Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 02:09 PM EDT

PDB ID	:	4XYJ
Title	:	Crystal structure of human phosphofructokinase-1 in complex with ATP and Mg, Northeast Structural Genomics Consortium Target HR9275
Authors	:	Forouhar, F.; Webb, B.A.; Szu, F.-E.; Seetharaman, J.; Barber, D.L.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2015-02-02
Resolution	:	3.10 Å(reported)

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

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

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

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

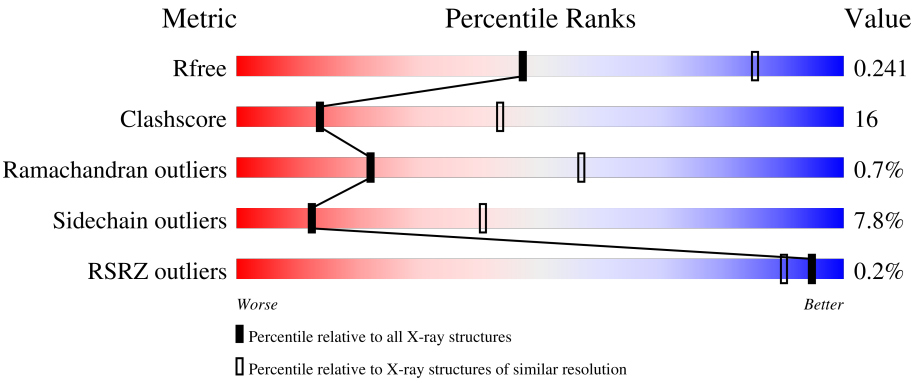
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	812	63% 29% • 5%
1	B	812	63% 28% • 5%
1	C	812	62% 28% • 6%
1	D	812	59% 31% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	812	60% 30% 6%
1	F	812	62% 28% 6%
1	G	812	% 61% 30% 6%
1	H	812	60% 28% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 47023 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	0	0
			5881	3689	1047	1106	39			
1	B	768	Total	C	N	O	S	0	0	0
			5880	3688	1047	1106	39			
1	C	760	Total	C	N	O	S	0	0	0
			5820	3652	1031	1098	39			
1	D	761	Total	C	N	O	S	0	0	0
			5825	3655	1032	1099	39			
1	E	765	Total	C	N	O	S	0	0	0
			5860	3675	1043	1103	39			
1	F	761	Total	C	N	O	S	0	0	0
			5823	3655	1030	1099	39			
1	G	760	Total	C	N	O	S	0	0	0
			5820	3652	1031	1098	39			
1	H	739	Total	C	N	O	S	0	0	0
			5644	3540	1003	1062	39			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q01813
A	-26	SER	-	expression tag	UNP Q01813
A	-25	TYR	-	expression tag	UNP Q01813
A	-24	TYR	-	expression tag	UNP Q01813
A	-23	HIS	-	expression tag	UNP Q01813
A	-22	HIS	-	expression tag	UNP Q01813
A	-21	HIS	-	expression tag	UNP Q01813
A	-20	HIS	-	expression tag	UNP Q01813
A	-19	HIS	-	expression tag	UNP Q01813
A	-18	HIS	-	expression tag	UNP Q01813
A	-17	ASP	-	expression tag	UNP Q01813
A	-16	TYR	-	expression tag	UNP Q01813
A	-15	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ILE	-	expression tag	UNP Q01813
A	-13	PRO	-	expression tag	UNP Q01813
A	-12	THR	-	expression tag	UNP Q01813
A	-11	THR	-	expression tag	UNP Q01813
A	-10	GLU	-	expression tag	UNP Q01813
A	-9	ASN	-	expression tag	UNP Q01813
A	-8	LEU	-	expression tag	UNP Q01813
A	-7	TYR	-	expression tag	UNP Q01813
A	-6	PHE	-	expression tag	UNP Q01813
A	-5	GLN	-	expression tag	UNP Q01813
A	-4	GLY	-	expression tag	UNP Q01813
A	-3	ALA	-	expression tag	UNP Q01813
A	-2	MET	-	expression tag	UNP Q01813
A	-1	ASP	-	expression tag	UNP Q01813
A	0	PRO	-	expression tag	UNP Q01813
B	-27	MET	-	initiating methionine	UNP Q01813
B	-26	SER	-	expression tag	UNP Q01813
B	-25	TYR	-	expression tag	UNP Q01813
B	-24	TYR	-	expression tag	UNP Q01813
B	-23	HIS	-	expression tag	UNP Q01813
B	-22	HIS	-	expression tag	UNP Q01813
B	-21	HIS	-	expression tag	UNP Q01813
B	-20	HIS	-	expression tag	UNP Q01813
B	-19	HIS	-	expression tag	UNP Q01813
B	-18	HIS	-	expression tag	UNP Q01813
B	-17	ASP	-	expression tag	UNP Q01813
B	-16	TYR	-	expression tag	UNP Q01813
B	-15	ASP	-	expression tag	UNP Q01813
B	-14	ILE	-	expression tag	UNP Q01813
B	-13	PRO	-	expression tag	UNP Q01813
B	-12	THR	-	expression tag	UNP Q01813
B	-11	THR	-	expression tag	UNP Q01813
B	-10	GLU	-	expression tag	UNP Q01813
B	-9	ASN	-	expression tag	UNP Q01813
B	-8	LEU	-	expression tag	UNP Q01813
B	-7	TYR	-	expression tag	UNP Q01813
B	-6	PHE	-	expression tag	UNP Q01813
B	-5	GLN	-	expression tag	UNP Q01813
B	-4	GLY	-	expression tag	UNP Q01813
B	-3	ALA	-	expression tag	UNP Q01813
B	-2	MET	-	expression tag	UNP Q01813
B	-1	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PRO	-	expression tag	UNP Q01813
C	-27	MET	-	initiating methionine	UNP Q01813
C	-26	SER	-	expression tag	UNP Q01813
C	-25	TYR	-	expression tag	UNP Q01813
C	-24	TYR	-	expression tag	UNP Q01813
C	-23	HIS	-	expression tag	UNP Q01813
C	-22	HIS	-	expression tag	UNP Q01813
C	-21	HIS	-	expression tag	UNP Q01813
C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	UNP Q01813
C	-13	PRO	-	expression tag	UNP Q01813
C	-12	THR	-	expression tag	UNP Q01813
C	-11	THR	-	expression tag	UNP Q01813
C	-10	GLU	-	expression tag	UNP Q01813
C	-9	ASN	-	expression tag	UNP Q01813
C	-8	LEU	-	expression tag	UNP Q01813
C	-7	TYR	-	expression tag	UNP Q01813
C	-6	PHE	-	expression tag	UNP Q01813
C	-5	GLN	-	expression tag	UNP Q01813
C	-4	GLY	-	expression tag	UNP Q01813
C	-3	ALA	-	expression tag	UNP Q01813
C	-2	MET	-	expression tag	UNP Q01813
C	-1	ASP	-	expression tag	UNP Q01813
C	0	PRO	-	expression tag	UNP Q01813
D	-27	MET	-	initiating methionine	UNP Q01813
D	-26	SER	-	expression tag	UNP Q01813
D	-25	TYR	-	expression tag	UNP Q01813
D	-24	TYR	-	expression tag	UNP Q01813
D	-23	HIS	-	expression tag	UNP Q01813
D	-22	HIS	-	expression tag	UNP Q01813
D	-21	HIS	-	expression tag	UNP Q01813
D	-20	HIS	-	expression tag	UNP Q01813
D	-19	HIS	-	expression tag	UNP Q01813
D	-18	HIS	-	expression tag	UNP Q01813
D	-17	ASP	-	expression tag	UNP Q01813
D	-16	TYR	-	expression tag	UNP Q01813
D	-15	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	ILE	-	expression tag	UNP Q01813
D	-13	PRO	-	expression tag	UNP Q01813
D	-12	THR	-	expression tag	UNP Q01813
D	-11	THR	-	expression tag	UNP Q01813
D	-10	GLU	-	expression tag	UNP Q01813
D	-9	ASN	-	expression tag	UNP Q01813
D	-8	LEU	-	expression tag	UNP Q01813
D	-7	TYR	-	expression tag	UNP Q01813
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813
E	-27	MET	-	initiating methionine	UNP Q01813
E	-26	SER	-	expression tag	UNP Q01813
E	-25	TYR	-	expression tag	UNP Q01813
E	-24	TYR	-	expression tag	UNP Q01813
E	-23	HIS	-	expression tag	UNP Q01813
E	-22	HIS	-	expression tag	UNP Q01813
E	-21	HIS	-	expression tag	UNP Q01813
E	-20	HIS	-	expression tag	UNP Q01813
E	-19	HIS	-	expression tag	UNP Q01813
E	-18	HIS	-	expression tag	UNP Q01813
E	-17	ASP	-	expression tag	UNP Q01813
E	-16	TYR	-	expression tag	UNP Q01813
E	-15	ASP	-	expression tag	UNP Q01813
E	-14	ILE	-	expression tag	UNP Q01813
E	-13	PRO	-	expression tag	UNP Q01813
E	-12	THR	-	expression tag	UNP Q01813
E	-11	THR	-	expression tag	UNP Q01813
E	-10	GLU	-	expression tag	UNP Q01813
E	-9	ASN	-	expression tag	UNP Q01813
E	-8	LEU	-	expression tag	UNP Q01813
E	-7	TYR	-	expression tag	UNP Q01813
E	-6	PHE	-	expression tag	UNP Q01813
E	-5	GLN	-	expression tag	UNP Q01813
E	-4	GLY	-	expression tag	UNP Q01813
E	-3	ALA	-	expression tag	UNP Q01813
E	-2	MET	-	expression tag	UNP Q01813
E	-1	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	PRO	-	expression tag	UNP Q01813
F	-27	MET	-	initiating methionine	UNP Q01813
F	-26	SER	-	expression tag	UNP Q01813
F	-25	TYR	-	expression tag	UNP Q01813
F	-24	TYR	-	expression tag	UNP Q01813
F	-23	HIS	-	expression tag	UNP Q01813
F	-22	HIS	-	expression tag	UNP Q01813
F	-21	HIS	-	expression tag	UNP Q01813
F	-20	HIS	-	expression tag	UNP Q01813
F	-19	HIS	-	expression tag	UNP Q01813
F	-18	HIS	-	expression tag	UNP Q01813
F	-17	ASP	-	expression tag	UNP Q01813
F	-16	TYR	-	expression tag	UNP Q01813
F	-15	ASP	-	expression tag	UNP Q01813
F	-14	ILE	-	expression tag	UNP Q01813
F	-13	PRO	-	expression tag	UNP Q01813
F	-12	THR	-	expression tag	UNP Q01813
F	-11	THR	-	expression tag	UNP Q01813
F	-10	GLU	-	expression tag	UNP Q01813
F	-9	ASN	-	expression tag	UNP Q01813
F	-8	LEU	-	expression tag	UNP Q01813
F	-7	TYR	-	expression tag	UNP Q01813
F	-6	PHE	-	expression tag	UNP Q01813
F	-5	GLN	-	expression tag	UNP Q01813
F	-4	GLY	-	expression tag	UNP Q01813
F	-3	ALA	-	expression tag	UNP Q01813
F	-2	MET	-	expression tag	UNP Q01813
F	-1	ASP	-	expression tag	UNP Q01813
F	0	PRO	-	expression tag	UNP Q01813
G	-27	MET	-	initiating methionine	UNP Q01813
G	-26	SER	-	expression tag	UNP Q01813
G	-25	TYR	-	expression tag	UNP Q01813
G	-24	TYR	-	expression tag	UNP Q01813
G	-23	HIS	-	expression tag	UNP Q01813
G	-22	HIS	-	expression tag	UNP Q01813
G	-21	HIS	-	expression tag	UNP Q01813
G	-20	HIS	-	expression tag	UNP Q01813
G	-19	HIS	-	expression tag	UNP Q01813
G	-18	HIS	-	expression tag	UNP Q01813
G	-17	ASP	-	expression tag	UNP Q01813
G	-16	TYR	-	expression tag	UNP Q01813
G	-15	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

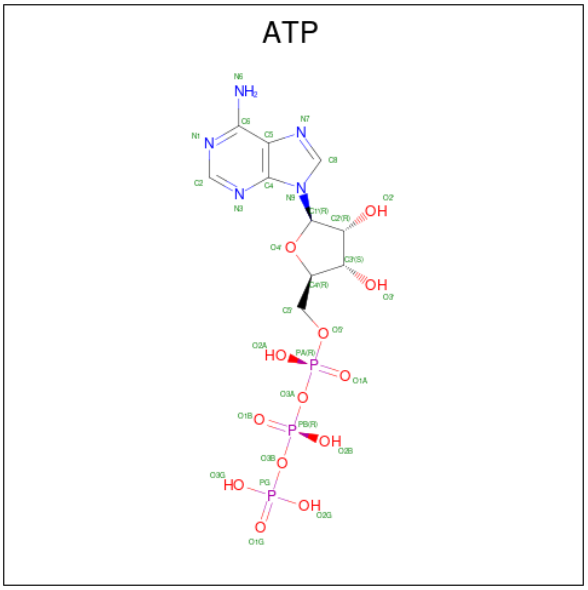
Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	ILE	-	expression tag	UNP Q01813
G	-13	PRO	-	expression tag	UNP Q01813
G	-12	THR	-	expression tag	UNP Q01813
G	-11	THR	-	expression tag	UNP Q01813
G	-10	GLU	-	expression tag	UNP Q01813
G	-9	ASN	-	expression tag	UNP Q01813
G	-8	LEU	-	expression tag	UNP Q01813
G	-7	TYR	-	expression tag	UNP Q01813
G	-6	PHE	-	expression tag	UNP Q01813
G	-5	GLN	-	expression tag	UNP Q01813
G	-4	GLY	-	expression tag	UNP Q01813
G	-3	ALA	-	expression tag	UNP Q01813
G	-2	MET	-	expression tag	UNP Q01813
G	-1	ASP	-	expression tag	UNP Q01813
G	0	PRO	-	expression tag	UNP Q01813
H	-27	MET	-	initiating methionine	UNP Q01813
H	-26	SER	-	expression tag	UNP Q01813
H	-25	TYR	-	expression tag	UNP Q01813
H	-24	TYR	-	expression tag	UNP Q01813
H	-23	HIS	-	expression tag	UNP Q01813
H	-22	HIS	-	expression tag	UNP Q01813
H	-21	HIS	-	expression tag	UNP Q01813
H	-20	HIS	-	expression tag	UNP Q01813
H	-19	HIS	-	expression tag	UNP Q01813
H	-18	HIS	-	expression tag	UNP Q01813
H	-17	ASP	-	expression tag	UNP Q01813
H	-16	TYR	-	expression tag	UNP Q01813
H	-15	ASP	-	expression tag	UNP Q01813
H	-14	ILE	-	expression tag	UNP Q01813
H	-13	PRO	-	expression tag	UNP Q01813
H	-12	THR	-	expression tag	UNP Q01813
H	-11	THR	-	expression tag	UNP Q01813
H	-10	GLU	-	expression tag	UNP Q01813
H	-9	ASN	-	expression tag	UNP Q01813
H	-8	LEU	-	expression tag	UNP Q01813
H	-7	TYR	-	expression tag	UNP Q01813
H	-6	PHE	-	expression tag	UNP Q01813
H	-5	GLN	-	expression tag	UNP Q01813
H	-4	GLY	-	expression tag	UNP Q01813
H	-3	ALA	-	expression tag	UNP Q01813
H	-2	MET	-	expression tag	UNP Q01813
H	-1	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	PRO	-	expression tag	UNP Q01813

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

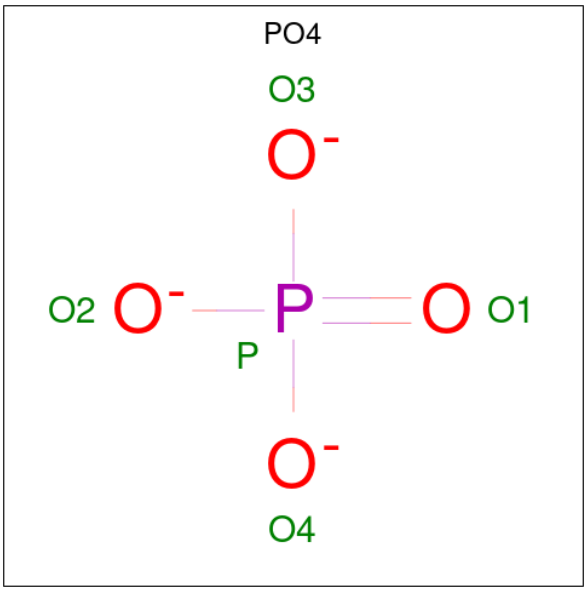


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	E	2	Total Mg 2 2	0	0
3	F	2	Total Mg 2 2	0	0
3	G	2	Total Mg 2 2	0	0
3	H	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0

- Molecule 5 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Co 1 1	0	0
5	F	1	Total Co 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	29	Total O 29 29	0	0
6	B	28	Total O 28 28	0	0
6	C	11	Total O 11 11	0	0
6	D	9	Total O 9 9	0	0
6	E	18	Total O 18 18	0	0
6	F	16	Total O 16 16	0	0
6	G	21	Total O 21 21	0	0

Continued on next page...

Continued from previous page...

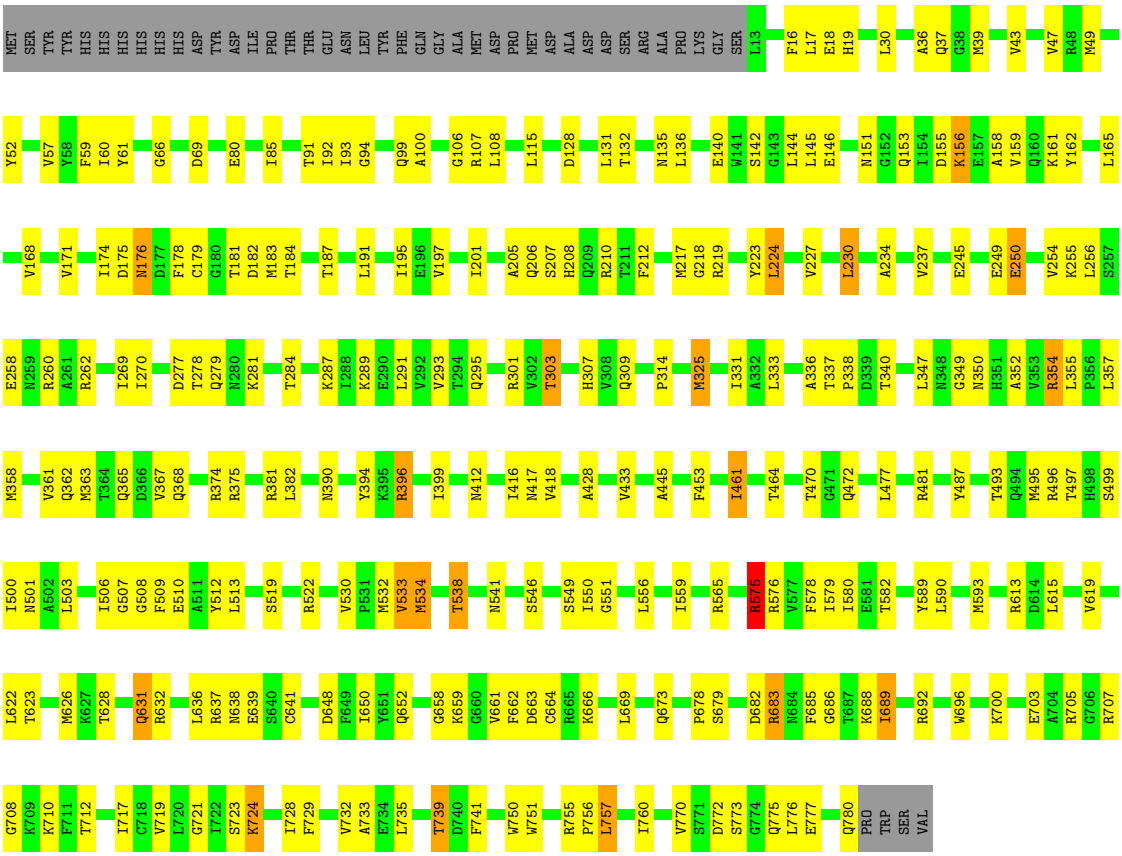
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	13	Total O 13 13	0	0

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.

