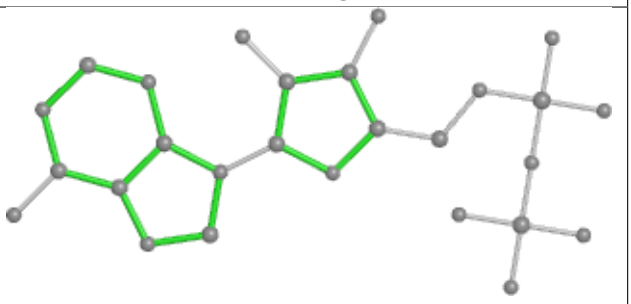
Bond lengths



Bond angles

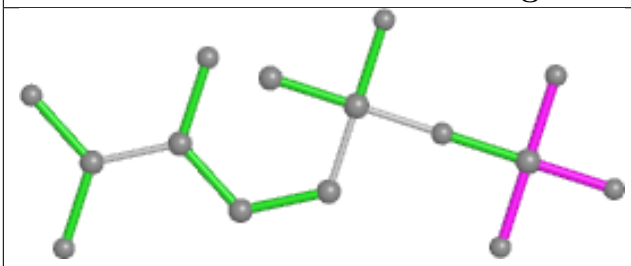


Torsions

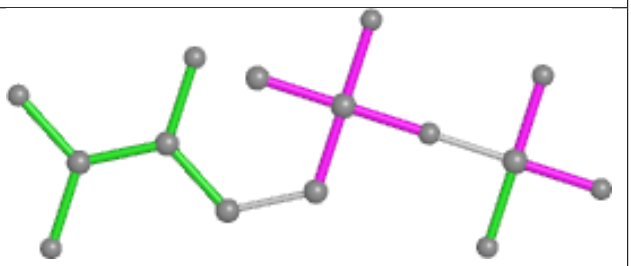


Rings

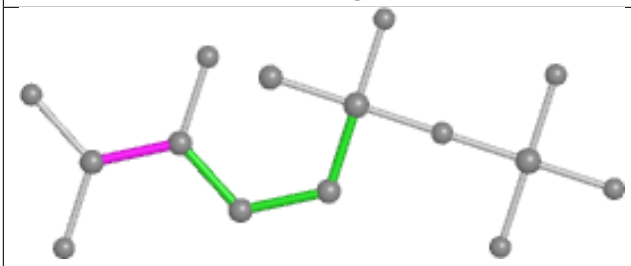
Ligand P3S C 3001



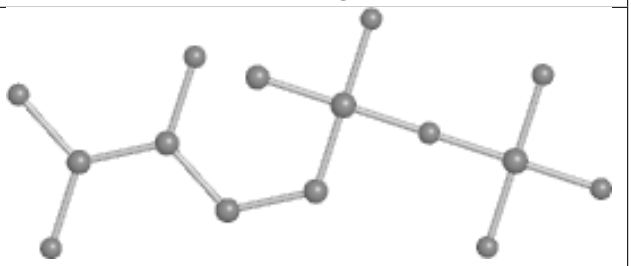
Bond lengths



Bond angles

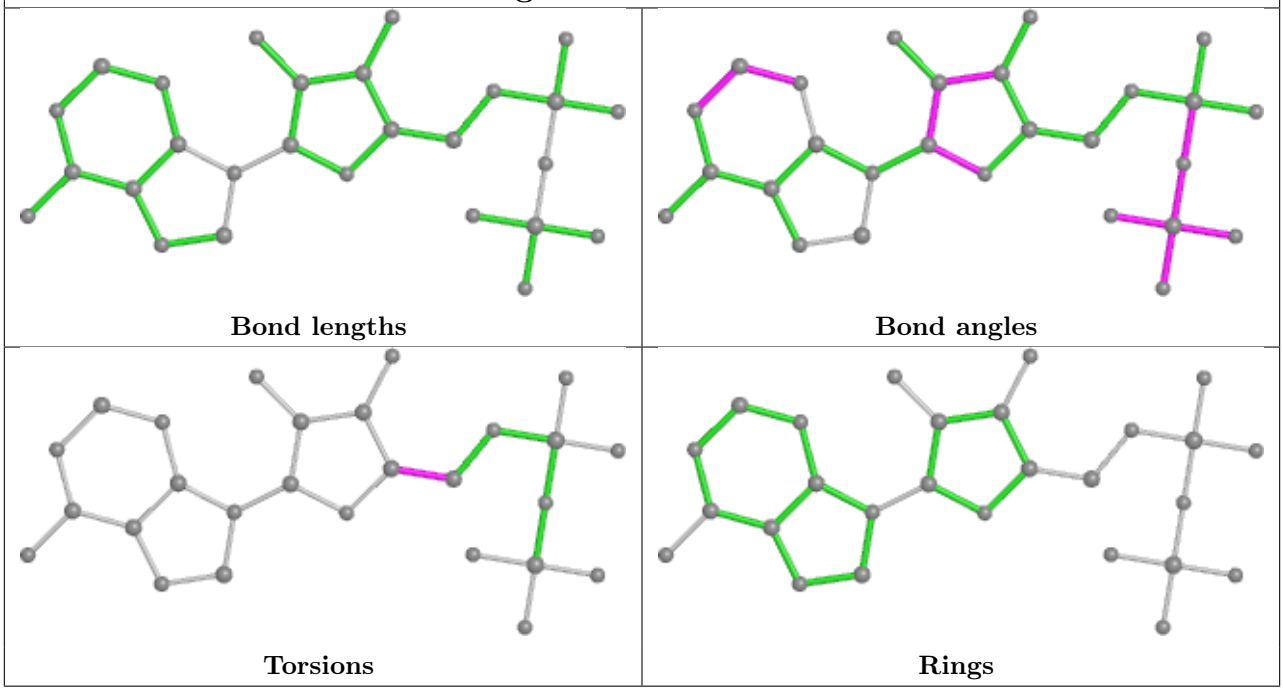


Torsions

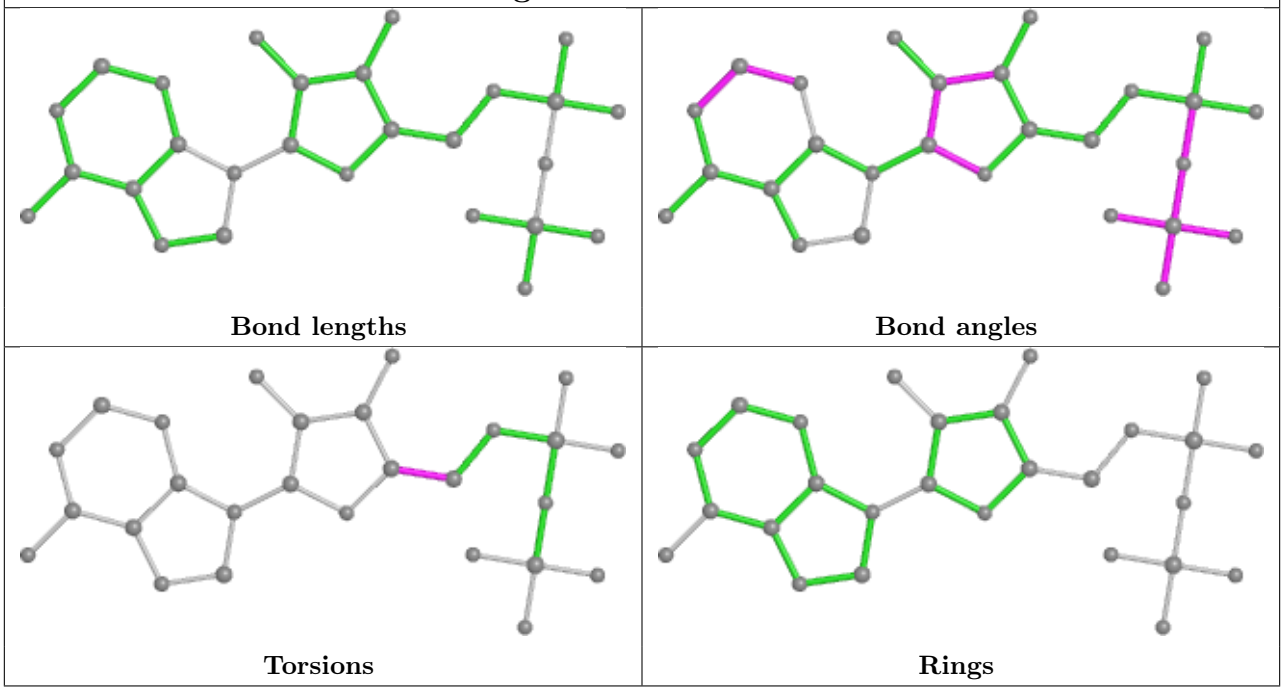


Rings

Ligand ADP F 4001



Ligand ADP D 4001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	637/729 (87%)	-0.49	0	100	100	2, 25, 71, 127	51 (8%)
1	B	637/729 (87%)	-0.43	0	100	100	2, 33, 89, 150	51 (8%)
1	C	637/729 (87%)	-0.35	1 (0%)	95	93	2, 31, 85, 149	51 (8%)
1	D	637/729 (87%)	-0.42	0	100	100	2, 29, 79, 148	51 (8%)
1	E	637/729 (87%)	-0.49	0	100	100	2, 32, 82, 169	51 (8%)
1	F	637/729 (87%)	-0.39	1 (0%)	95	93	2, 31, 81, 129	51 (8%)
All	All	3822/4374 (87%)	-0.43	2 (0%)	95	95	2, 30, 82, 169	306 (8%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	200	LEU	3.6
1	C	549	ARG	2.2

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)

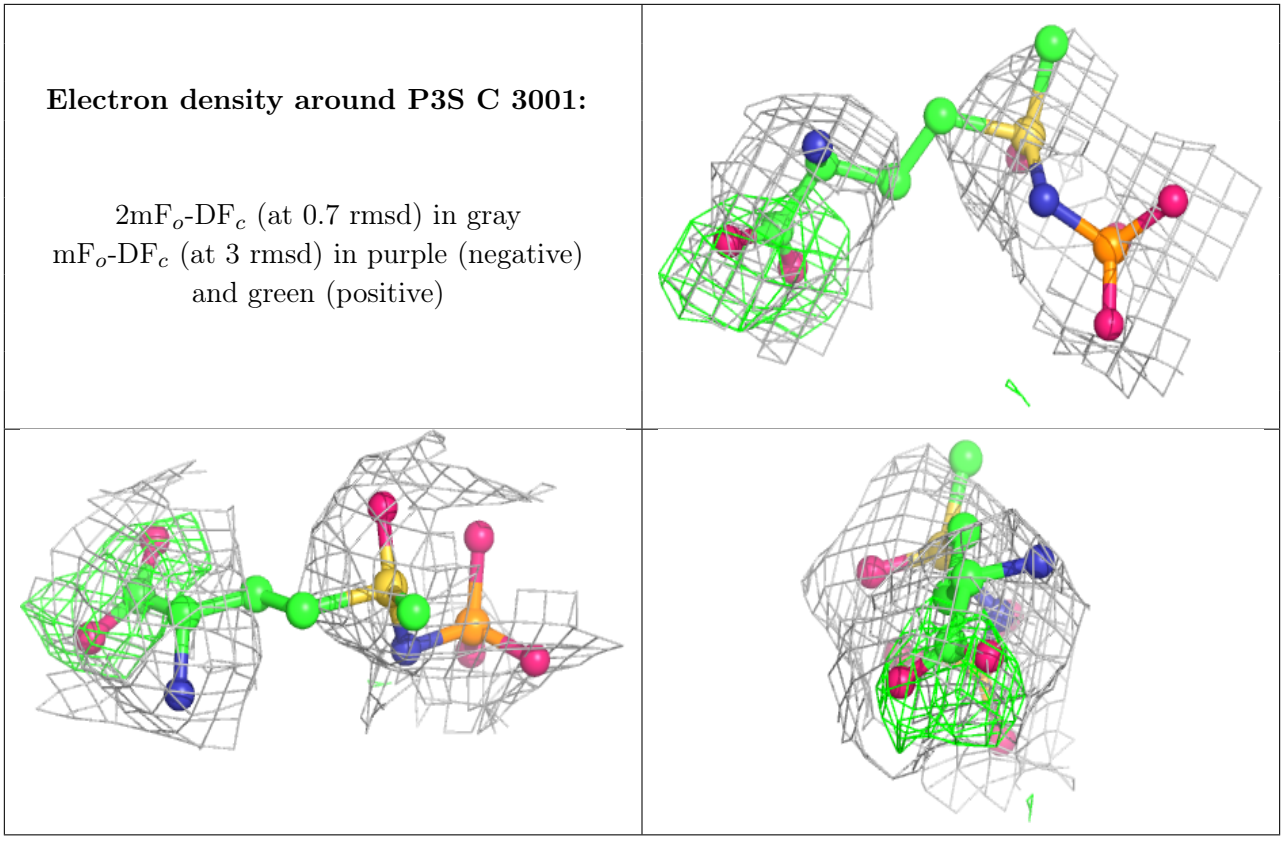
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	1001	1/1	0.72	0.20	15,15,15,15	0
2	MG	E	2001	1/1	0.76	0.23	41,41,41,41	0
3	P3S	C	3001	15/15	0.79	0.25	118,128,135,138	0
3	P3S	E	3001	15/15	0.80	0.30	118,128,135,138	0
4	ADP	B	4001	27/27	0.80	0.32	102,116,127,128	0
2	MG	F	2001	1/1	0.81	0.24	30,30,30,30	0
4	ADP	D	4001	27/27	0.81	0.33	93,107,117,118	0
4	ADP	C	4001	27/27	0.82	0.25	99,113,124,125	0
4	ADP	A	4001	27/27	0.82	0.29	80,94,104,106	0
4	ADP	E	4001	27/27	0.82	0.29	99,113,123,125	0
4	ADP	F	4001	27/27	0.82	0.30	88,102,113,114	0
3	P3S	A	3001	15/15	0.83	0.33	118,128,135,138	0
3	P3S	B	3001	15/15	0.83	0.23	118,128,135,138	0
3	P3S	D	3001	15/15	0.85	0.28	118,128,135,138	0
2	MG	C	1001	1/1	0.88	0.15	8,8,8,8	0
2	MG	F	1001	1/1	0.88	0.14	23,23,23,23	0
3	P3S	F	3001	15/15	0.88	0.32	118,128,135,138	0
5	CL	D	6001	1/1	0.89	0.16	4,4,4,4	0
2	MG	B	2001	1/1	0.90	0.15	52,52,52,52	0
2	MG	D	1001	1/1	0.90	0.20	10,10,10,10	0
2	MG	A	2001	1/1	0.91	0.14	37,37,37,37	0
2	MG	E	1001	1/1	0.91	0.08	10,10,10,10	0
2	MG	C	2001	1/1	0.91	0.30	33,33,33,33	0
5	CL	B	6001	1/1	0.92	0.07	5,5,5,5	0
2	MG	A	1001	1/1	0.92	0.17	3,3,3,3	0
2	MG	D	2001	1/1	0.94	0.31	32,32,32,32	0
5	CL	C	6001	1/1	0.94	0.09	10,10,10,10	0
5	CL	A	6001	1/1	0.94	0.12	2,2,2,2	0
5	CL	B	5001	1/1	0.95	0.25	1,1,1,1	0
5	CL	E	6001	1/1	0.95	0.13	5,5,5,5	0
5	CL	E	5001	1/1	0.96	0.15	1,1,1,1	0
5	CL	F	6001	1/1	0.96	0.13	1,1,1,1	0
5	CL	A	730	1/1	0.97	0.21	1,1,1,1	0
5	CL	A	5001	1/1	0.97	0.18	1,1,1,1	0
5	CL	D	5001	1/1	0.98	0.19	1,1,1,1	0
5	CL	C	5001	1/1	0.99	0.26	1,1,1,1	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.