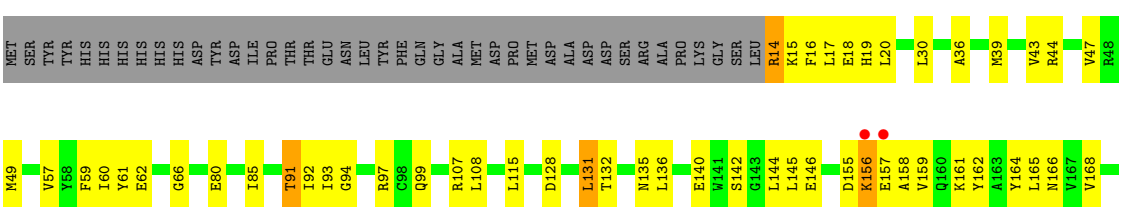
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

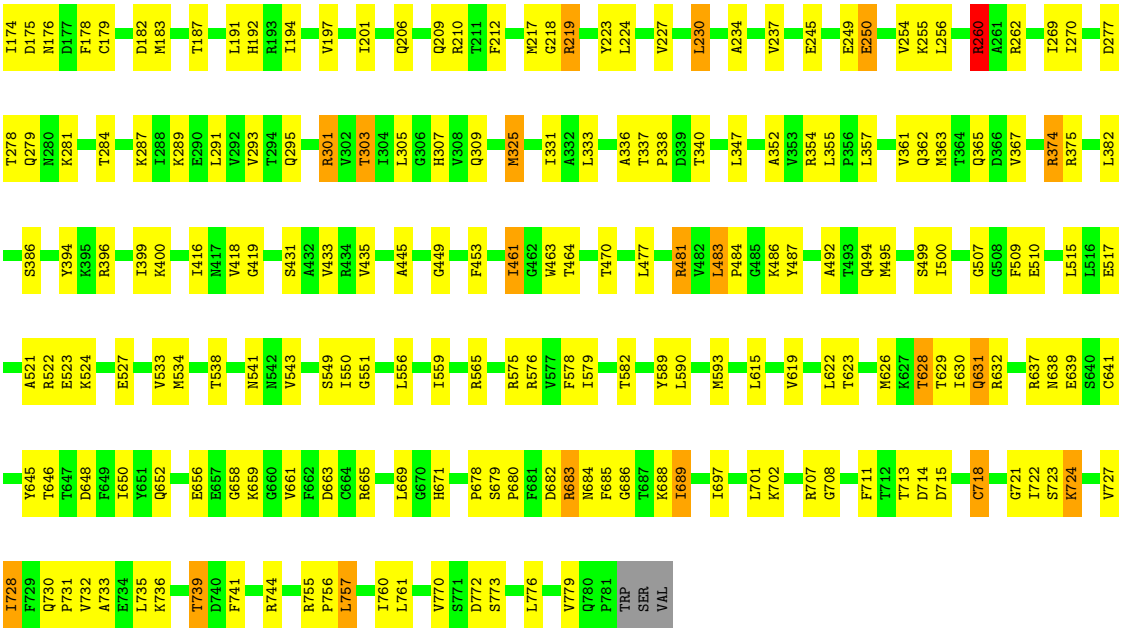
Chain A:



• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

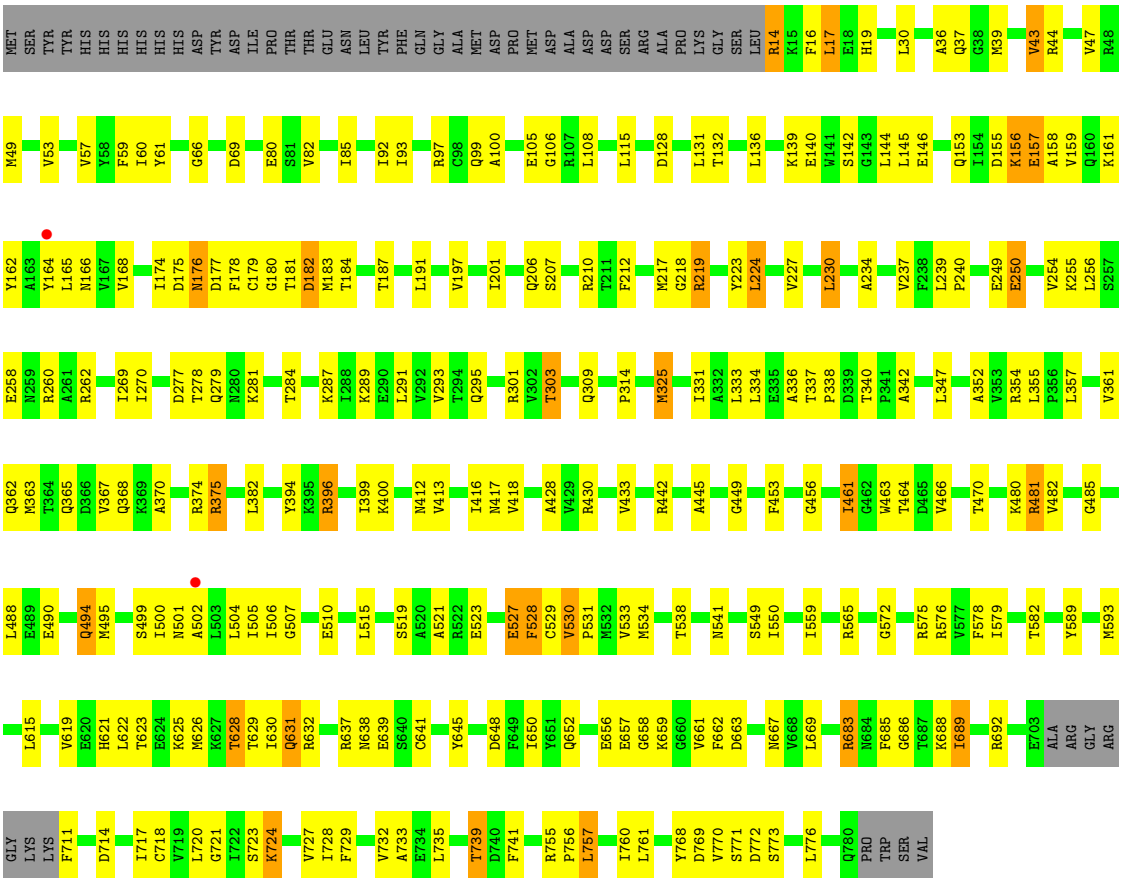
Chain B:





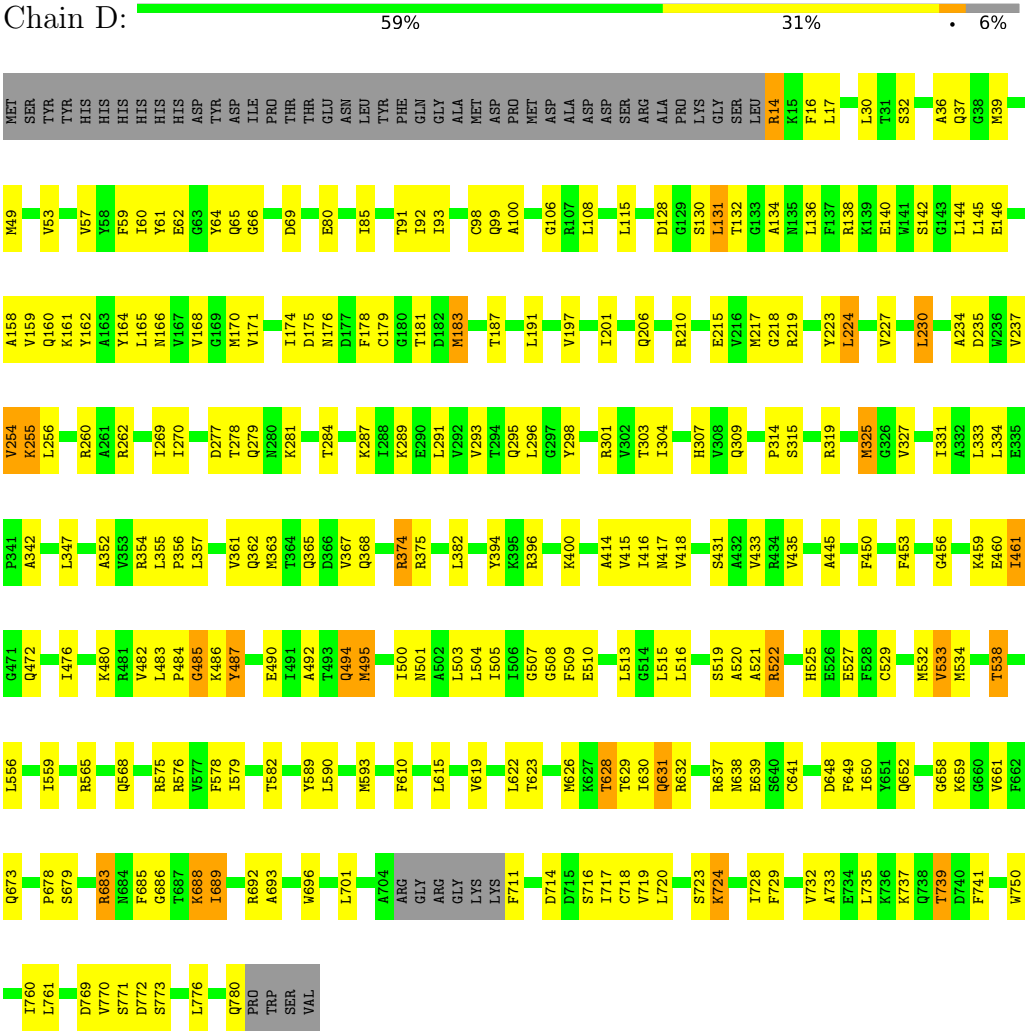
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain C:



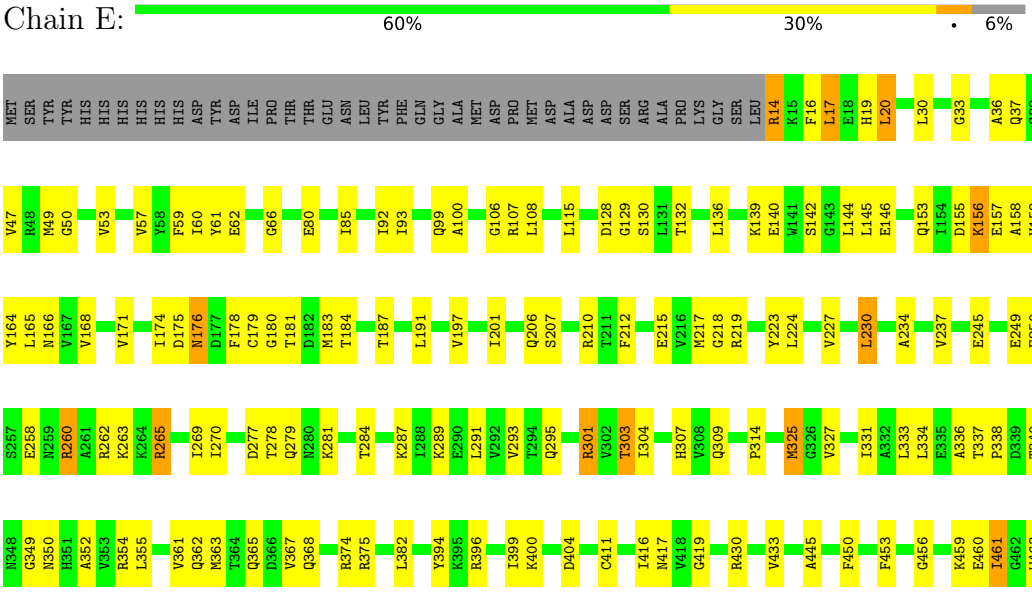
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

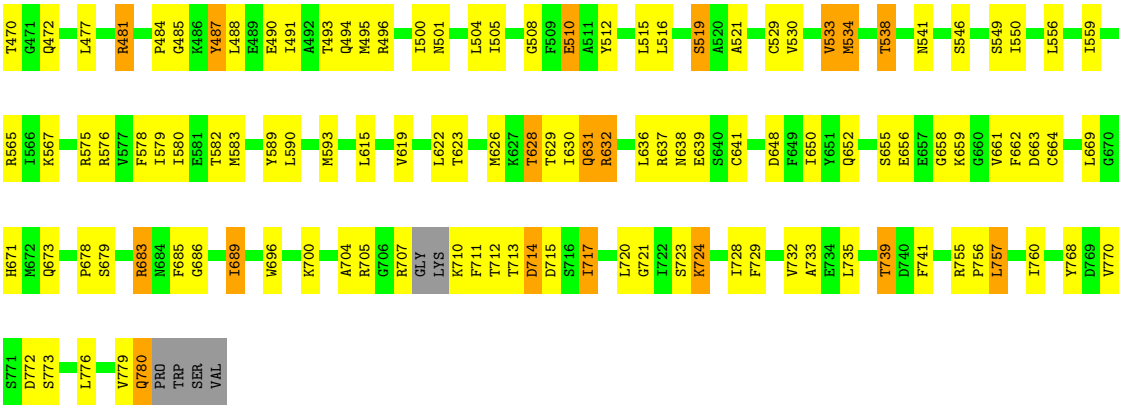
Chain D:



• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

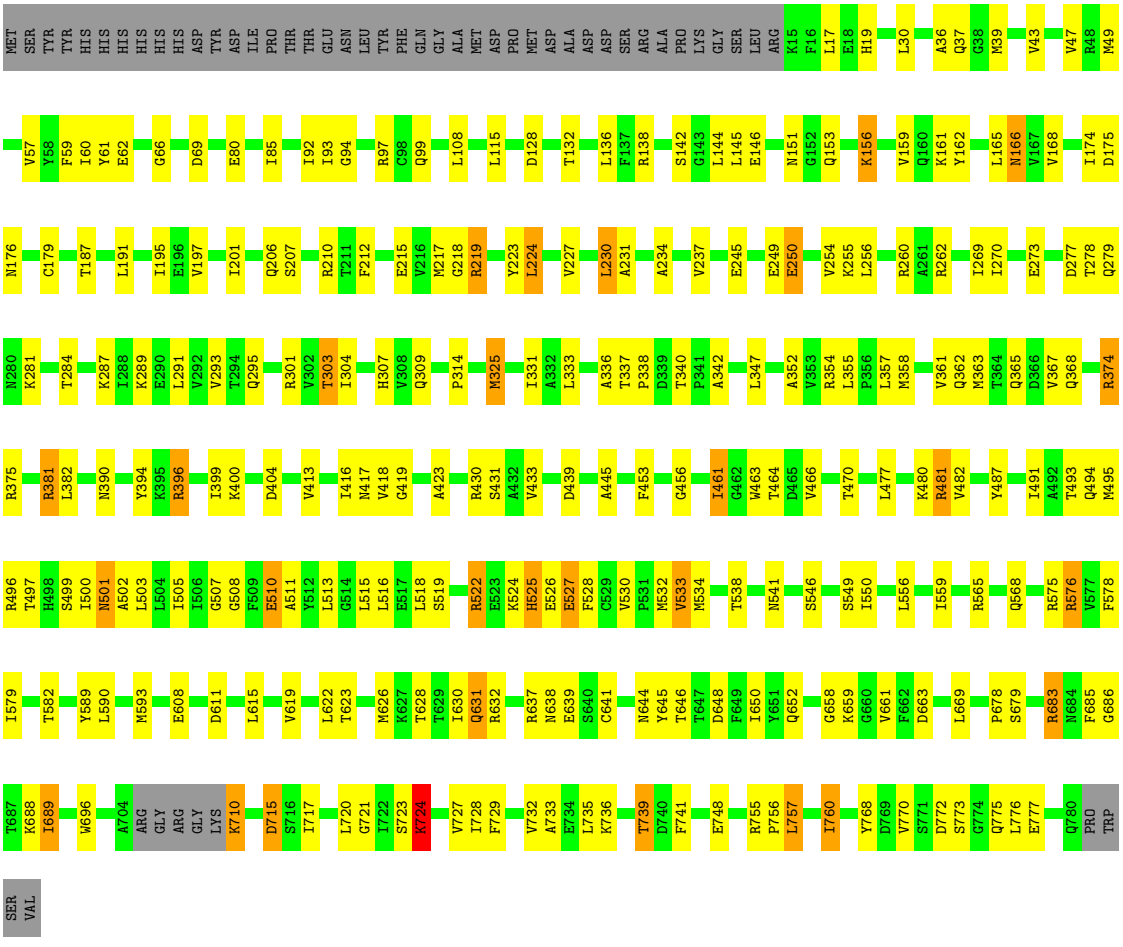
Chain E:





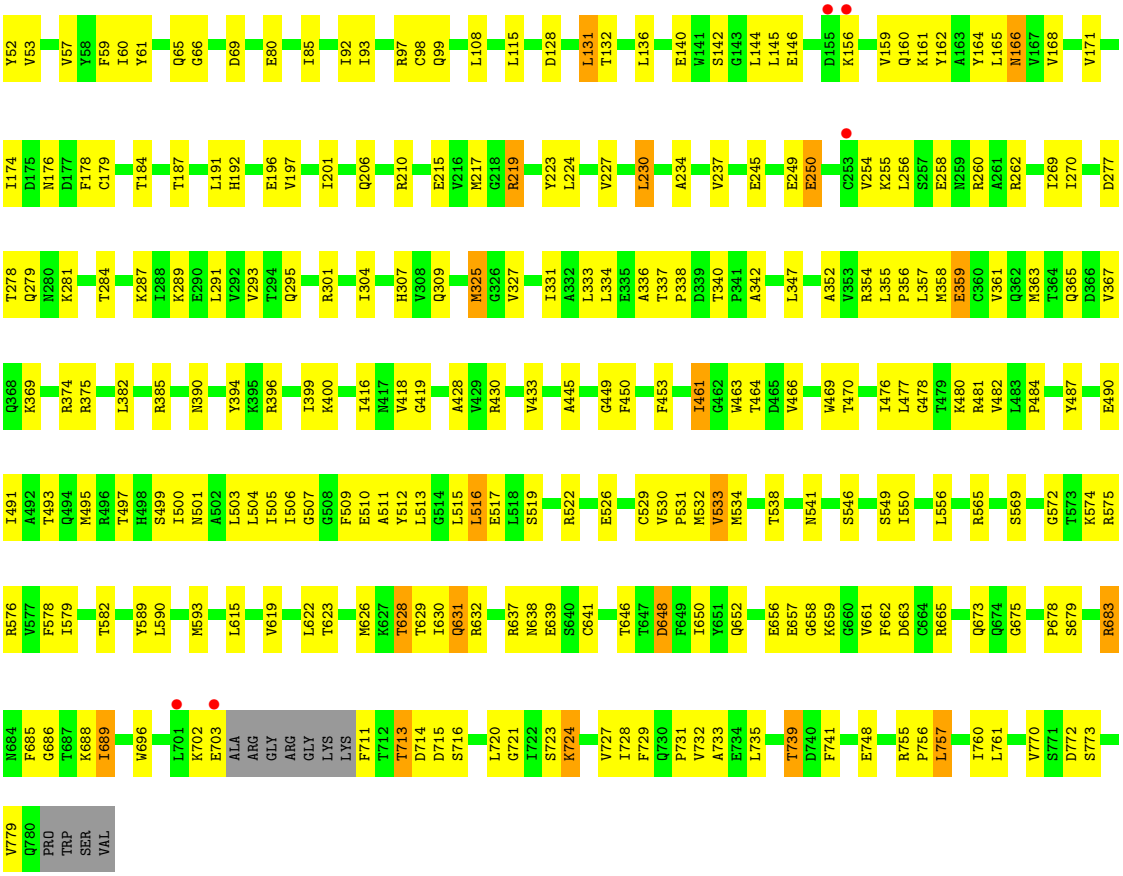
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain F:



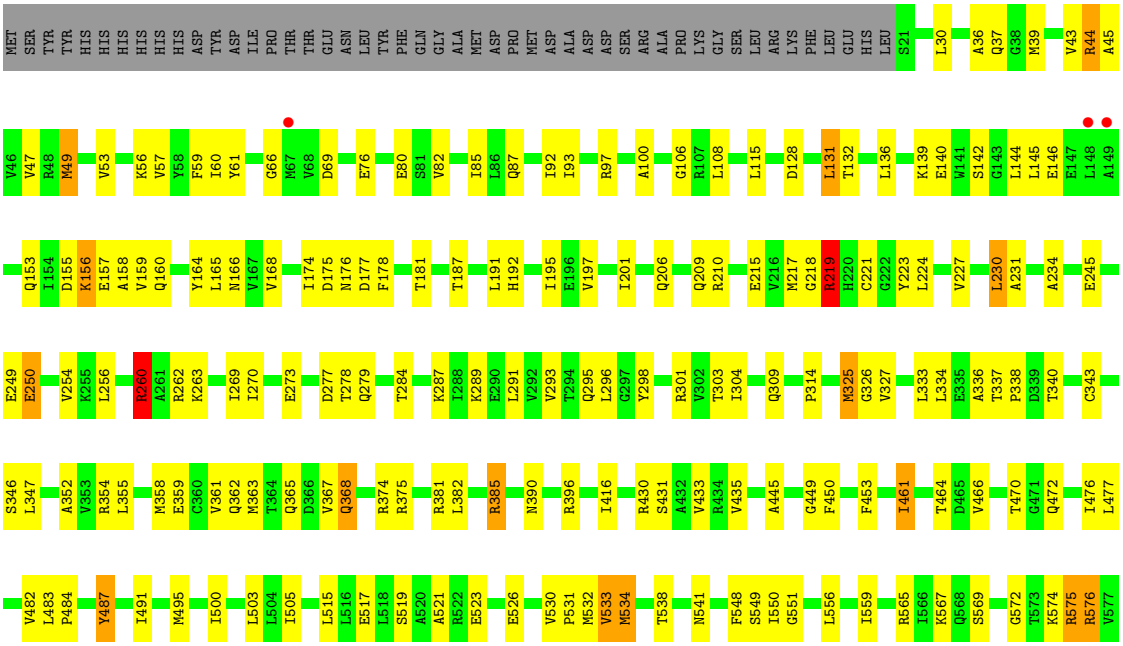
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

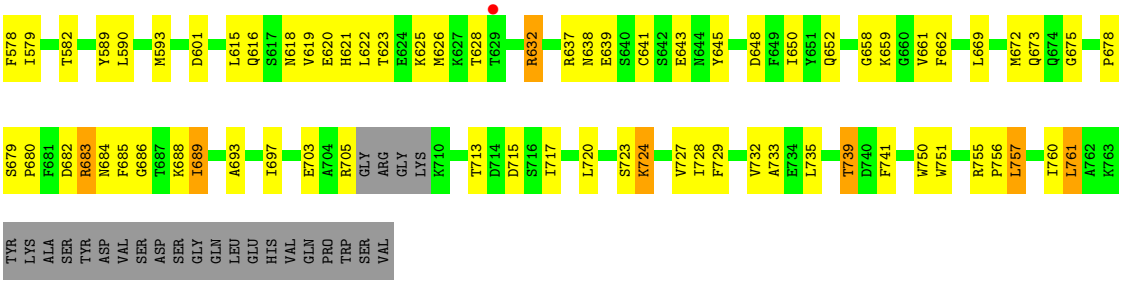
Chain G:



• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain H:




F578 I579 T582 Y589 L590 M593 D601 L615 Q616 S617 N618 V619 E620 H621 L622 T623 E624 K625 M626 K627 T628 T629 R632 R637 N638 E639 S640 C641 S642 E643 N644 Y645 D648 F649 I650 Y651 Q652 G658 K659 G660 V661 F662 L669 M672 Q673 Q674 G675 P678
S679 P680 F681 D682 R683 N684 F685 G686 T687 K688 I689 A693 I697 E703 A704 R705 GLY ARG GLY LYS K710 T713 D714 D715 S716 I717 L720 S723 K724 V727 I728 F729 V732 A733 E734 L735 T739 D740 F741 W750 W751 R755 P756 L757 I760 L761 A762 K763
TYR LYS ALA SER TYR ASP VAL SER ASP SER GLY GLN LEU GLU HIS VAL GLN PRO TRP SER VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.20Å 159.33Å 170.53Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	49.69 – 3.10 49.69 – 3.08	Depositor EDS
% Data completeness (in resolution range)	85.0 (49.69-3.10) 84.2 (49.69-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.07Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.221 , 0.246 0.215 , 0.241	Depositor DCC
R_{free} test set	12011 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	47023	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, ATP, CO

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	0.46	1/5977 (0.0%)	1.25	29/8067 (0.4%)
1	B	0.45	0/5977	0.75	8/8068 (0.1%)
1	C	0.42	0/5915	0.77	12/7986 (0.2%)
1	D	0.42	0/5920	0.75	8/7993 (0.1%)
1	E	0.42	0/5955	0.85	12/8037 (0.1%)
1	F	0.42	0/5918	0.86	12/7990 (0.2%)
1	G	0.41	0/5915	0.70	8/7986 (0.1%)
1	H	0.43	0/5734	0.83	12/7741 (0.2%)
All	All	0.43	1/47311 (0.0%)	0.86	101/63868 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	4
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	3
1	G	0	1
1	H	0	6
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	CYS	CB-SG	-5.67	1.72	1.81

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	ARG	NE-CZ-NH2	-27.87	106.36	120.30
1	A	575	ARG	NE-CZ-NH2	-26.89	106.85	120.30
1	H	219	ARG	NE-CZ-NH1	-26.18	107.21	120.30
1	A	613	ARG	NE-CZ-NH1	-26.11	107.24	120.30
1	F	138	ARG	NE-CZ-NH2	-26.08	107.26	120.30
1	A	396	ARG	NE-CZ-NH1	26.06	133.33	120.30
1	A	575	ARG	NE-CZ-NH1	25.59	133.09	120.30
1	H	219	ARG	NE-CZ-NH2	25.36	132.98	120.30
1	F	138	ARG	NE-CZ-NH1	24.92	132.76	120.30
1	A	613	ARG	NE-CZ-NH2	24.86	132.73	120.30
1	A	692	ARG	NE-CZ-NH2	-24.35	108.12	120.30
1	A	381	ARG	NE-CZ-NH2	22.47	131.53	120.30
1	A	692	ARG	NE-CZ-NH1	22.46	131.53	120.30
1	A	381	ARG	NE-CZ-NH1	-22.33	109.14	120.30
1	E	260	ARG	NE-CZ-NH2	-22.09	109.25	120.30
1	A	565	ARG	NE-CZ-NH1	-21.22	109.69	120.30
1	E	260	ARG	NE-CZ-NH1	21.01	130.81	120.30
1	E	565	ARG	NE-CZ-NH1	-20.83	109.88	120.30
1	A	354	ARG	NE-CZ-NH1	-20.52	110.04	120.30
1	A	354	ARG	NE-CZ-NH2	20.18	130.39	120.30
1	C	683	ARG	NE-CZ-NH1	-20.07	110.26	120.30
1	A	565	ARG	NE-CZ-NH2	19.76	130.18	120.30
1	E	565	ARG	NE-CZ-NH2	18.76	129.68	120.30
1	C	683	ARG	NE-CZ-NH2	17.87	129.24	120.30
1	F	374	ARG	NE-CZ-NH2	-17.27	111.66	120.30
1	B	374	ARG	NE-CZ-NH2	-17.09	111.76	120.30
1	F	374	ARG	NE-CZ-NH1	17.04	128.82	120.30
1	D	374	ARG	NE-CZ-NH2	-16.62	111.99	120.30
1	B	374	ARG	NE-CZ-NH1	16.55	128.58	120.30
1	D	374	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	E	375	ARG	NE-CZ-NH2	-14.13	113.24	120.30
1	H	375	ARG	NE-CZ-NH1	-14.05	113.27	120.30
1	C	375	ARG	NE-CZ-NH2	-13.91	113.34	120.30
1	D	375	ARG	NE-CZ-NH1	-13.89	113.36	120.30
1	A	396	ARG	CD-NE-CZ	13.72	142.80	123.60
1	A	375	ARG	NE-CZ-NH2	13.38	126.99	120.30
1	F	375	ARG	NE-CZ-NH2	-13.36	113.62	120.30
1	B	375	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	D	375	ARG	NE-CZ-NH2	13.29	126.94	120.30
1	H	219	ARG	CD-NE-CZ	13.18	142.04	123.60
1	G	375	ARG	NE-CZ-NH1	-13.14	113.73	120.30
1	H	375	ARG	NE-CZ-NH2	13.05	126.83	120.30
1	C	375	ARG	NE-CZ-NH1	12.91	126.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	375	ARG	NE-CZ-NH1	12.91	126.76	120.30
1	F	375	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	G	375	ARG	NE-CZ-NH2	12.72	126.66	120.30
1	A	375	ARG	NE-CZ-NH1	-12.72	113.94	120.30
1	A	613	ARG	CD-NE-CZ	12.38	140.93	123.60
1	A	575	ARG	CD-NE-CZ	12.38	140.93	123.60
1	B	375	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	F	138	ARG	CD-NE-CZ	12.00	140.40	123.60
1	A	381	ARG	CD-NE-CZ	11.58	139.81	123.60
1	C	374	ARG	NE-CZ-NH1	-10.69	114.95	120.30
1	E	374	ARG	NE-CZ-NH1	-10.44	115.08	120.30
1	A	692	ARG	CD-NE-CZ	10.29	138.00	123.60
1	G	374	ARG	NE-CZ-NH1	-10.13	115.23	120.30
1	E	260	ARG	CD-NE-CZ	10.12	137.76	123.60
1	A	374	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	A	565	ARG	CD-NE-CZ	10.02	137.63	123.60
1	E	565	ARG	CD-NE-CZ	9.97	137.57	123.60
1	H	374	ARG	NE-CZ-NH1	-9.90	115.35	120.30
1	G	374	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	C	374	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	H	374	ARG	NE-CZ-NH2	8.99	124.79	120.30
1	A	374	ARG	NE-CZ-NH2	8.95	124.78	120.30
1	E	374	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	F	374	ARG	CD-NE-CZ	8.76	135.87	123.60
1	B	374	ARG	CD-NE-CZ	8.57	135.60	123.60
1	A	354	ARG	CD-NE-CZ	8.47	135.46	123.60
1	D	374	ARG	CD-NE-CZ	8.45	135.43	123.60
1	C	683	ARG	CD-NE-CZ	7.69	134.37	123.60
1	A	396	ARG	CG-CD-NE	-7.43	96.21	111.80
1	F	565	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	H	565	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	565	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	375	ARG	CD-NE-CZ	6.87	133.22	123.60
1	F	565	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	G	375	ARG	CD-NE-CZ	6.81	133.14	123.60
1	G	565	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	D	565	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	E	375	ARG	CD-NE-CZ	6.78	133.08	123.60
1	C	565	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	D	375	ARG	CD-NE-CZ	6.72	133.00	123.60
1	D	565	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	375	ARG	CD-NE-CZ	6.65	132.91	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	375	ARG	CD-NE-CZ	6.64	132.90	123.60
1	C	565	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	F	375	ARG	CD-NE-CZ	6.61	132.85	123.60
1	C	375	ARG	CD-NE-CZ	6.58	132.81	123.60
1	H	565	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	G	565	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	565	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	F	138	ARG	CG-CD-NE	-5.40	100.45	111.80
1	C	374	ARG	CD-NE-CZ	5.35	131.09	123.60
1	A	354	ARG	CG-CD-NE	5.34	123.02	111.80
1	G	374	ARG	CD-NE-CZ	5.33	131.07	123.60
1	H	374	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	374	ARG	CD-NE-CZ	5.26	130.97	123.60
1	C	683	ARG	CB-CG-CD	-5.26	97.91	111.60
1	H	219	ARG	CG-CD-NE	-5.20	100.88	111.80
1	E	374	ARG	CD-NE-CZ	5.09	130.73	123.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	219	ARG	Sidechain
1	B	260	ARG	Sidechain
1	B	665	ARG	Sidechain
1	B	97	ARG	Sidechain
1	C	396	ARG	Sidechain
1	C	442	ARG	Sidechain
1	D	138	ARG	Sidechain
1	D	487	TYR	Sidechain
1	E	265	ARG	Sidechain
1	E	301	ARG	Sidechain
1	F	219	ARG	Sidechain
1	F	381	ARG	Sidechain
1	F	576	ARG	Sidechain
1	G	14	ARG	Sidechain
1	H	260	ARG	Sidechain
1	H	381	ARG	Sidechain
1	H	385	ARG	Sidechain
1	H	44	ARG	Sidechain
1	H	575	ARG	Sidechain
1	H	576	ARG	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	5881	0	5912	195	0
1	B	5880	0	5908	186	0
1	C	5820	0	5837	183	0
1	D	5825	0	5842	197	0
1	E	5860	0	5884	211	0
1	F	5823	0	5842	191	0
1	G	5820	0	5837	198	0
1	H	5644	0	5678	180	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
6	A	29	0	0	0	0
6	B	28	0	0	1	0
6	C	11	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	9	0	0	0	0
6	E	18	0	0	0	0
6	F	16	0	0	0	0
6	G	21	0	0	1	0
6	H	13	0	0	2	0
All	All	47023	0	46836	1489	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1489) 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:307:HIS:HE1	1:B:303:THR:HG22	1.04	1.16
1:B:481:ARG:HH11	1:B:481:ARG:HB2	1.01	1.13
1:H:166:ASN:ND2	1:H:336:ALA:HB3	1.63	1.12
1:H:166:ASN:HD21	1:H:336:ALA:CB	1.64	1.10
1:E:710:LYS:HE2	1:E:710:LYS:HA	1.38	1.02
1:A:307:HIS:CE1	1:B:303:THR:HG22	1.96	1.01
1:H:166:ASN:HD21	1:H:336:ALA:HB3	0.83	0.98
1:F:501:ASN:O	1:F:530:VAL:HB	1.66	0.95
1:A:303:THR:HG22	1:B:307:HIS:HE1	1.31	0.94
1:E:307:HIS:HE1	1:F:303:THR:HG22	1.33	0.93
1:B:132:THR:HG22	1:B:361:VAL:HG13	1.51	0.92
1:D:14:ARG:HB2	1:D:14:ARG:NH1	1.85	0.91
1:B:481:ARG:HB2	1:B:481:ARG:NH1	1.85	0.91
1:A:307:HIS:HE1	1:B:303:THR:CG2	1.83	0.91
1:E:164:TYR:CD2	1:E:338:PRO:HB3	2.06	0.91
1:B:164:TYR:CD2	1:B:338:PRO:HB3	2.08	0.87
1:B:481:ARG:HH11	1:B:481:ARG:CB	1.86	0.86
1:G:713:THR:HG23	1:G:716:SER:HB3	1.56	0.86
1:E:132:THR:HG22	1:E:361:VAL:HG13	1.54	0.86
1:E:171:VAL:HG21	1:E:181:THR:HG21	1.57	0.85
1:B:132:THR:CG2	1:B:361:VAL:HG13	2.07	0.85
1:F:419:GLY:HA2	1:F:510:GLU:HG3	1.57	0.85
1:B:735:LEU:O	1:B:739:THR:HG22	1.77	0.85
1:F:735:LEU:O	1:F:739:THR:HG22	1.76	0.84
1:A:735:LEU:O	1:A:739:THR:HG22	1.77	0.84
1:G:17:LEU:HD21	1:G:49:MET:HE3	1.57	0.84
1:C:735:LEU:O	1:C:739:THR:HG22	1.78	0.84
1:H:132:THR:HG22	1:H:361:VAL:HG13	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:THR:HG22	1:F:361:VAL:HG13	1.58	0.82
1:E:735:LEU:O	1:E:739:THR:HG22	1.79	0.82
1:A:501:ASN:O	1:A:530:VAL:HB	1.79	0.82
1:D:735:LEU:O	1:D:739:THR:HG22	1.79	0.82
1:A:510:GLU:HA	1:A:513:LEU:HD12	1.60	0.81
1:G:132:THR:HG22	1:G:361:VAL:HG13	1.62	0.81
1:G:735:LEU:O	1:G:739:THR:HG22	1.80	0.81
1:H:735:LEU:O	1:H:739:THR:HG22	1.81	0.81
1:C:481:ARG:HH11	1:C:481:ARG:HB2	1.44	0.81
1:E:174:ILE:HD11	1:E:217:MET:SD	2.21	0.81
1:G:174:ILE:HD11	1:G:217:MET:SD	2.21	0.81
1:E:411:CYS:HA	1:E:501:ASN:OD1	1.80	0.80
1:E:207:SER:HB3	1:F:62:GLU:OE2	1.82	0.79
1:F:49:MET:SD	1:F:760:ILE:HD11	2.21	0.79
1:A:132:THR:HG22	1:A:361:VAL:HG13	1.64	0.79
1:A:519:SER:O	1:A:522:ARG:HG2	1.81	0.78
1:B:174:ILE:HD11	1:B:217:MET:SD	2.23	0.78
1:E:212:PHE:HE1	1:E:303:THR:HG23	1.48	0.78
1:D:132:THR:HG22	1:D:361:VAL:HG13	1.66	0.77
1:G:678:PRO:HG2	1:G:683:ARG:HD2	1.67	0.77
1:E:166:ASN:ND2	1:E:336:ALA:HB3	2.00	0.76
1:A:678:PRO:HG2	1:A:683:ARG:HD2	1.68	0.76
1:H:678:PRO:HG2	1:H:683:ARG:HD2	1.66	0.76
1:E:678:PRO:HG2	1:E:683:ARG:HD2	1.67	0.76
1:F:678:PRO:HG2	1:F:683:ARG:HD2	1.67	0.76
1:B:723:SER:CB	1:B:728:ILE:HD11	2.15	0.76
1:D:678:PRO:HG2	1:D:683:ARG:HD2	1.67	0.76
1:C:519:SER:HB2	1:C:717:ILE:HD12	1.67	0.76
1:E:217:MET:HG3	1:E:309:GLN:NE2	2.01	0.76
1:C:132:THR:HG22	1:C:361:VAL:HG13	1.67	0.75
1:H:217:MET:HG3	1:H:309:GLN:NE2	2.02	0.75
1:B:217:MET:HG3	1:B:309:GLN:NE2	2.03	0.74
1:B:678:PRO:HG2	1:B:683:ARG:HD2	1.68	0.74
1:D:14:ARG:HB2	1:D:14:ARG:CZ	2.16	0.74
1:C:145:LEU:HB3	1:C:159:VAL:HG23	1.70	0.74
1:G:217:MET:HG3	1:G:309:GLN:NE2	2.03	0.73
1:G:179:CYS:SG	1:G:367:VAL:HG21	2.28	0.73
1:F:174:ILE:HD11	1:F:217:MET:SD	2.27	0.73
1:H:145:LEU:HB3	1:H:159:VAL:HG23	1.71	0.73
1:E:419:GLY:HA2	1:E:510:GLU:HG3	1.69	0.73
1:D:174:ILE:HD11	1:D:217:MET:SD	2.29	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:MET:HG3	1:A:309:GLN:NE2	2.04	0.72
1:H:177:ASP:HB3	1:H:221:CYS:HB2	1.69	0.72
1:F:217:MET:HG3	1:F:309:GLN:NE2	2.04	0.72
1:C:16:PHE:HB2	1:C:19:HIS:CD2	2.24	0.72
1:D:145:LEU:HB3	1:D:159:VAL:HG23	1.70	0.72
1:H:505:ILE:HD12	1:H:515:LEU:HD21	1.71	0.72
1:A:49:MET:SD	1:A:760:ILE:HD11	2.30	0.71
1:E:145:LEU:HB3	1:E:159:VAL:HG23	1.71	0.71
1:G:145:LEU:HB3	1:G:159:VAL:HG23	1.72	0.71
1:G:419:GLY:HA2	1:G:510:GLU:HG3	1.71	0.71
1:C:174:ILE:HD11	1:C:217:MET:SD	2.29	0.71
1:G:17:LEU:HD21	1:G:49:MET:CE	2.20	0.71
1:F:513:LEU:HD23	1:F:516:LEU:HD12	1.72	0.71
1:G:166:ASN:HD21	1:G:336:ALA:HB3	1.54	0.71
1:B:166:ASN:ND2	1:B:336:ALA:HB3	2.06	0.70
1:D:532:MET:HB2	1:D:717:ILE:HG12	1.72	0.70
1:C:433:VAL:CG2	1:C:461:ILE:HD12	2.21	0.70
1:C:212:PHE:HE1	1:C:303:THR:HG23	1.54	0.70
1:C:724:LYS:H	1:C:724:LYS:HD2	1.56	0.70
1:D:217:MET:HG3	1:D:309:GLN:NE2	2.06	0.70
1:F:433:VAL:HG22	1:F:461:ILE:HD12	1.73	0.70
1:B:145:LEU:HB3	1:B:159:VAL:HG23	1.72	0.70
1:G:724:LYS:H	1:G:724:LYS:HD2	1.57	0.70
1:C:303:THR:CG2	1:D:307:HIS:HE1	2.04	0.70
1:C:515:LEU:HD11	1:C:534:MET:HB2	1.74	0.70
1:F:413:VAL:HG22	1:F:502:ALA:HB3	1.74	0.70
1:A:145:LEU:HB3	1:A:159:VAL:HG23	1.73	0.70
1:E:303:THR:CG2	1:F:307:HIS:HE1	2.05	0.69
1:E:724:LYS:H	1:E:724:LYS:HD2	1.56	0.69
1:F:456:GLY:HA2	1:F:494:GLN:HG2	1.72	0.69
1:D:164:TYR:CD2	1:D:338:PRO:HB3	2.27	0.69
1:F:480:LYS:HB3	1:F:482:VAL:HG23	1.73	0.69
1:G:433:VAL:CG2	1:G:461:ILE:HD12	2.22	0.69
1:G:505:ILE:HG21	1:G:511:ALA:HB1	1.73	0.69
1:E:132:THR:CG2	1:E:361:VAL:HG13	2.21	0.69
1:F:145:LEU:HB3	1:F:159:VAL:HG23	1.73	0.69
1:F:433:VAL:CG2	1:F:461:ILE:HD12	2.23	0.69
1:A:724:LYS:H	1:A:724:LYS:HD2	1.57	0.69
1:C:303:THR:HG22	1:D:307:HIS:HE1	1.57	0.69
1:H:53:VAL:HG21	1:H:334:LEU:HD11	1.73	0.69
1:F:515:LEU:HD11	1:F:534:MET:HB2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:433:VAL:HG22	1:G:461:ILE:HD12	1.75	0.69
1:H:757:LEU:CD2	1:H:761:LEU:HG	2.23	0.69
1:B:723:SER:HB3	1:B:728:ILE:HD11	1.75	0.68
1:G:531:PRO:HG3	1:G:711:PHE:CE2	2.28	0.68
1:C:217:MET:HG3	1:C:309:GLN:NE2	2.08	0.68
1:H:337:THR:O	1:H:340:THR:HG22	1.94	0.68
1:F:212:PHE:HE1	1:F:303:THR:HG23	1.57	0.68
1:E:307:HIS:HE1	1:F:303:THR:CG2	2.06	0.68
1:G:418:VAL:O	1:G:507:GLY:HA3	1.94	0.68
1:A:533:VAL:HG22	1:A:696:TRP:CZ3	2.28	0.68
1:H:757:LEU:HD23	1:H:761:LEU:HG	1.75	0.68
1:D:433:VAL:CG2	1:D:461:ILE:HD12	2.23	0.68
1:E:707:ARG:HB2	1:E:707:ARG:HH11	1.57	0.68
1:E:179:CYS:O	1:E:181:THR:HG23	1.94	0.68
1:B:718:CYS:HB3	1:B:730:GLN:O	1.93	0.68
1:C:156:LYS:O	1:C:159:VAL:HG12	1.94	0.68
1:D:433:VAL:HG22	1:D:461:ILE:HD12	1.76	0.68
1:H:250:GLU:O	1:H:254:VAL:HG23	1.94	0.68
1:D:337:THR:O	1:D:340:THR:HG22	1.93	0.68
1:E:519:SER:HB2	1:E:717:ILE:HD12	1.76	0.68
1:F:337:THR:O	1:F:340:THR:HG22	1.93	0.67
1:F:541:ASN:HA	1:F:549:SER:OG	1.94	0.67
1:F:775:GLN:O	1:F:777:GLU:HG3	1.94	0.67
1:A:94:GLY:HA2	1:B:206:GLN:OE1	1.94	0.67
1:F:496:ARG:HB2	1:F:527:GLU:HG2	1.76	0.67
1:C:433:VAL:HG22	1:C:461:ILE:HD12	1.75	0.67