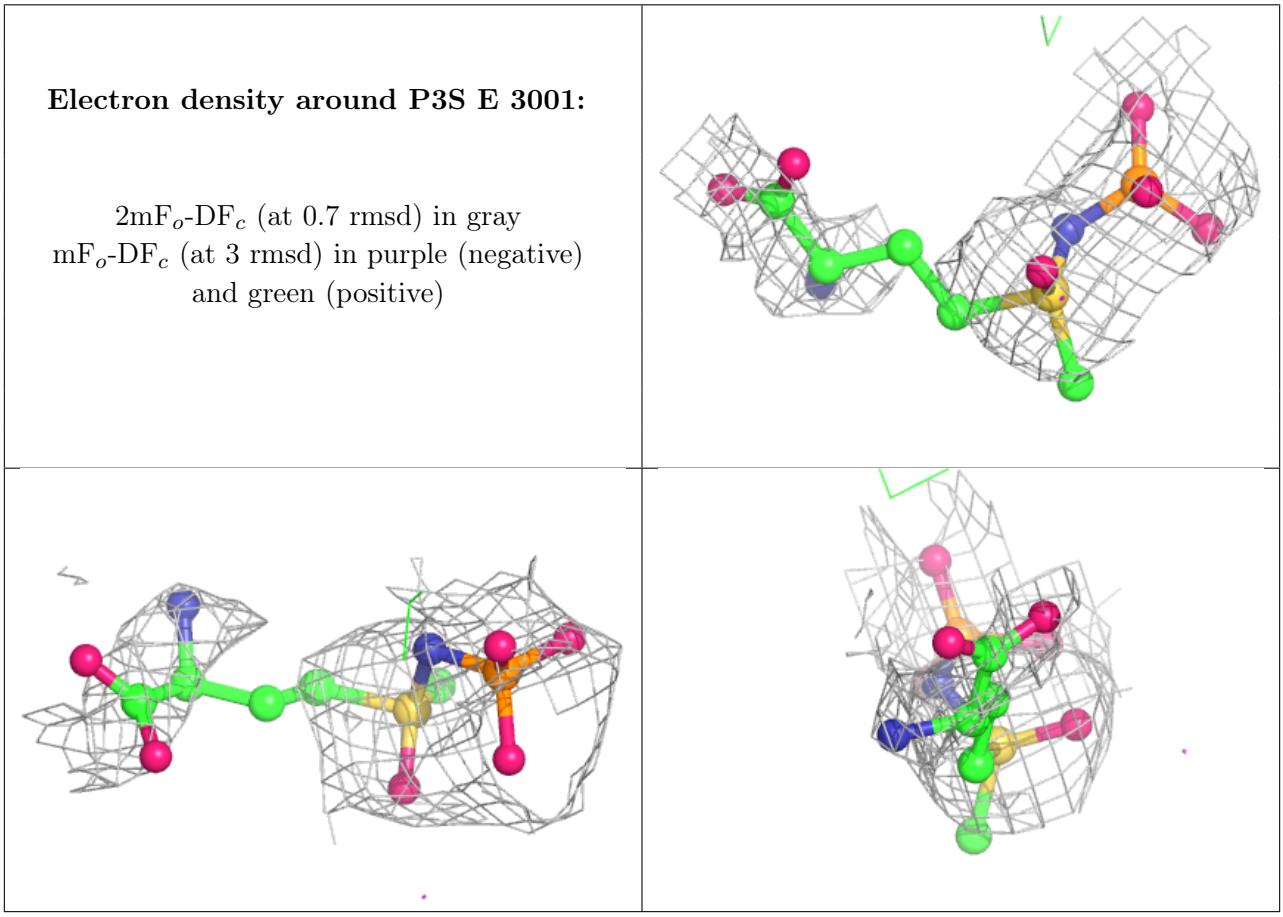
Electron density around P3S C 3001:

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



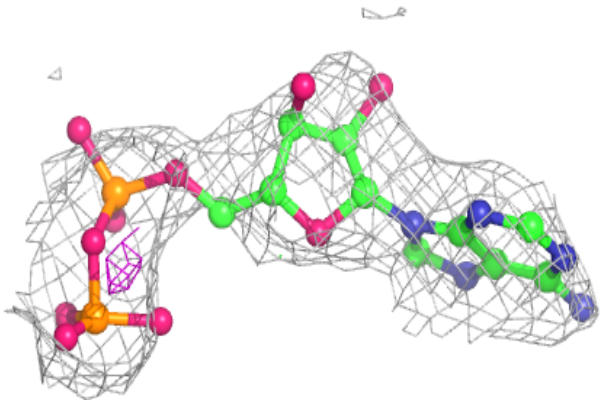
Electron density around P3S E 3001:

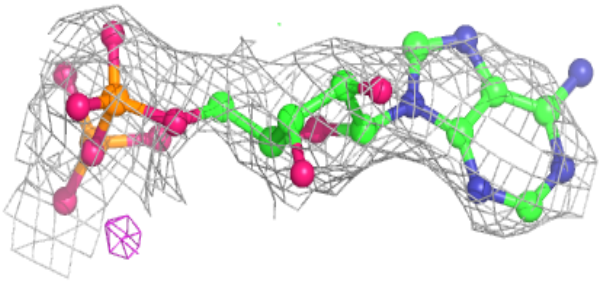
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