1:D:456:GLY:HA2	1:D:494:GLN:HG2	1.75	0.67
1:E:433:VAL:HG22	1:E:461:ILE:HD12	1.76	0.67
1:H:168:VAL:CG1	1:H:333:LEU:HD13	2.24	0.67
1:B:724:LYS:H	1:B:724:LYS:HD2	1.60	0.67
1:H:433:VAL:CG2	1:H:461:ILE:HD12	2.24	0.67
1:B:49:MET:SD	1:B:760:ILE:HD11	2.35	0.67
1:D:16:PHE:HD1	1:D:769:ASP:HA	1.60	0.67
1:A:541:ASN:HA	1:A:549:SER:OG	1.95	0.67
1:H:541:ASN:HA	1:H:549:SER:OG	1.95	0.67
1:B:128:ASP:O	1:B:132:THR:HG23	1.94	0.66
1:B:250:GLU:O	1:B:254:VAL:HG23	1.95	0.66
1:C:572:GLY:HA2	1:D:476:ILE:O	1.95	0.66
1:D:128:ASP:O	1:D:132:THR:HG23	1.95	0.66
1:G:337:THR:O	1:G:340:THR:HG22	1.95	0.66
1:B:337:THR:O	1:B:340:THR:HG22	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:GLU:O	1:C:254:VAL:HG23	1.95	0.66
1:E:156:LYS:O	1:E:159:VAL:HG12	1.96	0.66
1:F:168:VAL:CG1	1:F:333:LEU:HD13	2.25	0.66
1:A:168:VAL:CG1	1:A:333:LEU:HD13	2.25	0.66
1:C:212:PHE:HE1	1:C:303:THR:CG2	2.08	0.66
1:D:49:MET:SD	1:D:760:ILE:HD11	2.36	0.66
1:H:187:THR:HG21	1:H:223:TYR:HE2	1.60	0.66
1:A:187:THR:HG21	1:A:223:TYR:HE2	1.61	0.66
1:G:512:TYR:CZ	1:G:516:LEU:HD11	2.30	0.66
1:B:156:LYS:O	1:B:159:VAL:HG12	1.96	0.66
1:C:212:PHE:CE1	1:C:303:THR:HG23	2.30	0.66
1:D:156:LYS:O	1:D:159:VAL:HG12	1.96	0.66
1:A:156:LYS:O	1:A:159:VAL:HG12	1.95	0.66
1:A:250:GLU:O	1:A:254:VAL:HG23	1.96	0.66
1:D:187:THR:HG21	1:D:223:TYR:HE2	1.60	0.66
1:E:433:VAL:CG2	1:E:461:ILE:HD12	2.26	0.66
1:E:515:LEU:HD11	1:E:534:MET:HB2	1.77	0.66
1:H:97:ARG:HH11	1:H:219:ARG:HH22	1.44	0.66
1:G:156:LYS:O	1:G:159:VAL:HG12	1.96	0.66
1:E:710:LYS:HE2	1:E:710:LYS:CA	2.21	0.66
1:C:187:THR:HG21	1:C:223:TYR:HE2	1.61	0.65
1:H:637:ARG:HD2	1:H:650:ILE:HD12	1.78	0.65
1:A:212:PHE:HE1	1:A:303:THR:CG2	2.10	0.65
1:E:128:ASP:HA	1:E:178:PHE:CD1	2.31	0.65
1:E:780:GLN:H	1:E:780:GLN:CD	1.99	0.65
1:D:415:VAL:HG23	1:D:504:LEU:HD23	1.79	0.65
1:E:250:GLU:O	1:E:254:VAL:HG23	1.96	0.65
1:G:97:ARG:HG3	1:G:97:ARG:HH21	1.59	0.65
1:A:303:THR:HG22	1:B:307:HIS:CE1	2.23	0.65
1:C:337:THR:O	1:C:340:THR:HG22	1.96	0.65
1:E:337:THR:O	1:E:340:THR:HG22	1.97	0.65
1:A:331:ILE:CD1	1:A:773:SER:HB2	2.27	0.65
1:E:230:LEU:H	1:E:230:LEU:HD23	1.61	0.65
1:F:250:GLU:O	1:F:254:VAL:HG23	1.96	0.65
1:F:720:LEU:HD11	1:F:727:VAL:HG12	1.78	0.65
1:C:97:ARG:HH21	1:C:97:ARG:HG3	1.62	0.65
1:D:770:VAL:HG22	1:D:773:SER:HB3	1.79	0.65
1:G:166:ASN:ND2	1:G:336:ALA:HB3	2.12	0.65
1:G:493:THR:O	1:G:497:THR:HG23	1.95	0.65
1:A:433:VAL:HG22	1:A:461:ILE:HD12	1.79	0.65
1:G:250:GLU:O	1:G:254:VAL:HG23	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:541:ASN:HA	1:G:549:SER:OG	1.97	0.65
1:B:433:VAL:CG2	1:B:461:ILE:HD12	2.27	0.64
1:D:206:GLN:HG3	1:D:210:ARG:HD3	1.79	0.64
1:F:156:LYS:O	1:F:159:VAL:HG12	1.96	0.64
1:H:433:VAL:HG22	1:H:461:ILE:HD12	1.78	0.64
1:H:156:LYS:O	1:H:159:VAL:HG12	1.97	0.64
1:G:522:ARG:HH21	1:G:529:CYS:HA	1.62	0.64
1:F:262:ARG:HG2	1:F:262:ARG:HH11	1.62	0.64
1:H:262:ARG:HG2	1:H:262:ARG:HH11	1.63	0.64
1:B:521:ALA:C	1:B:523:GLU:H	1.98	0.64
1:C:481:ARG:HH11	1:C:481:ARG:CB	2.10	0.64
1:E:212:PHE:CE1	1:E:303:THR:HG23	2.31	0.64
1:F:212:PHE:HE1	1:F:303:THR:CG2	2.10	0.64
1:F:756:PRO:O	1:F:760:ILE:HG23	1.97	0.64
1:C:770:VAL:HG22	1:C:773:SER:HB3	1.80	0.64
1:G:363:MET:O	1:G:367:VAL:HG23	1.97	0.64
1:E:53:VAL:HG21	1:E:334:LEU:HD11	1.80	0.64
1:F:212:PHE:CE1	1:F:303:THR:HG23	2.33	0.64
1:G:720:LEU:HD11	1:G:727:VAL:HG12	1.80	0.64
1:C:128:ASP:O	1:C:132:THR:HG23	1.98	0.64
1:C:418:VAL:O	1:C:507:GLY:HA3	1.98	0.64
1:F:546:SER:HB2	1:F:721:GLY:HA3	1.80	0.64
1:A:176:ASN:ND2	1:A:184:THR:HG23	2.13	0.63
1:D:166:ASN:ND2	1:D:336:ALA:HB3	2.13	0.63
1:H:720:LEU:HD11	1:H:727:VAL:HG12	1.80	0.63
1:E:179:CYS:C	1:E:181:THR:H	2.02	0.63
1:H:56:LYS:HD2	1:H:76:GLU:OE1	1.98	0.63
1:B:187:THR:HG21	1:B:223:TYR:HE2	1.63	0.63
1:C:179:CYS:O	1:C:181:THR:HG23	1.98	0.63
1:G:262:ARG:HG2	1:G:262:ARG:HH11	1.63	0.63
1:G:770:VAL:HG22	1:G:773:SER:HB3	1.79	0.63
1:F:97:ARG:HH21	1:F:97:ARG:HG3	1.62	0.63
1:H:97:ARG:HH21	1:H:97:ARG:HG3	1.63	0.63
1:A:132:THR:CG2	1:A:361:VAL:HG13	2.28	0.63
1:B:212:PHE:HE1	1:B:303:THR:HG23	1.63	0.63
1:D:672:MET:HB2	1:D:673:GLN:HE22	1.63	0.63
1:F:487:TYR:O	1:F:491:ILE:HG13	1.99	0.63
1:H:174:ILE:HD11	1:H:217:MET:SD	2.39	0.63
1:A:262:ARG:HG2	1:A:262:ARG:HH11	1.63	0.63
1:C:206:GLN:HG3	1:C:210:ARG:HD3	1.80	0.63
1:E:207:SER:CB	1:F:94:GLY:HA3	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:THR:HG21	1:G:223:TYR:HE2	1.63	0.63
1:B:99:GLN:NE2	1:B:99:GLN:HA	2.14	0.63
1:B:168:VAL:CG1	1:B:333:LEU:HD13	2.28	0.63
1:A:128:ASP:O	1:A:132:THR:HG23	1.98	0.62
1:A:206:GLN:HG3	1:A:210:ARG:HD3	1.80	0.62
1:E:128:ASP:O	1:E:132:THR:HG23	1.98	0.62
1:C:515:LEU:CD1	1:C:534:MET:HB2	2.28	0.62
1:E:307:HIS:CE1	1:F:303:THR:HG22	2.25	0.62
1:G:637:ARG:HD2	1:G:650:ILE:HD12	1.81	0.62
1:A:337:THR:O	1:A:340:THR:HG22	1.98	0.62
1:E:187:THR:HG21	1:E:223:TYR:HE2	1.62	0.62
1:F:132:THR:CG2	1:F:361:VAL:HG13	2.29	0.62
1:B:486:LYS:HB2	1:B:487:TYR:CE2	2.35	0.62
1:D:262:ARG:HH11	1:D:262:ARG:HG2	1.65	0.62
1:D:363:MET:O	1:D:367:VAL:HG23	1.99	0.62
1:E:541:ASN:HA	1:E:549:SER:OG	1.98	0.62
1:F:363:MET:O	1:F:367:VAL:HG23	2.00	0.62
1:G:128:ASP:O	1:G:132:THR:HG23	1.99	0.62
1:F:361:VAL:O	1:F:365:GLN:HG3	1.99	0.62
1:B:331:ILE:CD1	1:B:773:SER:HB2	2.30	0.62
1:D:541:ASN:HA	1:D:549:SER:OG	2.00	0.62
1:G:99:GLN:HA	1:G:99:GLN:NE2	2.14	0.62
1:A:433:VAL:CG2	1:A:461:ILE:HD12	2.30	0.62
1:C:30:LEU:HB3	1:C:60:ILE:HB	1.81	0.62
1:G:503:LEU:HB3	1:G:532:MET:HG2	1.82	0.62
1:B:718:CYS:HB3	1:B:730:GLN:C	2.20	0.62
1:D:155:ASP:OD2	1:D:157:GLU:HG2	1.99	0.62
1:F:166:ASN:HD21	1:F:336:ALA:HB3	1.65	0.62
1:B:363:MET:O	1:B:367:VAL:HG23	2.00	0.62
1:B:433:VAL:HG22	1:B:461:ILE:HD12	1.80	0.62
1:F:151:ASN:HB2	1:F:153:GLN:NE2	2.14	0.62
1:G:367:VAL:HG22	1:G:382:LEU:HB3	1.81	0.62
1:H:361:VAL:O	1:H:365:GLN:HG3	2.00	0.62
1:A:230:LEU:HD23	1:A:230:LEU:H	1.65	0.61
1:B:770:VAL:HG22	1:B:773:SER:HB3	1.82	0.61
1:E:99:GLN:NE2	1:E:99:GLN:HA	2.14	0.61
1:E:128:ASP:HA	1:E:178:PHE:HD1	1.63	0.61
1:F:187:THR:HG21	1:F:223:TYR:HE2	1.63	0.61
1:C:49:MET:SD	1:C:760:ILE:HD11	2.40	0.61
1:D:131:LEU:HD23	1:D:178:PHE:CE2	2.35	0.61
1:D:533:VAL:HG22	1:D:696:TRP:CZ3	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:GLN:HG3	1:H:210:ARG:HD3	1.83	0.61
1:C:262:ARG:HG2	1:C:262:ARG:HH11	1.64	0.61
1:F:128:ASP:O	1:F:132:THR:HG23	2.00	0.61
1:H:363:MET:O	1:H:367:VAL:HG23	2.00	0.61
1:A:16:PHE:HB3	1:A:18:GLU:OE2	2.01	0.61
1:B:212:PHE:HE1	1:B:303:THR:CG2	2.13	0.61
1:F:519:SER:HB2	1:F:717:ILE:HD12	1.82	0.61
1:C:495:MET:HG2	1:C:500:ILE:HD12	1.82	0.61
1:E:206:GLN:HG3	1:E:210:ARG:HD3	1.80	0.61
1:F:230:LEU:HD23	1:F:230:LEU:H	1.65	0.61
1:F:206:GLN:HG3	1:F:210:ARG:HD3	1.81	0.61
1:A:770:VAL:HG22	1:A:773:SER:HB3	1.83	0.61
1:C:97:ARG:HH11	1:C:219:ARG:HH22	1.49	0.61
1:C:541:ASN:HA	1:C:549:SER:OG	2.01	0.61
1:E:770:VAL:HG22	1:E:773:SER:HB3	1.81	0.61
1:H:132:THR:CG2	1:H:361:VAL:HG13	2.28	0.61
1:A:174:ILE:HD11	1:A:217:MET:SD	2.41	0.61
1:A:255:LYS:NZ	1:A:399:ILE:HA	2.16	0.60
1:C:367:VAL:HG22	1:C:382:LEU:HB3	1.81	0.60
1:E:49:MET:SD	1:E:760:ILE:HD11	2.40	0.60
1:G:495:MET:HG2	1:G:500:ILE:HD12	1.82	0.60
1:H:284:THR:HG23	1:H:287:LYS:H	1.66	0.60
1:H:367:VAL:HG22	1:H:382:LEU:HB3	1.83	0.60
1:B:331:ILE:HD11	1:B:773:SER:HB2	1.83	0.60
1:E:303:THR:HG22	1:F:307:HIS:HE1	1.64	0.60
1:F:770:VAL:HG22	1:F:773:SER:HB3	1.82	0.60
1:G:230:LEU:HD23	1:G:230:LEU:H	1.65	0.60
1:A:503:LEU:HB3	1:A:532:MET:HG2	1.82	0.60
1:B:17:LEU:HD21	1:B:49:MET:CE	2.31	0.60
1:B:671:HIS:HE1	6:B:917:HOH:O	1.84	0.60
1:G:192:HIS:HD2	6:G:917:HOH:O	1.84	0.60
1:C:361:VAL:O	1:C:365:GLN:HG3	2.01	0.60
1:E:30:LEU:HB3	1:E:60:ILE:HB	1.84	0.60
1:E:262:ARG:HG2	1:E:262:ARG:HH11	1.65	0.60
1:A:363:MET:O	1:A:367:VAL:HG23	2.01	0.60
1:D:168:VAL:CG1	1:D:333:LEU:HD13	2.32	0.60
1:F:17:LEU:HD13	1:F:768:TYR:CD1	2.37	0.60
1:F:685:PHE:O	1:F:689:ILE:HG13	2.01	0.60
1:E:713:THR:OG1	1:E:714:ASP:N	2.34	0.60
1:E:623:THR:HG23	1:E:661:VAL:HG11	1.83	0.60
1:D:367:VAL:HG22	1:D:382:LEU:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:LEU:HD21	1:E:49:MET:CE	2.32	0.60
1:E:367:VAL:HG22	1:E:382:LEU:HB3	1.84	0.60
1:E:361:VAL:O	1:E:365:GLN:HG3	2.02	0.59
1:E:487:TYR:O	1:E:491:ILE:HG13	2.02	0.59
1:F:30:LEU:HB3	1:F:60:ILE:HB	1.84	0.59
1:A:30:LEU:HB3	1:A:60:ILE:HB	1.84	0.59
1:C:685:PHE:O	1:C:689:ILE:HG13	2.01	0.59
1:D:284:THR:HG23	1:D:287:LYS:H	1.66	0.59
1:H:450:PHE:CE1	1:H:484:PRO:HD3	2.37	0.59
1:C:720:LEU:HD11	1:C:727:VAL:HG12	1.84	0.59
1:E:363:MET:O	1:E:367:VAL:HG23	2.02	0.59
1:G:30:LEU:HB3	1:G:60:ILE:HB	1.84	0.59
1:A:212:PHE:HE1	1:A:303:THR:HG22	1.67	0.59
1:B:30:LEU:HB3	1:B:60:ILE:HB	1.84	0.59
1:B:262:ARG:HG2	1:B:262:ARG:HH11	1.66	0.59
1:B:637:ARG:HD2	1:B:650:ILE:HD12	1.85	0.59
1:D:30:LEU:HB3	1:D:60:ILE:HB	1.84	0.59
1:D:685:PHE:O	1:D:689:ILE:HG13	2.03	0.59
1:F:367:VAL:HG22	1:F:382:LEU:HB3	1.84	0.59
1:G:168:VAL:CG1	1:G:333:LEU:HD13	2.33	0.59
1:B:212:PHE:CE1	1:B:303:THR:HG23	2.38	0.59
1:E:685:PHE:O	1:E:689:ILE:HG13	2.01	0.59
1:A:331:ILE:HD11	1:A:773:SER:HB2	1.84	0.59
1:A:493:THR:O	1:A:497:THR:HG23	2.01	0.59
1:D:230:LEU:HD23	1:D:230:LEU:H	1.67	0.59
1:D:637:ARG:HD2	1:D:650:ILE:HD12	1.85	0.59
1:G:361:VAL:O	1:G:365:GLN:HG3	2.03	0.59
1:H:128:ASP:O	1:H:132:THR:HG23	2.02	0.59
1:D:501:ASN:O	1:D:701:LEU:HD21	2.02	0.59
1:G:623:THR:HG23	1:G:661:VAL:HG11	1.85	0.59
1:H:166:ASN:ND2	1:H:336:ALA:CB	2.41	0.59
1:B:230:LEU:HD23	1:B:230:LEU:H	1.67	0.59
1:H:623:THR:HG23	1:H:661:VAL:HG11	1.84	0.59
1:H:30:LEU:HB3	1:H:60:ILE:HB	1.85	0.58
1:H:574:LYS:HA	6:H:903:HOH:O	2.02	0.58
1:B:541:ASN:HA	1:B:549:SER:OG	2.03	0.58
1:C:99:GLN:NE2	1:C:99:GLN:HA	2.17	0.58
1:E:481:ARG:HH11	1:E:481:ARG:HB2	1.68	0.58
1:A:367:VAL:HG22	1:A:382:LEU:HB3	1.85	0.58
1:G:166:ASN:HD21	1:G:336:ALA:CB	2.16	0.58
1:C:61:TYR:O	1:C:66:GLY:HA3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLN:HA	1:A:99:GLN:NE2	2.19	0.58
1:G:206:GLN:HG3	1:G:210:ARG:HD3	1.85	0.58
1:G:501:ASN:O	1:G:530:VAL:HB	2.02	0.58
1:A:522:ARG:CZ	1:A:717:ILE:HD11	2.34	0.58
1:B:284:THR:HG23	1:B:287:LYS:H	1.69	0.58
1:E:456:GLY:HA2	1:E:494:GLN:HG2	1.86	0.58
1:F:331:ILE:CD1	1:F:773:SER:HB2	2.34	0.58
1:G:53:VAL:HG21	1:G:334:LEU:HD11	1.86	0.58
1:B:361:VAL:O	1:B:365:GLN:HG3	2.03	0.58
1:B:623:THR:HG23	1:B:661:VAL:HG11	1.85	0.58
1:C:648:ASP:O	1:C:652:GLN:HG3	2.04	0.58
1:B:131:LEU:HD23	1:B:178:PHE:CE2	2.39	0.57
1:E:164:TYR:CE2	1:E:338:PRO:HB3	2.38	0.57
1:F:495:MET:HG2	1:F:500:ILE:HD12	1.84	0.57
1:A:361:VAL:O	1:A:365:GLN:HG3	2.04	0.57
1:A:623:THR:HG23	1:A:661:VAL:HG11	1.85	0.57
1:A:756:PRO:O	1:A:760:ILE:HG23	2.04	0.57
1:B:684:ASN:O	1:B:688:LYS:HG3	2.04	0.57
1:F:47:VAL:HA	1:F:57:VAL:HG11	1.86	0.57
1:G:49:MET:SD	1:G:760:ILE:HD11	2.44	0.57
1:G:61:TYR:O	1:G:66:GLY:HA3	2.04	0.57
1:A:533:VAL:HG22	1:A:696:TRP:CE3	2.38	0.57
1:C:363:MET:O	1:C:367:VAL:HG23	2.04	0.57
1:C:428:ALA:HB1	1:C:506:ILE:HD13	1.85	0.57
1:A:18:GLU:H	1:A:18:GLU:CD	2.08	0.57
1:C:623:THR:HG23	1:C:661:VAL:HG11	1.86	0.57
1:C:637:ARG:HD2	1:C:650:ILE:HD12	1.86	0.57
1:E:303:THR:HG22	1:F:307:HIS:CE1	2.39	0.57
1:A:546:SER:HB2	1:A:721:GLY:HA3	1.86	0.57
1:B:685:PHE:O	1:B:689:ILE:HG13	2.05	0.57
1:H:36:ALA:O	1:H:39:MET:HG3	2.05	0.57
1:H:61:TYR:O	1:H:66:GLY:HA3	2.03	0.57
1:B:61:TYR:O	1:B:66:GLY:HA3	2.03	0.57
1:D:53:VAL:HG21	1:D:334:LEU:HD11	1.86	0.57
1:F:99:GLN:HA	1:F:99:GLN:NE2	2.19	0.57
1:H:648:ASP:O	1:H:652:GLN:HG3	2.04	0.57
1:D:361:VAL:O	1:D:365:GLN:HG3	2.05	0.57
1:E:61:TYR:O	1:E:66:GLY:HA3	2.05	0.57
1:C:531:PRO:HG3	1:C:711:PHE:CE2	2.40	0.57
1:D:456:GLY:HA2	1:D:494:GLN:CG	2.34	0.57
1:D:623:THR:HG23	1:D:661:VAL:HG11	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:PRO:O	1:D:760:ILE:HG23	2.05	0.57
1:E:14:ARG:HG3	1:E:14:ARG:HH11	1.70	0.57
1:E:277:ASP:OD2	1:E:281:LYS:HB2	2.04	0.57
1:F:637:ARG:HD2	1:F:650:ILE:HD12	1.85	0.57
1:H:601:ASP:CG	1:H:622:LEU:HD13	2.24	0.57
1:A:495:MET:HA	1:A:500:ILE:HD12	1.87	0.56
1:C:303:THR:HG22	1:D:307:HIS:CE1	2.39	0.56
1:D:14:ARG:HB2	1:D:14:ARG:HH11	1.69	0.56
1:E:263:LYS:HG2	1:E:265:ARG:HH12	1.69	0.56
1:H:192:HIS:CE1	1:H:680:PRO:HD2	2.40	0.56
1:A:85:ILE:HG21	1:A:92:ILE:HD13	1.86	0.56
1:B:367:VAL:HG22	1:B:382:LEU:HB3	1.86	0.56
1:B:576:ARG:HD3	1:B:663:ASP:OD1	2.04	0.56
1:C:97:ARG:HH11	1:C:219:ARG:NH2	2.03	0.56
1:C:576:ARG:HD3	1:C:663:ASP:OD1	2.05	0.56
1:E:47:VAL:HA	1:E:57:VAL:HG11	1.87	0.56
1:A:648:ASP:O	1:A:652:GLN:HG3	2.06	0.56
1:G:685:PHE:O	1:G:689:ILE:HG13	2.06	0.56
1:H:495:MET:HG2	1:H:500:ILE:HD12	1.86	0.56
1:C:490:GLU:N	1:C:490:GLU:OE1	2.39	0.56
1:B:255:LYS:NZ	1:B:399:ILE:HA	2.20	0.56
1:E:207:SER:HB3	1:F:94:GLY:HA3	1.88	0.56
1:E:689:ILE:HG22	1:E:720:LEU:CD2	2.36	0.56
1:F:255:LYS:NZ	1:F:399:ILE:HA	2.21	0.56
1:G:665:ARG:HD2	1:H:672:MET:CE	2.35	0.56
1:A:303:THR:CG2	1:B:307:HIS:HE1	2.11	0.56
1:E:255:LYS:NZ	1:E:399:ILE:HA	2.21	0.56
1:E:637:ARG:HD2	1:E:650:ILE:HD12	1.85	0.56
1:G:576:ARG:HD3	1:G:663:ASP:OD1	2.06	0.56
1:B:483:LEU:HB3	1:B:484:PRO:HD2	1.88	0.56
1:B:495:MET:HE3	1:B:500:ILE:HB	1.88	0.56
1:B:756:PRO:O	1:B:760:ILE:HG23	2.05	0.56
1:C:230:LEU:HD23	1:C:230:LEU:H	1.71	0.56
1:H:47:VAL:HA	1:H:57:VAL:HG11	1.87	0.56
1:H:358:MET:HG3	1:H:359:GLU:N	2.21	0.56
1:E:648:ASP:O	1:E:652:GLN:HG3	2.06	0.55
1:F:61:TYR:O	1:F:66:GLY:HA3	2.06	0.55
1:A:207:SER:HB3	1:B:62:GLU:OE2	2.06	0.55
1:B:534:MET:CE	1:B:543:VAL:HG11	2.35	0.55
1:D:522:ARG:HH12	1:D:716:SER:HB2	1.70	0.55
1:E:168:VAL:CG1	1:E:333:LEU:HD13	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:576:ARG:HD3	1:E:663:ASP:OD1	2.06	0.55
1:A:47:VAL:HA	1:A:57:VAL:HG11	1.87	0.55
1:A:637:ARG:HD2	1:A:650:ILE:HD12	1.88	0.55
1:F:17:LEU:HB3	1:F:768:TYR:HB3	1.89	0.55
1:C:284:THR:HG23	1:C:287:LYS:H	1.71	0.55
1:C:621:HIS:CE1	1:C:625:LYS:HE2	2.41	0.55
1:D:132:THR:CG2	1:D:361:VAL:HG13	2.35	0.55
1:D:576:ARG:HD3	1:D:663:ASP:OD1	2.06	0.55
1:E:284:THR:HG23	1:E:287:LYS:H	1.71	0.55
1:E:756:PRO:O	1:E:760:ILE:HG23	2.06	0.55
1:F:576:ARG:HD3	1:F:663:ASP:OD1	2.07	0.55
1:H:756:PRO:O	1:H:760:ILE:HG23	2.05	0.55
1:B:534:MET:HE2	1:B:543:VAL:HG11	1.89	0.55
1:C:428:ALA:CB	1:C:506:ILE:HD13	2.36	0.55
1:F:648:ASP:O	1:F:652:GLN:HG3	2.07	0.55
1:B:209:GLN:OE1	1:B:260:ARG:HD2	2.07	0.55
1:G:428:ALA:HB1	1:G:506:ILE:HD13	1.88	0.55
1:H:197:VAL:O	1:H:201:ILE:HD13	2.07	0.55
1:B:168:VAL:HG12	1:B:333:LEU:HD13	1.89	0.55
1:C:36:ALA:O	1:C:39:MET:HG3	2.07	0.55
1:D:61:TYR:O	1:D:66:GLY:HA3	2.07	0.55
1:D:519:SER:C	1:D:521:ALA:H	2.10	0.55
1:A:284:THR:HG23	1:A:287:LYS:H	1.72	0.55
1:B:36:ALA:O	1:B:39:MET:HG3	2.07	0.55
1:B:521:ALA:C	1:B:523:GLU:N	2.60	0.55
1:E:85:ILE:HG21	1:E:92:ILE:HD13	1.88	0.55
1:E:710:LYS:HA	1:E:710:LYS:CE	2.25	0.55
1:G:576:ARG:HG2	1:G:578:PHE:CE1	2.42	0.55
1:G:164:TYR:CD2	1:G:338:PRO:HB3	2.42	0.55
1:A:176:ASN:HA	1:A:184:THR:HG21	1.88	0.54
1:A:495:MET:HG2	1:A:500:ILE:HD12	1.89	0.54
1:C:413:VAL:HG22	1:C:502:ALA:HB3	1.87	0.54
1:G:234:ALA:HB2	1:G:270:ILE:HD13	1.89	0.54
1:H:230:LEU:HD23	1:H:230:LEU:H	1.72	0.54
1:H:515:LEU:HD11	1:H:534:MET:HB2	1.87	0.54
1:B:47:VAL:HA	1:B:57:VAL:HG11	1.88	0.54
1:H:209:GLN:OE1	1:H:260:ARG:HG2	2.07	0.54
1:H:234:ALA:HB2	1:H:270:ILE:HD13	1.87	0.54
1:B:648:ASP:O	1:B:652:GLN:HG3	2.07	0.54
1:C:412:ASN:HB2	1:C:499:SER:O	2.07	0.54
1:E:416:ILE:CG2	1:E:505:ILE:HG12	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:445:ALA:HB2	1:H:461:ILE:HD13	1.89	0.54
1:A:652:GLN:HE22	1:D:649:PHE:HB2	1.70	0.54
1:C:718:CYS:SG	1:C:729:PHE:HB3	2.47	0.54
1:E:155:ASP:HB3	1:E:158:ALA:HB2	1.89	0.54
1:G:36:ALA:O	1:G:39:MET:HG3	2.08	0.54
1:D:36:ALA:O	1:D:39:MET:HG3	2.07	0.54
1:F:623:THR:HG23	1:F:661:VAL:HG11	1.89	0.54
1:G:97:ARG:HG3	1:G:97:ARG:NH2	2.22	0.54
1:C:85:ILE:HG21	1:C:92:ILE:HD13	1.90	0.54
1:C:168:VAL:CG1	1:C:333:LEU:HD13	2.38	0.54
1:D:519:SER:O	1:D:522:ARG:HG2	2.07	0.54
1:G:572:GLY:HA2	1:H:476:ILE:O	2.07	0.54
1:C:132:THR:CG2	1:C:361:VAL:HG13	2.37	0.54
1:C:234:ALA:HB2	1:C:270:ILE:HD13	1.87	0.54
1:D:197:VAL:O	1:D:201:ILE:HD13	2.08	0.54
1:D:47:VAL:HA	1:D:57:VAL:HG11	1.88	0.54
1:D:485:GLY:O	1:D:487:TYR:N	2.40	0.54
1:F:234:ALA:HB2	1:F:270:ILE:HD13	1.90	0.54
1:G:255:LYS:NZ	1:G:399:ILE:HA	2.22	0.54
1:A:36:ALA:O	1:A:39:MET:HG3	2.09	0.53
1:A:496:ARG:HG2	1:A:496:ARG:HH21	1.72	0.53
1:A:576:ARG:HD3	1:A:663:ASP:OD1	2.08	0.53
1:A:615:LEU:O	1:A:619:VAL:HG23	2.08	0.53
1:B:17:LEU:HD21	1:B:49:MET:HE3	1.88	0.53
1:B:175:ASP:OD1	1:B:218:GLY:HA2	2.09	0.53
1:C:164:TYR:CD2	1:C:338:PRO:HB3	2.43	0.53
1:H:685:PHE:O	1:H:689:ILE:HG13	2.08	0.53
1:F:284:THR:HG23	1:F:287:LYS:H	1.72	0.53
1:H:155:ASP:OD2	1:H:157:GLU:HG2	2.08	0.53
1:A:212:PHE:CE1	1:A:303:THR:CG2	2.90	0.53
1:D:17:LEU:HD21	1:D:49:MET:CE	2.39	0.53
1:E:155:ASP:HB3	1:E:158:ALA:CB	2.39	0.53
1:F:97:ARG:HG3	1:F:97:ARG:NH2	2.23	0.53
1:G:755:ARG:HG3	1:G:755:ARG:HH11	1.72	0.53
1:H:192:HIS:HA	1:H:680:PRO:HG2	1.90	0.53
1:G:515:LEU:HD11	1:G:534:MET:HB2	1.91	0.53
1:A:522:ARG:NH2	1:A:717:ILE:HD11	2.24	0.53
1:E:679:SER:O	1:E:683:ARG:HG2	2.08	0.53
1:G:756:PRO:O	1:G:760:ILE:HG23	2.08	0.53
1:C:97:ARG:HG3	1:C:97:ARG:NH2	2.24	0.53
1:C:255:LYS:NZ	1:C:399:ILE:HA	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:ILE:N	1:C:579:ILE:HD12	2.23	0.53
1:F:197:VAL:O	1:F:201:ILE:HD13	2.09	0.53
1:F:331:ILE:HD11	1:F:773:SER:HB2	1.90	0.53
1:G:284:THR:HG23	1:G:287:LYS:H	1.73	0.53
1:F:503:LEU:HD23	1:F:532:MET:HE2	1.91	0.53
1:G:331:ILE:HD11	1:G:773:SER:HB2	1.90	0.53
1:H:576:ARG:HG2	1:H:578:PHE:CE1	2.44	0.53
1:A:755:ARG:N	1:A:756:PRO:HD2	2.24	0.53
1:B:197:VAL:O	1:B:201:ILE:HD13	2.08	0.53
1:F:720:LEU:CD1	1:F:727:VAL:HG12	2.39	0.53
1:G:720:LEU:CD1	1:G:727:VAL:HG12	2.39	0.53
1:C:481:ARG:HB2	1:C:481:ARG:NH1	2.20	0.53
1:D:179:CYS:SG	1:D:367:VAL:HG21	2.49	0.53
1:D:576:ARG:HG2	1:D:578:PHE:CE1	2.43	0.52
1:E:17:LEU:HD21	1:E:49:MET:HE3	1.90	0.52
1:D:356:PRO:HD3	1:D:776:LEU:CD2	2.40	0.52
1:E:33:GLY:HA3	2:E:801:ATP:O2B	2.09	0.52
1:E:541:ASN:HA	1:E:549:SER:HG	1.74	0.52
1:F:710:LYS:O	1:F:710:LYS:HD3	2.10	0.52
1:E:331:ILE:HD11	1:E:773:SER:HB2	1.92	0.52
1:G:47:VAL:HA	1:G:57:VAL:HG11	1.90	0.52
1:G:519:SER:O	1:G:522:ARG:HG2	2.09	0.52
1:A:135:ASN:ND2	1:A:358:MET:SD	2.77	0.52
1:A:175:ASP:OD1	1:A:218:GLY:HA2	2.09	0.52
1:E:519:SER:HB2	1:E:717:ILE:CD1	2.38	0.52
1:E:615:LEU:O	1:E:619:VAL:HG23	2.09	0.52
1:G:59:PHE:CG	1:G:93:ILE:HD11	2.44	0.52
1:H:168:VAL:HG12	1:H:333:LEU:HD13	1.91	0.52
1:A:197:VAL:O	1:A:201:ILE:HD13	2.09	0.52
1:D:85:ILE:HG21	1:D:92:ILE:HD13	1.91	0.52
1:D:492:ALA:CB	1:D:525:HIS:HD2	2.22	0.52
1:H:567:LYS:HA	1:H:632:ARG:HD2	1.92	0.52
1:A:390:ASN:OD1	1:A:688:LYS:HD3	2.09	0.52
1:E:207:SER:HB2	1:F:94:GLY:HA3	1.92	0.52
1:B:85:ILE:HG21	1:B:92:ILE:HD13	1.92	0.52
1:G:503:LEU:HD12	1:G:504:LEU:N	2.25	0.52
1:H:526:GLU:O	1:H:526:GLU:HG2	2.09	0.52
1:B:59:PHE:CG	1:B:93:ILE:HD11	2.45	0.52
1:C:47:VAL:HA	1:C:57:VAL:HG11	1.90	0.52
1:G:171:VAL:HG11	1:G:184:THR:HG21	1.92	0.52
1:A:534:MET:SD	1:A:719:VAL:HG22	2.50	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:VAL:HG21	1:C:461:ILE:HD12	1.91	0.52
1:H:679:SER:O	1:H:683:ARG:HG2	2.10	0.52
1:A:254:VAL:O	1:A:258:GLU:HG3	2.11	0.51
1:B:445:ALA:HB2	1:B:461:ILE:HD13	1.92	0.51
1:C:331:ILE:CD1	1:C:773:SER:HB2	2.40	0.51
1:E:505:ILE:O	1:E:534:MET:HA	2.10	0.51
1:H:164:TYR:CZ	1:H:337:THR:O	2.63	0.51
1:B:363:MET:SD	1:B:779:VAL:HG21	2.49	0.51
1:E:36:ALA:O	1:E:39:MET:HG3	2.09	0.51
1:E:582:THR:O	1:E:639:GLU:HG3	2.11	0.51
1:G:15:LYS:HD3	1:G:15:LYS:H	1.75	0.51
1:B:164:TYR:CE2	1:B:338:PRO:HB3	2.45	0.51
1:C:331:ILE:HD11	1:C:773:SER:HB2	1.91	0.51
1:E:488:LEU:HD13	1:E:521:ALA:HB2	1.92	0.51
1:E:504:LEU:HD12	1:E:505:ILE:N	2.24	0.51
1:H:616:GLN:O	1:H:620:GLU:HG3	2.10	0.51
1:B:615:LEU:O	1:B:619:VAL:HG23	2.09	0.51
1:C:197:VAL:O	1:C:201:ILE:HD13	2.11	0.51
1:E:245:GLU:HA	1:E:245:GLU:OE2	2.10	0.51
1:F:36:ALA:O	1:F:39:MET:HG3	2.11	0.51
1:E:234:ALA:HB2	1:E:270:ILE:HD13	1.93	0.51
1:H:85:ILE:HG21	1:H:92:ILE:HD13	1.91	0.51
1:H:720:LEU:CD1	1:H:727:VAL:HG12	2.39	0.51
1:A:445:ALA:HB2	1:A:461:ILE:HD13	1.93	0.51
1:C:227:VAL:HA	1:C:230:LEU:CD2	2.41	0.51
1:C:717:ILE:HG22	1:C:717:ILE:O	2.11	0.51
1:C:721:GLY:O	1:C:727:VAL:HA	2.10	0.51
1:E:179:CYS:O	1:E:181:THR:N	2.44	0.51
1:G:85:ILE:HG21	1:G:92:ILE:HD13	1.93	0.51
1:G:490:GLU:OE1	1:G:490:GLU:N	2.28	0.51
1:H:37:GLN:HB3	1:H:314:PRO:HB3	1.93	0.51
1:H:755:ARG:N	1:H:756:PRO:HD2	2.26	0.51
1:C:14:ARG:HH12	1:C:771:SER:CB	2.23	0.51
1:E:230:LEU:H	1:E:230:LEU:CD2	2.23	0.51
1:A:234:ALA:HB2	1:A:270:ILE:HD13	1.93	0.51
1:B:44:ARG:HH12	1:B:761:LEU:HD13	1.74	0.51
1:B:234:ALA:HB2	1:B:270:ILE:HD13	1.93	0.51
1:A:17:LEU:HD21	1:A:49:MET:CE	2.41	0.51
1:A:61:TYR:O	1:A:66:GLY:HA3	2.10	0.51
1:A:724:LYS:HD2	1:A:724:LYS:N	2.25	0.51
1:B:576:ARG:HG2	1:B:578:PHE:CE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:ALA:HB2	1:D:525:HIS:CD2	2.46	0.51
1:F:755:ARG:HG3	1:F:755:ARG:HH11	1.76	0.51
1:A:775:GLN:O	1:A:777:GLU:HG3	2.11	0.51
1:F:576:ARG:HG2	1:F:578:PHE:CE1	2.46	0.51
1:G:227:VAL:HA	1:G:230:LEU:HD21	1.93	0.51
1:C:153:GLN:OE1	1:C:153:GLN:HA	2.11	0.50
1:F:728:ILE:HD12	1:F:729:PHE:H	1.75	0.50
1:G:445:ALA:HB2	1:G:461:ILE:HD13	1.93	0.50
1:H:530:VAL:HB	1:H:531:PRO:CD	2.42	0.50
1:A:508:GLY:HA3	1:A:538:THR:HG23	1.93	0.50
1:E:755:ARG:HG3	1:E:755:ARG:HH11	1.75	0.50
1:H:445:ALA:HB2	1:H:461:ILE:CD1	2.41	0.50
1:H:755:ARG:HG3	1:H:755:ARG:HH11	1.76	0.50
1:C:576:ARG:HG2	1:C:578:PHE:CE1	2.45	0.50
1:F:582:THR:O	1:F:639:GLU:HG3	2.12	0.50
1:G:675:GLY:O	1:H:569:SER:HB2	2.10	0.50
1:A:723:SER:O	1:A:724:LYS:C	2.50	0.50
1:B:715:ASP:HA	1:B:731:PRO:HB3	1.92	0.50
1:D:414:ALA:O	1:D:503:LEU:HD12	2.10	0.50
1:E:19:HIS:O	1:E:20:LEU:C	2.50	0.50
1:F:723:SER:O	1:F:724:LYS:C	2.50	0.50
1:G:166:ASN:OD1	1:G:336:ALA:CB	2.58	0.50
1:G:615:LEU:O	1:G:619:VAL:HG23	2.12	0.50
1:H:390:ASN:OD1	1:H:688:LYS:HD3	2.11	0.50
1:H:582:THR:O	1:H:639:GLU:HG3	2.11	0.50
1:A:445:ALA:HB2	1:A:461:ILE:CD1	2.42	0.50
1:B:579:ILE:HD12	1:B:579:ILE:N	2.27	0.50
1:C:59:PHE:CG	1:C:93:ILE:HD11	2.47	0.50
1:C:755:ARG:N	1:C:756:PRO:HD2	2.26	0.50
1:C:756:PRO:O	1:C:760:ILE:HG23	2.11	0.50
1:D:648:ASP:O	1:D:652:GLN:HG3	2.11	0.50
1:G:724:LYS:HD2	1:G:724:LYS:N	2.26	0.50
1:A:245:GLU:HG3	1:E:707:ARG:NH2	2.27	0.50
1:B:755:ARG:HG3	1:B:755:ARG:HH11	1.77	0.50
1:C:501:ASN:HA	1:C:530:VAL:HG11	1.93	0.50
1:D:755:ARG:N	1:D:756:PRO:HD2	2.27	0.50
1:E:156:LYS:HA	1:E:156:LYS:HE2	1.94	0.50
1:B:179:CYS:SG	1:B:382:LEU:O	2.68	0.50
1:E:227:VAL:HA	1:E:230:LEU:HD21	1.94	0.50
1:A:575:ARG:HH11	1:A:631:GLN:HG2	1.76	0.50
1:A:755:ARG:HG3	1:A:755:ARG:HH11	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:618:ASN:N	1:H:618:ASN:HD22	2.10	0.50
1:A:207:SER:HB3	1:B:94:GLY:HA3	1.93	0.50
1:A:576:ARG:HG2	1:A:578:PHE:CE1	2.47	0.50
1:B:515:LEU:CD1	1:B:534:MET:HB2	2.42	0.50
1:E:445:ALA:HB2	1:E:461:ILE:HD13	1.94	0.50
1:E:559:ILE:HG12	1:E:669:LEU:HD11	1.94	0.50
1:F:156:LYS:HE2	1:F:156:LYS:HA	1.94	0.50
1:C:724:LYS:HD2	1:C:724:LYS:N	2.26	0.49
1:D:227:VAL:HA	1:D:230:LEU:HD21	1.94	0.49
1:G:533:VAL:HG22	1:G:696:TRP:CE3	2.47	0.49
1:G:739:THR:HG23	1:G:741:PHE:CE1	2.47	0.49
1:H:156:LYS:HA	1:H:156:LYS:HE2	1.93	0.49
1:A:37:GLN:HB3	1:A:314:PRO:HB3	1.94	0.49
1:A:206:GLN:NE2	1:A:208:HIS:CE1	2.81	0.49
1:B:418:VAL:O	1:B:507:GLY:HA3	2.12	0.49
1:B:724:LYS:HD2	1:B:724:LYS:N	2.26	0.49
1:C:582:THR:O	1:C:639:GLU:HG3	2.12	0.49
1:D:739:THR:HG23	1:D:741:PHE:CE1	2.47	0.49
1:E:707:ARG:NH1	1:E:707:ARG:CB	2.75	0.49
1:F:533:VAL:HG22	1:F:696:TRP:CZ3	2.47	0.49
1:G:665:ARG:HD2	1:H:672:MET:HE1	1.93	0.49
1:A:59:PHE:CG	1:A:93:ILE:HD11	2.47	0.49
1:A:227:VAL:HA	1:A:230:LEU:CD2	2.43	0.49
1:A:685:PHE:O	1:A:689:ILE:HG13	2.13	0.49
1:C:156:LYS:HA	1:C:156:LYS:HE2	1.94	0.49
1:G:576:ARG:HG2	1:G:578:PHE:CZ	2.46	0.49
1:G:715:ASP:HA	1:G:731:PRO:HB3	1.95	0.49
1:A:176:ASN:ND2	1:A:184:THR:CG2	2.75	0.49
1:D:234:ALA:HB2	1:D:270:ILE:HD13	1.95	0.49
1:D:245:GLU:OE2	1:D:245:GLU:HA	2.12	0.49
1:D:433:VAL:HG21	1:D:461:ILE:HD12	1.95	0.49
1:G:245:GLU:OE2	1:G:245:GLU:HA	2.11	0.49
1:C:14:ARG:NH1	1:C:771:SER:CB	2.75	0.49
1:E:723:SER:O	1:E:724:LYS:C	2.51	0.49
1:E:724:LYS:H	1:E:724:LYS:CD	2.24	0.49
1:F:559:ILE:HG12	1:F:669:LEU:HD11	1.94	0.49
1:G:569:SER:HB2	1:H:675:GLY:O	2.13	0.49
1:D:175:ASP:OD1	1:D:218:GLY:HA2	2.12	0.49
1:E:168:VAL:HA	1:E:343:CYS:O	2.13	0.49
1:E:331:ILE:CD1	1:E:773:SER:HB2	2.43	0.49