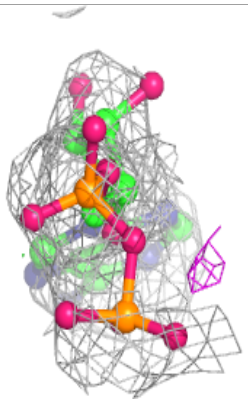


Electron density around ADP B 4001:

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

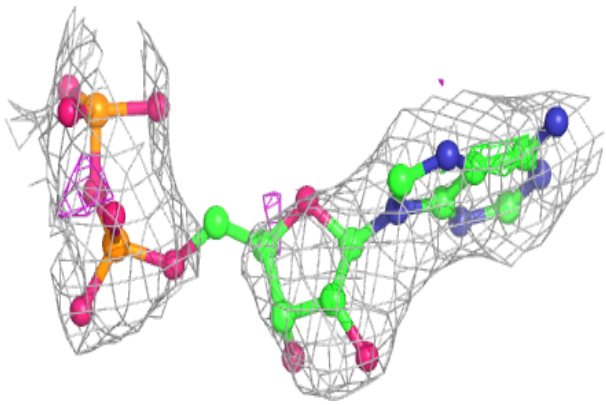


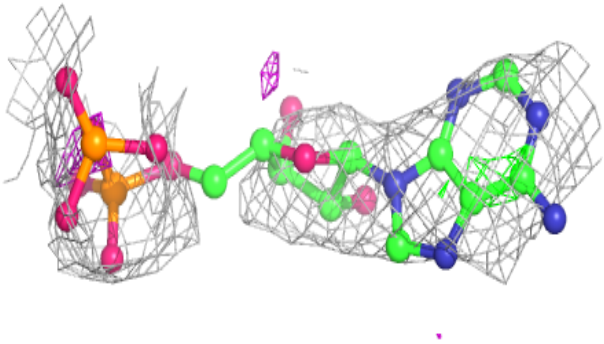


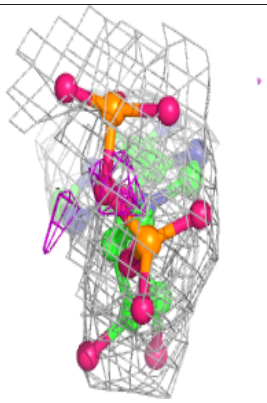


Electron density around ADP D 4001:

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

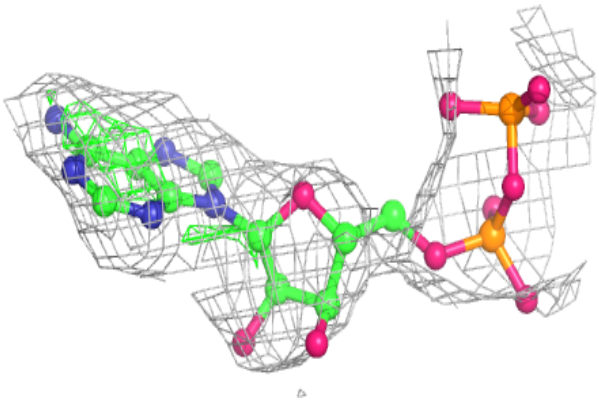


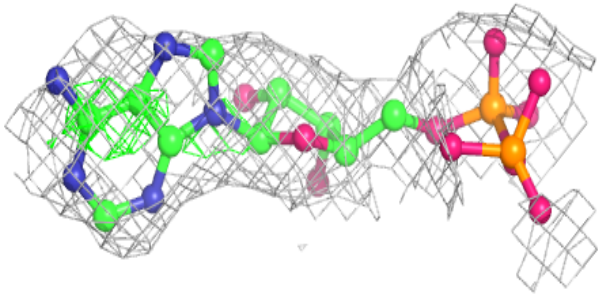


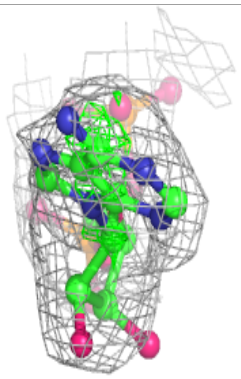


Electron density around ADP C 4001:

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

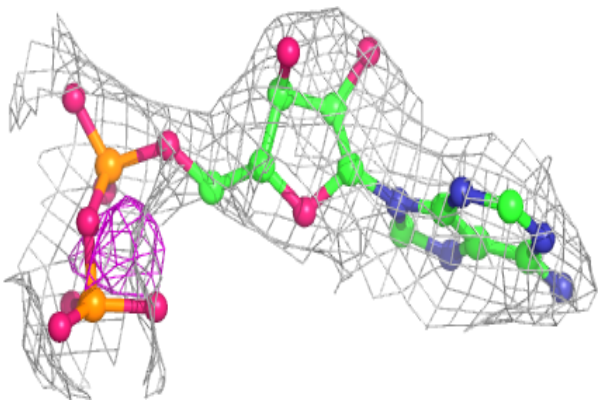


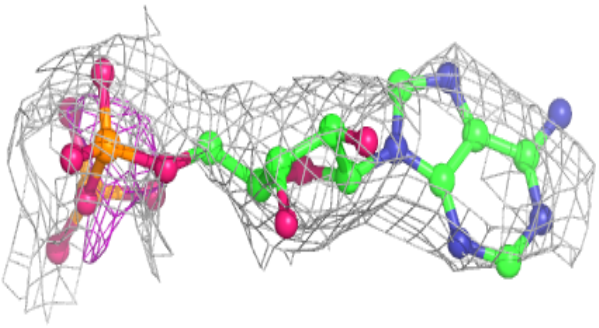


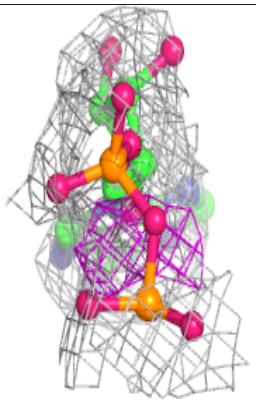


Electron density around ADP A 4001:

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

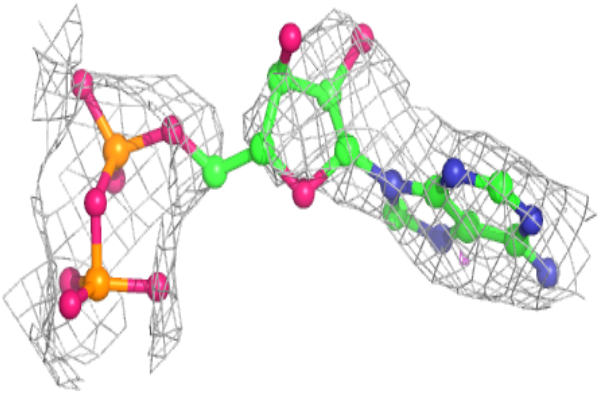


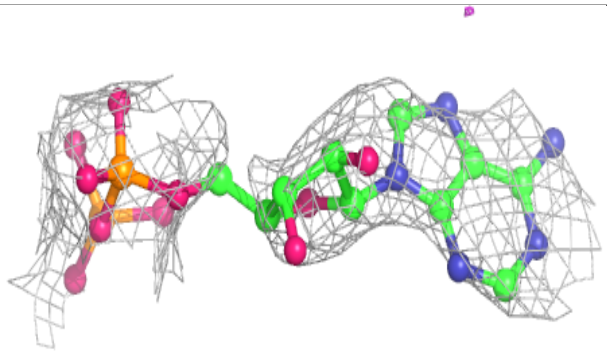


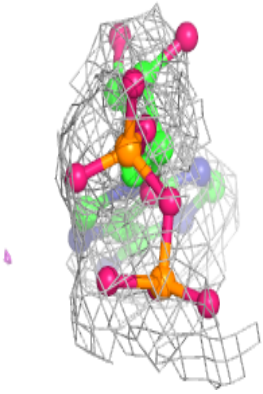


Electron density around ADP E 4001:

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

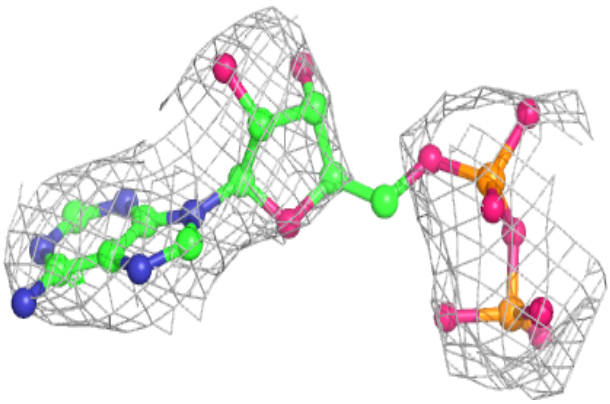


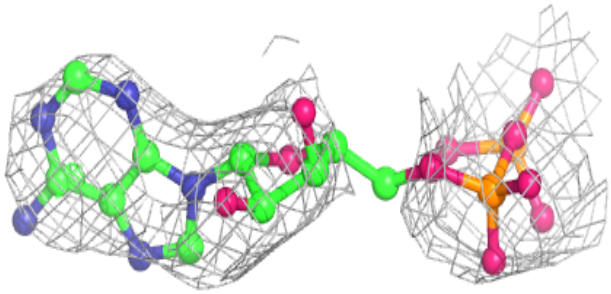


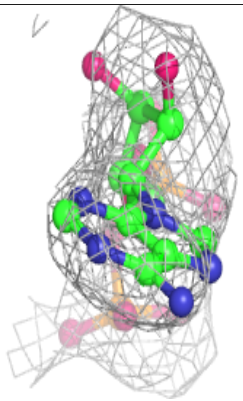


Electron density around ADP F 4001:

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

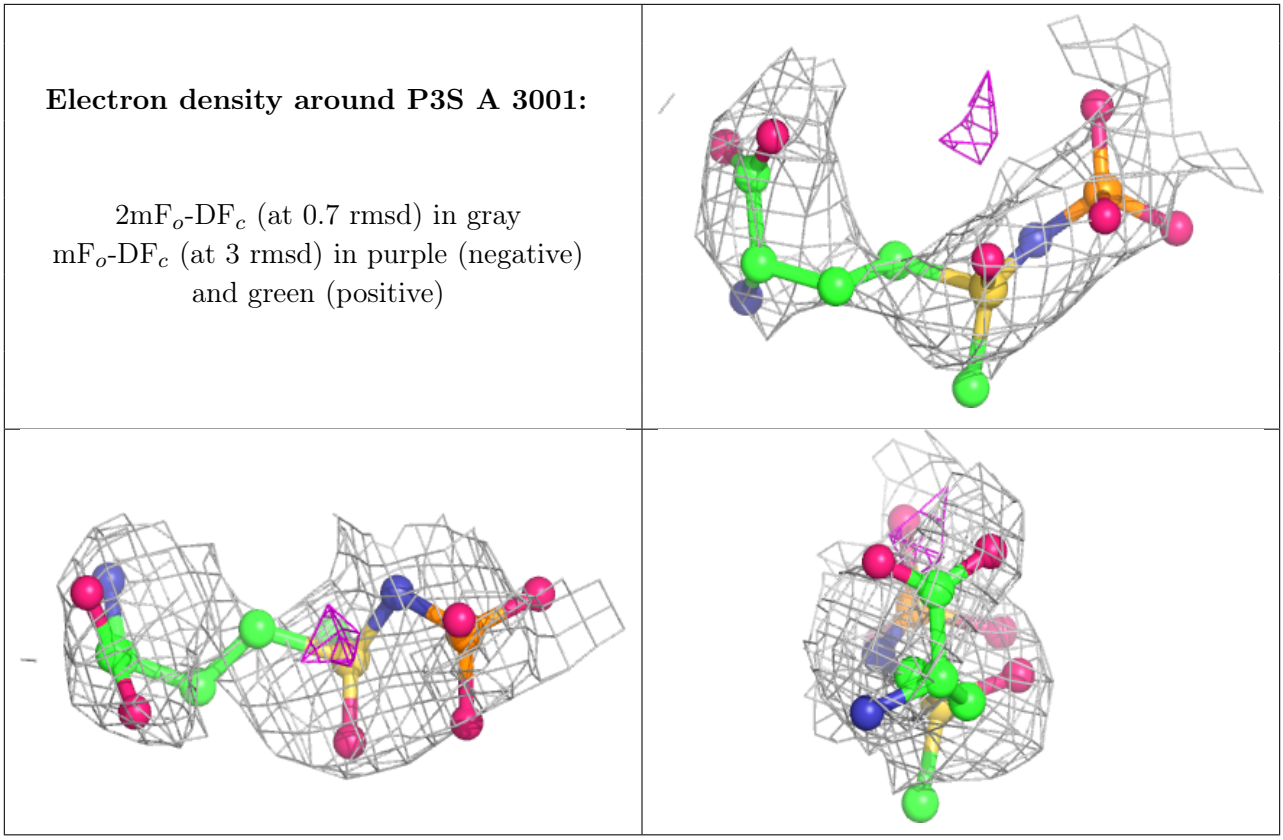






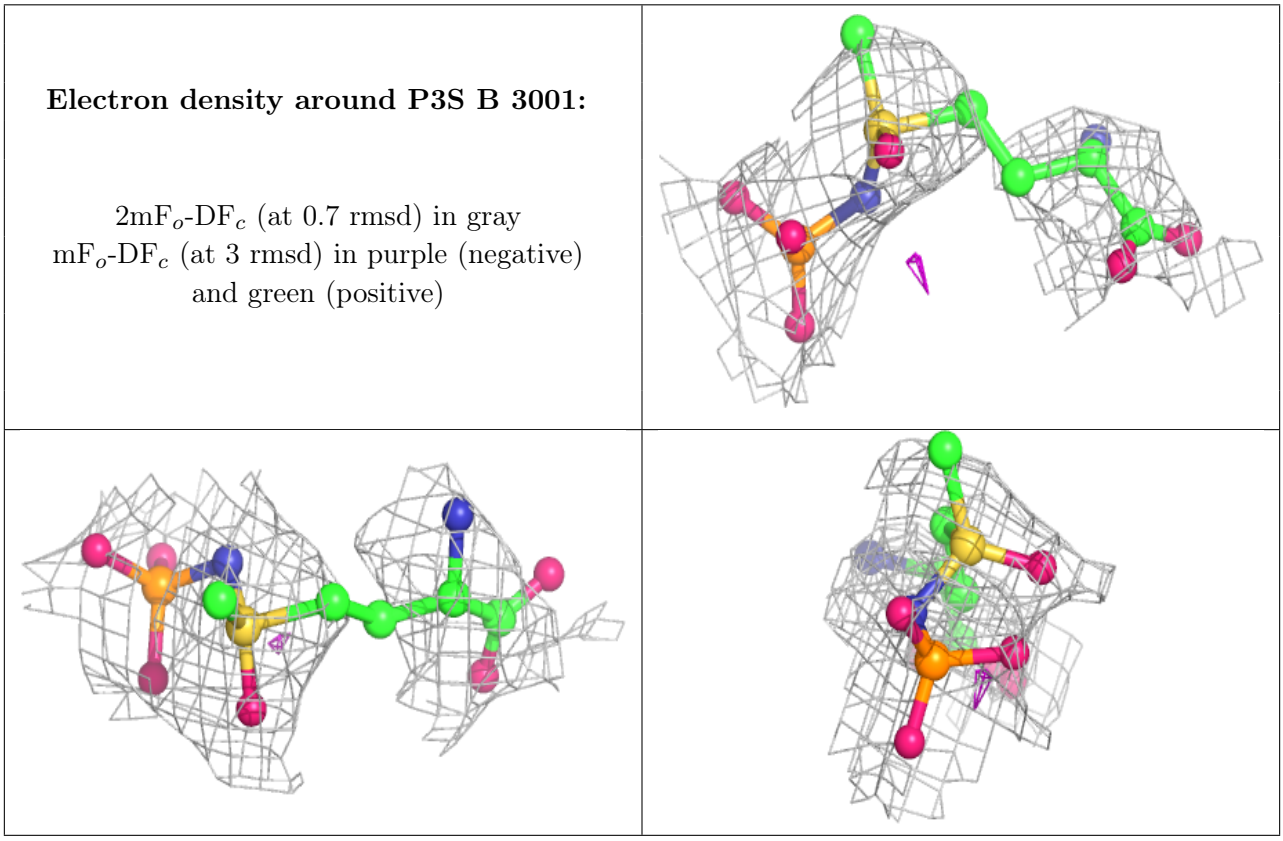
Electron density around P3S A 3001:

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



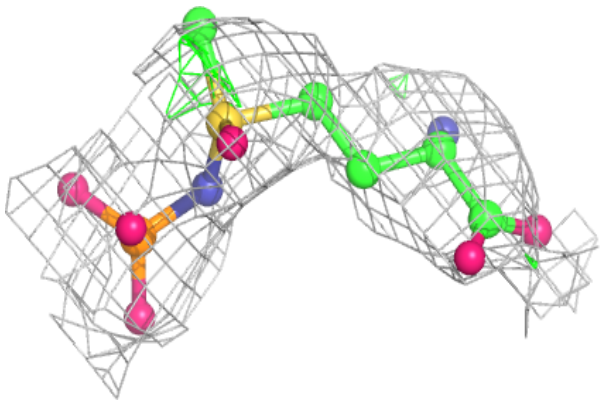
Electron density around P3S B 3001:

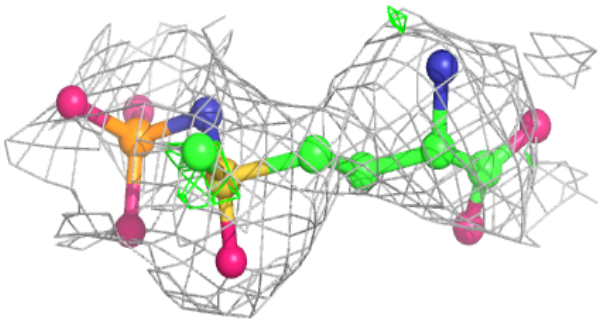
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

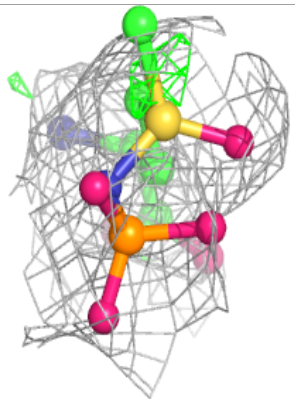


Electron density around P3S D 3001:

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

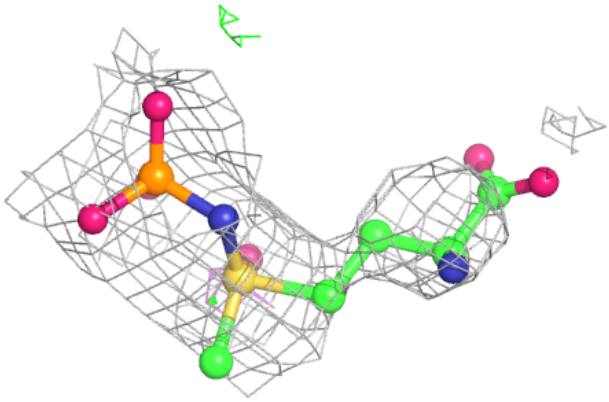


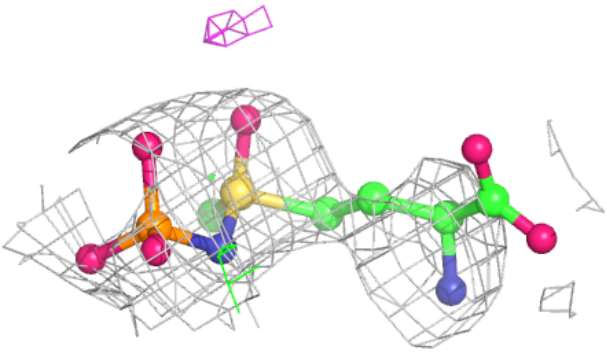


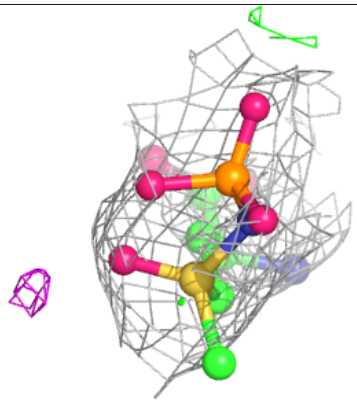


Electron density around P3S F 3001:

$2mF_o$-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.