1:B:206:GLN:HG3	1:B:210:ARG:HD3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:PHE:HE1	1:E:303:THR:CG2	2.20	0.49
1:F:576:ARG:HG2	1:F:578:PHE:CZ	2.48	0.49
1:F:755:ARG:N	1:F:756:PRO:HD2	2.28	0.49
1:B:487:TYR:N	1:B:487:TYR:CD2	2.80	0.49
1:B:656:GLU:HG2	1:C:645:TYR:CZ	2.48	0.49
1:C:667:ASN:OD1	1:D:672:MET:HG3	2.13	0.49
1:C:728:ILE:HD12	1:C:729:PHE:H	1.77	0.49
1:D:227:VAL:HA	1:D:230:LEU:CD2	2.43	0.49
1:D:755:ARG:HG3	1:D:755:ARG:HH11	1.76	0.49
1:E:445:ALA:HB2	1:E:461:ILE:CD1	2.43	0.49
1:F:59:PHE:CG	1:F:93:ILE:HD11	2.48	0.49
1:F:85:ILE:HG21	1:F:92:ILE:HD13	1.94	0.49
1:F:227:VAL:HA	1:F:230:LEU:HD21	1.94	0.49
1:H:59:PHE:CG	1:H:93:ILE:HD11	2.46	0.49
1:C:175:ASP:OD1	1:C:218:GLY:HA2	2.13	0.49
1:C:723:SER:O	1:C:724:LYS:C	2.51	0.49
1:D:155:ASP:HB3	1:D:158:ALA:HB2	1.95	0.49
1:H:97:ARG:HG3	1:H:97:ARG:NH2	2.26	0.49
1:A:582:THR:O	1:A:639:GLU:HG3	2.13	0.49
1:B:161:LYS:HE3	1:B:162:TYR:CZ	2.48	0.49
1:B:445:ALA:HB2	1:B:461:ILE:CD1	2.43	0.49
1:D:37:GLN:HB3	1:D:314:PRO:HB3	1.95	0.49
1:F:255:LYS:HZ2	1:F:399:ILE:HA	1.76	0.49
1:A:724:LYS:H	1:A:724:LYS:CD	2.25	0.48
1:C:227:VAL:HA	1:C:230:LEU:HD21	1.94	0.48
1:D:161:LYS:HE3	1:D:162:TYR:CZ	2.48	0.48
1:D:723:SER:O	1:D:724:LYS:C	2.52	0.48
1:E:175:ASP:OD1	1:E:218:GLY:HA2	2.13	0.48
1:G:445:ALA:HB2	1:G:461:ILE:CD1	2.43	0.48
1:C:724:LYS:H	1:C:724:LYS:CD	2.26	0.48
1:D:628:THR:HB	1:D:629:THR:H	1.35	0.48
1:E:576:ARG:HG2	1:E:578:PHE:CE1	2.47	0.48
1:F:445:ALA:HB2	1:F:461:ILE:HD13	1.94	0.48
1:G:331:ILE:CD1	1:G:773:SER:HB2	2.42	0.48
1:B:723:SER:O	1:B:724:LYS:C	2.52	0.48
1:C:615:LEU:O	1:C:619:VAL:HG23	2.14	0.48
1:F:245:GLU:OE2	1:F:245:GLU:HA	2.12	0.48
1:F:645:TYR:CE1	1:G:656:GLU:HG2	2.48	0.48
1:G:582:THR:O	1:G:639:GLU:HG3	2.13	0.48
1:H:262:ARG:HB3	1:H:464:THR:HG21	1.96	0.48
1:H:541:ASN:OD1	1:H:548:PHE:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:SER:O	1:A:683:ARG:HG2	2.14	0.48
1:B:354:ARG:C	1:B:355:LEU:HD12	2.33	0.48
1:C:739:THR:HG23	1:C:741:PHE:CE1	2.49	0.48
1:D:331:ILE:CD1	1:D:773:SER:HB2	2.44	0.48
1:F:445:ALA:HB2	1:F:461:ILE:CD1	2.43	0.48
1:G:16:PHE:HB3	1:G:18:GLU:OE2	2.13	0.48
1:G:17:LEU:CD2	1:G:49:MET:CE	2.91	0.48
1:D:142:SER:O	1:D:146:GLU:HG2	2.14	0.48
1:F:161:LYS:HE3	1:F:162:TYR:CZ	2.49	0.48
1:G:723:SER:O	1:G:724:LYS:C	2.52	0.48
1:H:217:MET:HA	1:H:273:GLU:HG3	1.96	0.48
1:A:161:LYS:HE3	1:A:162:TYR:CZ	2.48	0.48
1:A:770:VAL:HG22	1:A:770:VAL:O	2.14	0.48
1:E:583:MET:SD	1:E:671:HIS:ND1	2.87	0.48
1:E:656:GLU:HG2	1:H:645:TYR:CZ	2.48	0.48
1:E:707:ARG:HH11	1:E:707:ARG:CB	2.24	0.48
1:G:17:LEU:HD23	1:G:52:TYR:CE1	2.49	0.48
1:G:428:ALA:CB	1:G:506:ILE:HD13	2.43	0.48
1:H:227:VAL:HA	1:H:230:LEU:CD2	2.44	0.48
1:H:358:MET:HG3	1:H:359:GLU:H	1.78	0.48
1:A:227:VAL:HA	1:A:230:LEU:HD21	1.95	0.48
1:B:156:LYS:HE2	1:B:156:LYS:HA	1.94	0.48
1:D:44:ARG:HH12	1:D:761:LEU:HD13	1.78	0.48
1:D:99:GLN:HA	1:D:99:GLN:NE2	2.27	0.48
1:D:576:ARG:HG2	1:D:578:PHE:CZ	2.48	0.48
1:F:227:VAL:HA	1:F:230:LEU:CD2	2.43	0.48
1:F:325:MET:CE	1:F:325:MET:HA	2.43	0.48
1:F:622:LEU:O	1:F:626:MET:HG2	2.13	0.48
1:H:131:LEU:HD23	1:H:178:PHE:CZ	2.48	0.48
1:D:59:PHE:CG	1:D:93:ILE:HD11	2.49	0.48
1:D:356:PRO:HD3	1:D:776:LEU:HD21	1.95	0.48
1:D:527:GLU:CD	1:D:527:GLU:H	2.17	0.48
1:D:582:THR:O	1:D:639:GLU:HG3	2.13	0.48
1:F:518:LEU:HD13	1:F:532:MET:CE	2.43	0.48
1:H:579:ILE:N	1:H:579:ILE:HD12	2.29	0.48
1:A:652:GLN:NE2	1:D:649:PHE:HB2	2.28	0.48
1:C:720:LEU:CD1	1:C:727:VAL:HG12	2.44	0.48
1:D:354:ARG:C	1:D:355:LEU:HD12	2.34	0.48
1:D:728:ILE:HD12	1:D:729:PHE:H	1.79	0.48
1:E:197:VAL:O	1:E:201:ILE:HD13	2.14	0.48
1:E:550:ILE:HD13	1:E:686:GLY:HA2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:589:TYR:CE1	1:F:593:MET:HG3	2.49	0.48
1:G:230:LEU:H	1:G:230:LEU:CD2	2.26	0.48
1:D:331:ILE:HD11	1:D:773:SER:HB2	1.96	0.48
1:E:354:ARG:C	1:E:355:LEU:HD12	2.34	0.48
1:G:724:LYS:H	1:G:724:LYS:CD	2.27	0.48
1:A:703:GLU:O	1:A:707:ARG:HB3	2.14	0.47
1:C:400:LYS:HB2	1:C:463:TRP:CZ2	2.49	0.47
1:D:168:VAL:HG12	1:D:333:LEU:HD13	1.96	0.47
1:E:179:CYS:C	1:E:181:THR:N	2.67	0.47
1:E:227:VAL:HA	1:E:230:LEU:CD2	2.44	0.47
1:E:400:LYS:HB2	1:E:463:TRP:CZ2	2.49	0.47
1:F:37:GLN:HB3	1:F:314:PRO:HB3	1.96	0.47
1:F:166:ASN:ND2	1:F:336:ALA:HB3	2.28	0.47
1:H:739:THR:HG23	1:H:741:PHE:CE1	2.49	0.47
1:A:207:SER:CB	1:B:94:GLY:HA3	2.44	0.47
1:B:155:ASP:HB3	1:B:158:ALA:HB2	1.96	0.47
1:C:354:ARG:C	1:C:355:LEU:HD12	2.34	0.47
1:C:456:GLY:HA2	1:C:494:GLN:HG2	1.96	0.47
1:D:256:LEU:HD21	1:D:269:ILE:HD11	1.96	0.47
1:E:255:LYS:HZ1	1:E:399:ILE:HA	1.78	0.47
1:E:728:ILE:HD12	1:E:729:PHE:H	1.79	0.47
1:G:97:ARG:HH11	1:G:219:ARG:HH22	1.62	0.47
1:G:262:ARG:HB3	1:G:464:THR:HG21	1.95	0.47
1:H:433:VAL:HG21	1:H:461:ILE:HD12	1.94	0.47
1:B:755:ARG:N	1:B:756:PRO:HD2	2.29	0.47
1:C:692:ARG:HG2	1:C:720:LEU:HD21	1.96	0.47
1:E:303:THR:CG2	1:F:307:HIS:CE1	2.91	0.47
1:E:579:ILE:N	1:E:579:ILE:HD12	2.30	0.47
1:E:755:ARG:N	1:E:756:PRO:HD2	2.29	0.47
1:H:683:ARG:HG2	1:H:683:ARG:H	1.47	0.47
1:A:579:ILE:N	1:A:579:ILE:HD12	2.29	0.47
1:B:433:VAL:HG21	1:B:461:ILE:HD12	1.97	0.47
1:C:157:GLU:HG3	1:C:158:ALA:N	2.30	0.47
1:C:161:LYS:HE3	1:C:162:TYR:CZ	2.49	0.47
1:D:14:ARG:HB3	1:D:771:SER:OG	2.14	0.47
1:D:550:ILE:HD13	1:D:686:GLY:HA2	1.96	0.47
1:E:450:PHE:CD1	1:E:484:PRO:HD3	2.49	0.47
1:F:179:CYS:SG	1:F:367:VAL:HG21	2.55	0.47
1:G:713:THR:CG2	1:G:716:SER:HB3	2.38	0.47
1:D:355:LEU:HD12	1:D:355:LEU:N	2.29	0.47
1:E:546:SER:HB2	1:E:721:GLY:HA3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:615:LEU:O	1:F:619:VAL:HG23	2.15	0.47
1:H:175:ASP:OD1	1:H:218:GLY:HA2	2.15	0.47
1:H:227:VAL:HA	1:H:230:LEU:HD21	1.96	0.47
1:B:638:ASN:HB3	1:B:641:CYS:HB3	1.97	0.47
1:D:156:LYS:HE2	1:D:156:LYS:HA	1.95	0.47
1:D:492:ALA:HB2	1:D:525:HIS:HD2	1.78	0.47
1:E:262:ARG:HB3	1:E:464:THR:HG21	1.97	0.47
1:E:776:LEU:HD13	1:E:776:LEU:C	2.34	0.47
1:F:519:SER:O	1:F:522:ARG:HD2	2.14	0.47
1:G:589:TYR:CE1	1:G:593:MET:HG3	2.49	0.47
1:G:679:SER:O	1:G:683:ARG:HG2	2.14	0.47
1:H:567:LYS:HG2	1:H:632:ARG:HG2	1.96	0.47
1:C:559:ILE:HG12	1:C:669:LEU:HD11	1.96	0.47
1:C:589:TYR:CE1	1:C:593:MET:HG3	2.49	0.47
1:D:445:ALA:HB2	1:D:461:ILE:HD13	1.96	0.47
1:G:227:VAL:HA	1:G:230:LEU:CD2	2.44	0.47
1:G:450:PHE:CD1	1:G:484:PRO:HD3	2.49	0.47
1:H:723:SER:O	1:H:724:LYS:C	2.52	0.47
1:A:277:ASP:OD2	1:A:281:LYS:HB2	2.15	0.47
1:B:192:HIS:CE1	1:B:680:PRO:HD2	2.50	0.47
1:C:16:PHE:CD2	1:C:769:ASP:HA	2.50	0.47
1:D:155:ASP:HB3	1:D:158:ALA:CB	2.45	0.47
1:D:579:ILE:HD12	1:D:579:ILE:N	2.30	0.47
1:F:683:ARG:H	1:F:683:ARG:HG2	1.47	0.47
1:G:44:ARG:HH12	1:G:761:LEU:HD13	1.80	0.47
1:G:192:HIS:O	1:G:196:GLU:HG3	2.15	0.47
1:G:495:MET:HA	1:G:500:ILE:HD12	1.96	0.47
1:G:770:VAL:HG22	1:G:770:VAL:O	2.15	0.47
1:H:728:ILE:HD12	1:H:729:PHE:H	1.80	0.47
1:C:755:ARG:HG3	1:C:755:ARG:HH11	1.79	0.47
1:E:658:GLY:O	1:E:659:LYS:C	2.52	0.47
1:F:230:LEU:H	1:F:230:LEU:CD2	2.27	0.47
1:G:354:ARG:C	1:G:355:LEU:HD12	2.35	0.47
1:G:648:ASP:O	1:G:652:GLN:HG3	2.14	0.47
1:A:155:ASP:HB3	1:A:158:ALA:HB2	1.97	0.47
1:C:255:LYS:HZ2	1:C:399:ILE:HA	1.79	0.47
1:C:256:LEU:HD21	1:C:269:ILE:HD11	1.96	0.47
1:C:621:HIS:HE1	1:C:625:LYS:HE2	1.80	0.47
1:E:689:ILE:HG22	1:E:720:LEU:HD23	1.97	0.47
1:F:518:LEU:HA	1:F:518:LEU:HD23	1.49	0.47
1:G:325:MET:HA	1:G:325:MET:CE	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:478:GLY:CA	1:H:572:GLY:HA3	2.45	0.47
1:G:481:ARG:NH1	1:G:481:ARG:HG3	2.30	0.47
1:H:49:MET:CE	1:H:327:VAL:HG13	2.45	0.47
1:H:100:ALA:O	1:H:106:GLY:HA3	2.15	0.47
1:H:615:LEU:O	1:H:619:VAL:HG23	2.15	0.47
1:A:307:HIS:CD2	1:B:301:ARG:HB3	2.50	0.46
1:B:576:ARG:HG2	1:B:578:PHE:CZ	2.49	0.46
1:C:504:LEU:HD12	1:C:505:ILE:N	2.30	0.46
1:H:550:ILE:HD13	1:H:686:GLY:HA2	1.97	0.46
1:A:255:LYS:HZ1	1:A:399:ILE:HA	1.79	0.46
1:A:256:LEU:HD21	1:A:269:ILE:HD11	1.97	0.46
1:B:256:LEU:HD21	1:B:269:ILE:HD11	1.98	0.46
1:B:589:TYR:CE1	1:B:593:MET:HG3	2.50	0.46
1:B:724:LYS:H	1:B:724:LYS:CD	2.26	0.46
1:C:576:ARG:HG2	1:C:578:PHE:CZ	2.51	0.46
1:D:325:MET:CE	1:D:325:MET:HA	2.45	0.46
1:E:168:VAL:HG12	1:E:333:LEU:HD13	1.97	0.46
1:G:132:THR:CG2	1:G:361:VAL:HG13	2.38	0.46
1:G:161:LYS:HE3	1:G:162:TYR:CZ	2.49	0.46
1:G:529:CYS:O	1:G:711:PHE:HB2	2.15	0.46
1:H:672:MET:HB2	1:H:673:GLN:HE22	1.81	0.46
1:A:728:ILE:HD12	1:A:729:PHE:H	1.79	0.46
1:C:166:ASN:ND2	1:C:336:ALA:HB3	2.29	0.46
1:C:488:LEU:HD23	1:C:488:LEU:HA	1.75	0.46
1:D:679:SER:O	1:D:683:ARG:HG2	2.15	0.46
1:F:249:GLU:CG	1:F:291:LEU:HD21	2.46	0.46
1:F:456:GLY:HA2	1:F:494:GLN:CG	2.42	0.46
1:G:683:ARG:HG2	1:G:683:ARG:H	1.48	0.46
1:G:755:ARG:N	1:G:756:PRO:HD2	2.30	0.46
1:H:483:LEU:HB3	1:H:517:GLU:OE1	2.15	0.46
1:A:340:THR:HG23	1:A:340:THR:O	2.14	0.46
1:B:622:LEU:O	1:B:626:MET:HG2	2.15	0.46
1:E:166:ASN:HD21	1:E:336:ALA:HB3	1.77	0.46
1:F:433:VAL:HG21	1:F:461:ILE:HD12	1.97	0.46
1:F:658:GLY:O	1:F:659:LYS:C	2.53	0.46
1:G:546:SER:HB2	1:G:721:GLY:HA3	1.96	0.46
1:A:142:SER:O	1:A:146:GLU:HG2	2.15	0.46
1:B:135:ASN:HB2	1:B:357:LEU:HD13	1.97	0.46
1:E:700:LYS:HD2	1:E:711:PHE:HE2	1.80	0.46
1:F:505:ILE:HD12	1:F:515:LEU:HD21	1.97	0.46
1:F:739:THR:HG23	1:F:741:PHE:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:GLY:O	1:A:659:LYS:C	2.53	0.46
1:B:582:THR:O	1:B:639:GLU:HG3	2.16	0.46
1:B:679:SER:O	1:B:683:ARG:HG2	2.15	0.46
1:C:155:ASP:HB3	1:C:158:ALA:HB2	1.97	0.46
1:D:450:PHE:CD2	1:D:484:PRO:HB3	2.51	0.46
1:F:175:ASP:OD1	1:F:218:GLY:HA2	2.16	0.46
1:F:679:SER:O	1:F:683:ARG:HG2	2.16	0.46
1:G:197:VAL:O	1:G:201:ILE:HD13	2.16	0.46
1:H:354:ARG:C	1:H:355:LEU:HD12	2.35	0.46
1:D:140:GLU:O	1:D:144:LEU:HG	2.16	0.46
1:F:496:ARG:HB2	1:F:527:GLU:CG	2.44	0.46
1:C:638:ASN:HB3	1:C:641:CYS:HB3	1.97	0.46
1:D:529:CYS:HB3	1:D:711:PHE:O	2.16	0.46
1:G:277:ASP:OD2	1:G:281:LYS:HB2	2.16	0.46
1:G:480:LYS:HB3	1:G:482:VAL:HG23	1.97	0.46
1:G:515:LEU:CD1	1:G:534:MET:HB2	2.46	0.46
1:B:132:THR:HG22	1:B:361:VAL:HG22	1.98	0.46
1:B:230:LEU:H	1:B:230:LEU:CD2	2.28	0.46
1:C:445:ALA:HB2	1:C:461:ILE:CD1	2.46	0.46
1:D:533:VAL:HG22	1:D:696:TRP:CE3	2.51	0.46
1:E:576:ARG:HG2	1:E:578:PHE:CZ	2.51	0.46
1:F:550:ILE:HD13	1:F:686:GLY:HA2	1.97	0.46
1:G:728:ILE:HD12	1:G:729:PHE:H	1.79	0.46
1:H:589:TYR:CE1	1:H:593:MET:HG3	2.50	0.46
1:A:289:LYS:O	1:A:293:VAL:HG23	2.15	0.46
1:B:355:LEU:HD12	1:B:355:LEU:N	2.31	0.46
1:D:289:LYS:O	1:D:293:VAL:HG23	2.15	0.46
1:E:59:PHE:CG	1:E:93:ILE:HD11	2.51	0.46
1:E:176:ASN:HA	1:E:184:THR:HG21	1.98	0.46
1:F:644:ASN:O	1:G:652:GLN:HB3	2.16	0.46
1:A:17:LEU:HD21	1:A:49:MET:HE3	1.98	0.45
1:A:135:ASN:HB2	1:A:357:LEU:HD13	1.97	0.45
1:A:230:LEU:H	1:A:230:LEU:CD2	2.27	0.45
1:A:550:ILE:HD13	1:A:686:GLY:HA2	1.98	0.45
1:C:488:LEU:HD22	1:C:528:PHE:CE1	2.51	0.45
1:D:483:LEU:HD21	1:D:510:GLU:HB2	1.98	0.45
1:D:505:ILE:HD12	1:D:515:LEU:HD21	1.97	0.45
1:E:49:MET:HG3	1:E:327:VAL:HG22	1.97	0.45
1:E:481:ARG:HB2	1:E:481:ARG:NH1	2.29	0.45
1:F:579:ILE:HD12	1:F:579:ILE:N	2.31	0.45
1:A:576:ARG:HG2	1:A:578:PHE:CZ	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:LEU:O	1:D:626:MET:HG2	2.16	0.45
1:E:161:LYS:HE3	1:E:162:TYR:CZ	2.52	0.45
1:E:488:LEU:HD13	1:E:521:ALA:CB	2.46	0.45
1:E:739:THR:HG23	1:E:741:PHE:CE1	2.51	0.45
1:F:289:LYS:O	1:F:293:VAL:HG23	2.17	0.45
1:G:433:VAL:HG21	1:G:461:ILE:HD12	1.94	0.45
1:H:108:LEU:HG	1:H:144:LEU:HD22	1.98	0.45
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.81	0.45
1:A:708:GLY:C	1:A:710:LYS:H	2.20	0.45
1:B:337:THR:HB	1:B:338:PRO:CD	2.46	0.45
1:B:419:GLY:HA2	1:B:510:GLU:HG3	1.98	0.45
1:B:645:TYR:CZ	1:C:656:GLU:HG2	2.51	0.45
1:B:739:THR:HG23	1:B:741:PHE:CE1	2.51	0.45
1:C:142:SER:O	1:C:146:GLU:HG2	2.17	0.45
1:C:262:ARG:HB3	1:C:464:THR:HG21	1.98	0.45
1:D:418:VAL:O	1:D:507:GLY:HA3	2.16	0.45
1:F:503:LEU:HB3	1:F:532:MET:HG2	1.99	0.45
1:H:181:THR:HG22	1:H:346:SER:OG	2.17	0.45
1:H:347:LEU:HD12	1:H:352:ALA:HA	1.99	0.45
1:H:638:ASN:HB3	1:H:641:CYS:HB3	1.98	0.45
1:B:658:GLY:O	1:B:659:LYS:C	2.55	0.45
1:C:480:LYS:HB3	1:C:482:VAL:HG23	1.98	0.45
1:G:622:LEU:O	1:G:626:MET:HG2	2.16	0.45
1:H:140:GLU:O	1:H:144:LEU:HG	2.16	0.45
1:H:263:LYS:HD3	1:H:263:LYS:HA	1.78	0.45
1:B:14:ARG:HG2	1:B:16:PHE:CZ	2.51	0.45
1:C:445:ALA:HB2	1:C:461:ILE:HD13	1.98	0.45
1:G:509:PHE:O	1:G:513:LEU:HG	2.17	0.45
1:G:628:THR:HB	1:G:629:THR:H	1.36	0.45
1:A:205:ALA:O	1:B:91:THR:N	2.42	0.45
1:A:245:GLU:OE2	1:A:245:GLU:HA	2.16	0.45
1:B:515:LEU:HD11	1:B:534:MET:HB2	1.98	0.45
1:D:254:VAL:HG12	1:D:255:LYS:N	2.30	0.45
1:F:262:ARG:HB3	1:F:464:THR:HG21	1.98	0.45
1:F:445:ALA:HB1	1:F:477:LEU:HD11	1.99	0.45
1:F:638:ASN:HB3	1:F:641:CYS:HB3	1.98	0.45
1:G:531:PRO:HG3	1:G:711:PHE:CD2	2.51	0.45
1:H:559:ILE:HG12	1:H:669:LEU:HD11	1.99	0.45
1:A:277:ASP:C	1:A:279:GLN:H	2.19	0.45
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.78	0.45
1:B:262:ARG:HB3	1:B:464:THR:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:HD12	1:C:352:ALA:HA	1.99	0.45
1:D:559:ILE:HG12	1:D:669:LEU:HD11	1.99	0.45
1:D:615:LEU:O	1:D:619:VAL:HG23	2.16	0.45
1:D:688:LYS:C	1:D:688:LYS:HD2	2.36	0.45
1:H:601:ASP:OD2	1:H:622:LEU:HD13	2.17	0.45
1:H:757:LEU:CD2	1:H:757:LEU:C	2.85	0.45
1:A:156:LYS:HE2	1:A:156:LYS:HA	1.98	0.45
1:B:17:LEU:C	1:B:19:HIS:H	2.20	0.45
1:B:135:ASN:CA	1:B:357:LEU:HD13	2.47	0.45
1:B:140:GLU:O	1:B:144:LEU:HG	2.17	0.45
1:E:493:THR:HG23	1:E:496:ARG:NH1	2.32	0.45
1:E:732:VAL:HG23	1:E:733:ALA:N	2.32	0.45
1:F:93:ILE:HD13	1:F:93:ILE:HA	1.81	0.45
1:F:256:LEU:HD21	1:F:269:ILE:HD11	1.99	0.45
1:H:136:LEU:C	1:H:136:LEU:HD23	2.38	0.45
1:H:658:GLY:O	1:H:659:LYS:C	2.55	0.45
1:B:227:VAL:HA	1:B:230:LEU:CD2	2.46	0.45
1:B:227:VAL:HA	1:B:230:LEU:HD21	1.98	0.45
1:B:289:LYS:O	1:B:293:VAL:HG23	2.16	0.45
1:B:628:THR:HB	1:B:629:THR:H	1.35	0.45
1:C:53:VAL:HG21	1:C:334:LEU:HD11	1.99	0.45
1:C:325:MET:HA	1:C:325:MET:CE	2.47	0.45
1:D:230:LEU:H	1:D:230:LEU:CD2	2.28	0.45
1:F:142:SER:O	1:F:146:GLU:HG2	2.17	0.45
1:F:354:ARG:C	1:F:355:LEU:HD12	2.37	0.45
1:F:526:GLU:C	1:F:528:PHE:N	2.70	0.45
1:H:336:ALA:HA	1:H:340:THR:HG21	1.98	0.45
1:H:355:LEU:HD12	1:H:355:LEU:N	2.31	0.45
1:H:658:GLY:O	1:H:661:VAL:HG12	2.17	0.45
1:A:428:ALA:CB	1:A:506:ILE:HD13	2.47	0.45
1:B:325:MET:HA	1:B:325:MET:CE	2.47	0.45
1:C:17:LEU:HB2	1:C:768:TYR:HB3	1.99	0.45
1:C:155:ASP:HB3	1:C:158:ALA:CB	2.47	0.45
1:C:277:ASP:OD2	1:C:281:LYS:HB2	2.17	0.45
1:D:445:ALA:HB2	1:D:461:ILE:CD1	2.47	0.45
1:G:142:SER:O	1:G:146:GLU:HG2	2.17	0.45
1:H:487:TYR:O	1:H:491:ILE:HG13	2.17	0.45
1:A:171:VAL:HG21	1:A:181:THR:HG21	1.99	0.44
1:A:250:GLU:CD	1:A:250:GLU:H	2.19	0.44
1:B:559:ILE:HG12	1:B:669:LEU:HD11	1.98	0.44
1:C:100:ALA:O	1:C:106:GLY:HA3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:TYR:CE1	1:E:593:MET:HG3	2.52	0.44
1:F:526:GLU:O	1:F:528:PHE:N	2.50	0.44
1:H:445:ALA:HB1	1:H:477:LEU:HD11	1.98	0.44
1:D:49:MET:HG3	1:D:327:VAL:HG22	2.00	0.44
1:D:347:LEU:HD12	1:D:352:ALA:HA	1.98	0.44
1:E:325:MET:HA	1:E:325:MET:CE	2.48	0.44
1:F:505:ILE:HD12	1:F:515:LEU:CD2	2.47	0.44
1:G:256:LEU:HD21	1:G:269:ILE:HD11	1.98	0.44
1:G:550:ILE:HD13	1:G:686:GLY:HA2	1.98	0.44
1:B:550:ILE:HD13	1:B:686:GLY:HA2	2.00	0.44
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.84	0.44
1:C:355:LEU:HD12	1:C:355:LEU:N	2.32	0.44
1:C:521:ALA:C	1:C:523:GLU:H	2.20	0.44
1:D:638:ASN:HB3	1:D:641:CYS:HB3	1.99	0.44
1:D:737:LYS:HE3	1:D:737:LYS:HB3	1.67	0.44
1:E:495:MET:CE	1:E:500:ILE:HB	2.47	0.44
1:F:277:ASP:OD2	1:F:281:LYS:HB2	2.17	0.44
1:G:481:ARG:HG3	1:G:481:ARG:HH11	1.81	0.44
1:G:757:LEU:C	1:G:757:LEU:CD2	2.85	0.44
1:A:481:ARG:HG3	1:A:510:GLU:OE1	2.17	0.44
1:A:589:TYR:CE1	1:A:593:MET:HG3	2.52	0.44
1:C:770:VAL:HG22	1:C:770:VAL:O	2.17	0.44
1:E:140:GLU:O	1:E:144:LEU:HG	2.17	0.44
1:E:142:SER:O	1:E:146:GLU:HG2	2.17	0.44
1:E:433:VAL:HG21	1:E:461:ILE:HD12	2.00	0.44
1:G:249:GLU:CG	1:G:291:LEU:HD21	2.48	0.44
1:H:45:ALA:HB3	1:H:326:GLY:HA3	2.00	0.44
1:H:262:ARG:O	1:H:263:LYS:HB2	2.18	0.44
1:A:418:VAL:O	1:A:507:GLY:HA3	2.18	0.44
1:B:336:ALA:HA	1:B:340:THR:HG21	2.00	0.44
1:C:181:THR:O	1:C:182:ASP:C	2.56	0.44
1:D:589:TYR:CE1	1:D:593:MET:HG3	2.52	0.44
1:G:255:LYS:HZ1	1:G:399:ILE:HA	1.82	0.44
1:G:515:LEU:O	1:G:517:GLU:N	2.51	0.44
1:H:142:SER:O	1:H:146:GLU:HG2	2.18	0.44
1:B:14:ARG:HH11	1:B:14:ARG:HB2	1.82	0.44
1:B:155:ASP:HB3	1:B:158:ALA:CB	2.48	0.44
1:B:347:LEU:HD12	1:B:352:ALA:HA	1.98	0.44
1:C:336:ALA:HA	1:C:340:THR:HG21	2.00	0.44
1:D:336:ALA:HA	1:D:340:THR:HG21	1.99	0.44
1:D:495:MET:HE3	1:D:500:ILE:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:LEU:O	1:D:532:MET:HA	2.18	0.44
1:E:533:VAL:HG13	1:E:696:TRP:CZ3	2.52	0.44
1:G:258:GLU:O	1:G:262:ARG:HG3	2.17	0.44
1:G:579:ILE:HD12	1:G:579:ILE:N	2.32	0.44
1:A:262:ARG:HB3	1:A:464:THR:HG21	1.98	0.44
1:A:703:GLU:HB3	1:E:404:ASP:CG	2.38	0.44
1:B:132:THR:HG22	1:B:361:VAL:CG1	2.34	0.44
1:B:340:THR:HG23	1:B:340:THR:O	2.18	0.44
1:B:400:LYS:HG3	1:B:463:TRP:CE3	2.53	0.44
1:C:628:THR:HB	1:C:629:THR:H	1.34	0.44
1:D:495:MET:CE	1:D:500:ILE:HB	2.48	0.44
1:F:396:ARG:NH1	1:F:439:ASP:OD2	2.51	0.44
1:G:347:LEU:HD12	1:G:352:ALA:HA	1.99	0.44
1:G:638:ASN:HB3	1:G:641:CYS:HB3	2.00	0.44
1:D:215:GLU:OE1	1:D:304:ILE:HG23	2.18	0.44
1:D:556:LEU:HD13	1:D:590:LEU:HD23	2.00	0.44
1:F:347:LEU:HD12	1:F:352:ALA:HA	1.99	0.44
1:G:277:ASP:C	1:G:279:GLN:H	2.21	0.44
1:H:195:ILE:HD11	1:H:231:ALA:HB3	2.00	0.44
1:H:289:LYS:O	1:H:293:VAL:HG23	2.18	0.44
1:A:445:ALA:HB1	1:A:477:LEU:HD11	1.99	0.44
1:A:559:ILE:HG12	1:A:669:LEU:HD11	2.00	0.44
1:C:527:GLU:C	1:C:529:CYS:H	2.22	0.44
1:D:187:THR:HG21	1:D:223:TYR:CE2	2.48	0.44
1:D:277:ASP:OD2	1:D:281:LYS:HB2	2.18	0.44
1:E:336:ALA:HA	1:E:340:THR:HG21	2.00	0.44
1:G:131:LEU:HD23	1:G:178:PHE:CE2	2.53	0.44
1:G:337:THR:HB	1:G:338:PRO:CD	2.48	0.44
1:H:168:VAL:HG11	1:H:333:LEU:HD13	1.98	0.44
1:B:683:ARG:HG2	1:B:683:ARG:H	1.48	0.43
1:B:770:VAL:HG22	1:B:770:VAL:O	2.17	0.43
1:E:490:GLU:OE1	1:E:490:GLU:N	2.47	0.43
1:E:515:LEU:HD22	1:E:717:ILE:HG23	2.00	0.43
1:F:342:ALA:O	1:F:357:LEU:HB2	2.18	0.43
1:F:390:ASN:OD1	1:F:688:LYS:HD3	2.17	0.43
1:F:508:GLY:O	1:F:511:ALA:HB3	2.18	0.43
1:G:18:GLU:CD	1:G:18:GLU:H	2.22	0.43
1:A:17:LEU:HD23	1:A:52:TYR:CE1	2.53	0.43
1:A:155:ASP:HB3	1:A:158:ALA:CB	2.48	0.43
1:B:551:GLY:H	1:B:682:ASP:CG	2.20	0.43
1:B:732:VAL:HG23	1:B:733:ALA:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:LEU:HG	1:E:144:LEU:HD22	2.01	0.43
1:E:512:TYR:CE2	1:E:516:LEU:HD11	2.53	0.43
1:E:638:ASN:HB3	1:E:641:CYS:HB3	2.00	0.43
1:F:17:LEU:C	1:F:19:HIS:H	2.22	0.43
1:F:418:VAL:O	1:F:507:GLY:HA3	2.18	0.43
1:A:503:LEU:O	1:A:532:MET:HA	2.18	0.43
1:A:509:PHE:HE2	1:A:513:LEU:HD21	1.83	0.43
1:A:575:ARG:HD2	1:A:631:GLN:OE1	2.18	0.43
1:B:522:ARG:NH2	1:B:711:PHE:O	2.52	0.43
1:C:108:LEU:HG	1:C:144:LEU:HD22	1.99	0.43
1:C:550:ILE:HD13	1:C:686:GLY:HA2	1.99	0.43
1:D:503:LEU:HD23	1:D:532:MET:CE	2.49	0.43
1:E:347:LEU:HD12	1:E:352:ALA:HA	2.00	0.43
1:E:630:ILE:HG22	1:E:631:GLN:N	2.33	0.43
1:E:704:ALA:O	1:E:705:ARG:C	2.57	0.43
1:F:262:ARG:HG2	1:F:262:ARG:NH1	2.32	0.43
1:F:336:ALA:HA	1:F:340:THR:HG21	2.00	0.43
1:H:249:GLU:CG	1:H:291:LEU:HD21	2.48	0.43
1:A:638:ASN:HB3	1:A:641:CYS:HB3	1.99	0.43
1:C:342:ALA:O	1:C:357:LEU:HB2	2.18	0.43
1:D:17:LEU:CD2	1:D:49:MET:HE1	2.49	0.43
1:D:340:THR:HG23	1:D:340:THR:O	2.18	0.43
1:D:658:GLY:O	1:D:659:LYS:C	2.56	0.43
1:E:456:GLY:HA2	1:E:494:GLN:CG	2.48	0.43
1:E:700:LYS:HD2	1:E:711:PHE:CE2	2.53	0.43
1:F:381:ARG:HE	1:F:381:ARG:HB3	1.61	0.43
1:G:262:ARG:HG2	1:G:262:ARG:NH1	2.31	0.43
1:H:325:MET:HA	1:H:325:MET:CE	2.47	0.43
1:H:703:GLU:C	1:H:705:ARG:H	2.21	0.43
1:A:355:LEU:HD12	1:A:355:LEU:N	2.33	0.43
1:A:519:SER:O	1:A:522:ARG:CG	2.62	0.43
1:B:333:LEU:HD12	1:B:333:LEU:HA	1.82	0.43
1:B:697:ILE:O	1:B:701:LEU:HG	2.17	0.43
1:B:757:LEU:C	1:B:757:LEU:CD2	2.87	0.43
1:E:62:GLU:OE2	1:F:207:SER:HB3	2.18	0.43
1:E:179:CYS:SG	1:E:367:VAL:HG21	2.58	0.43
1:E:770:VAL:HG22	1:E:770:VAL:O	2.18	0.43
1:F:355:LEU:HD12	1:F:355:LEU:N	2.32	0.43
1:G:15:LYS:H	1:G:15:LYS:CD	2.31	0.43
1:G:732:VAL:HG23	1:G:733:ALA:N	2.33	0.43
1:A:354:ARG:C	1:A:355:LEU:HD12	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LEU:O	1:A:626:MET:HG2	2.18	0.43
1:C:176:ASN:ND2	1:C:184:THR:HG23	2.34	0.43
1:C:237:VAL:HG23	1:C:394:TYR:CE2	2.53	0.43
1:C:506:ILE:HG22	1:C:506:ILE:O	2.19	0.43
1:E:510:GLU:H	1:E:510:GLU:HG2	1.58	0.43
1:F:108:LEU:HG	1:F:144:LEU:HD22	2.01	0.43
1:G:136:LEU:C	1:G:136:LEU:HD23	2.39	0.43
1:G:289:LYS:O	1:G:293:VAL:HG23	2.19	0.43
1:G:505:ILE:CG2	1:G:511:ALA:HB1	2.46	0.43
1:H:250:GLU:CD	1:H:250:GLU:H	2.22	0.43
1:A:556:LEU:HD13	1:A:590:LEU:HD23	2.01	0.43
1:D:153:GLN:HE21	1:D:153:GLN:HB2	1.52	0.43
1:D:262:ARG:HB3	1:D:464:THR:HG21	2.01	0.43
1:E:14:ARG:HH22	1:E:16:PHE:HZ	1.66	0.43
1:E:622:LEU:O	1:E:626:MET:HG2	2.18	0.43
1:G:215:GLU:OE1	1:G:304:ILE:HG23	2.19	0.43
1:H:215:GLU:OE1	1:H:304:ILE:HG23	2.18	0.43
1:H:256:LEU:HD21	1:H:269:ILE:HD11	2.00	0.43
1:H:296:LEU:HD13	1:H:298:TYR:CE2	2.53	0.43
1:A:155:ASP:OD2	1:A:156:LYS:N	2.52	0.43
1:A:325:MET:CE	1:A:325:MET:HA	2.48	0.43
1:A:700:LYS:O	1:A:703:GLU:HG2	2.18	0.43
1:C:495:MET:HA	1:C:500:ILE:HD12	2.00	0.43
1:D:249:GLU:CG	1:D:291:LEU:HD21	2.48	0.43
1:D:333:LEU:HD12	1:D:333:LEU:HA	1.83	0.43
1:D:485:GLY:C	1:D:487:TYR:H	2.22	0.43
1:D:678:PRO:O	1:D:683:ARG:HD3	2.19	0.43
1:F:400:LYS:HB2	1:F:463:TRP:CZ2	2.53	0.43
1:F:757:LEU:C	1:F:757:LEU:CD2	2.87	0.43
1:F:770:VAL:HG22	1:F:770:VAL:O	2.19	0.43
1:H:556:LEU:HD12	1:H:556:LEU:HA	1.92	0.43
1:A:307:HIS:CE1	1:B:303:THR:CG2	2.75	0.43
1:A:757:LEU:C	1:A:757:LEU:CD2	2.87	0.43
1:B:249:GLU:CG	1:B:291:LEU:HD21	2.49	0.43
1:B:509:PHE:CE2	1:B:744:ARG:HG2	2.54	0.43
1:D:277:ASP:C	1:D:279:GLN:H	2.22	0.43
1:D:732:VAL:HG23	1:D:733:ALA:N	2.33	0.43
1:E:556:LEU:HD13	1:E:590:LEU:HD23	2.00	0.43
1:E:628:THR:HB	1:E:629:THR:H	1.33	0.43
1:E:779:VAL:HG13	1:E:779:VAL:O	2.18	0.43
1:F:224:LEU:HD23	1:F:224:LEU:HA	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:VAL:HG23	1:G:394:TYR:CE2	2.53	0.43
1:G:336:ALA:HA	1:G:340:THR:HG21	1.99	0.43
1:G:400:LYS:HB2	1:G:463:TRP:CZ2	2.53	0.43
1:G:658:GLY:O	1:G:659:LYS:C	2.57	0.43
1:H:574:LYS:HD3	6:H:903:HOH:O	2.19	0.43
1:A:347:LEU:HD12	1:A:352:ALA:HA	2.01	0.43
1:A:487:TYR:CD2	1:A:487:TYR:N	2.87	0.43
1:D:400:LYS:HB2	1:D:463:TRP:CZ2	2.54	0.43
1:D:770:VAL:HG22	1:D:770:VAL:O	2.18	0.43
1:E:355:LEU:HD12	1:E:355:LEU:N	2.33	0.43
1:E:673:GLN:N	1:E:673:GLN:CD	2.72	0.43
1:H:521:ALA:C	1:H:523:GLU:H	2.21	0.43
1:A:336:ALA:HA	1:A:340:THR:HG21	2.01	0.42
1:A:509:PHE:O	1:A:512:TYR:HB3	2.19	0.42
1:B:277:ASP:C	1:B:279:GLN:H	2.22	0.42
1:B:277:ASP:OD2	1:B:281:LYS:HB2	2.18	0.42
1:C:175:ASP:O	1:C:176:ASN:HB3	2.19	0.42
1:D:693:ALA:HB2	1:D:720:LEU:HD23	2.00	0.42
1:E:237:VAL:HG23	1:E:394:TYR:CE2	2.54	0.42
1:E:508:GLY:HA3	1:E:538:THR:HG23	2.01	0.42
1:F:760:ILE:C	1:F:760:ILE:HD12	2.39	0.42
1:G:515:LEU:HA	1:G:515:LEU:HD23	1.71	0.42
1:H:503:LEU:HD23	1:H:532:MET:HE2	2.01	0.42
1:C:128:ASP:HA	1:C:178:PHE:CD1	2.54	0.42
1:C:249:GLU:CG	1:C:291:LEU:HD21	2.49	0.42
1:E:411:CYS:CA	1:E:501:ASN:OD1	2.61	0.42
1:E:529:CYS:SG	1:E:712:THR:HG22	2.59	0.42
1:F:590:LEU:HD23	1:F:590:LEU:HA	1.87	0.42
1:A:739:THR:HG23	1:A:741:PHE:CE1	2.53	0.42
1:B:255:LYS:HZ1	1:B:399:ILE:HA	1.84	0.42
1:B:492:ALA:O	1:B:527:GLU:HG2	2.19	0.42
1:B:757:LEU:HD23	1:B:761:LEU:HG	2.01	0.42
1:D:342:ALA:O	1:D:357:LEU:HB2	2.19	0.42
1:F:416:ILE:HG12	1:F:417:ASN:N	2.35	0.42
1:F:503:LEU:O	1:F:532:MET:HA	2.19	0.42
1:F:525:HIS:CD2	1:F:525:HIS:N	2.87	0.42
1:F:658:GLY:O	1:F:661:VAL:HG12	2.19	0.42
1:G:342:ALA:O	1:G:357:LEU:HB2	2.18	0.42
1:H:487:TYR:CD2	1:H:487:TYR:N	2.87	0.42
1:H:551:GLY:H	1:H:682:ASP:CG	2.22	0.42
1:A:303:THR:CG2	1:B:307:HIS:CE1	2.96	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ILE:HD12	1:A:773:SER:HB2	1.98	0.42
1:B:445:ALA:HB1	1:B:477:LEU:HD11	2.00	0.42
1:C:39:MET:O	1:C:43:VAL:HG13	2.19	0.42
1:D:431:SER:O	1:D:435:VAL:HG23	2.20	0.42
1:E:249:GLU:CG	1:E:291:LEU:HD21	2.50	0.42
1:E:430:ARG:HD2	1:E:466:VAL:O	2.20	0.42
1:H:262:ARG:HG2	1:H:262:ARG:NH1	2.32	0.42
1:H:340:THR:O	1:H:340:THR:HG23	2.19	0.42
1:H:416:ILE:HD11	1:H:449:GLY:C	2.40	0.42
1:H:503:LEU:O	1:H:532:MET:HA	2.19	0.42
1:A:533:VAL:CG2	1:A:696:TRP:CE3	3.02	0.42
1:C:37:GLN:HB3	1:C:314:PRO:HB3	2.02	0.42
1:C:289:LYS:O	1:C:293:VAL:HG23	2.19	0.42
1:C:630:ILE:HG22	1:C:631:GLN:N	2.35	0.42
1:F:136:LEU:HD23	1:F:136:LEU:C	2.40	0.42
1:F:333:LEU:HD12	1:F:333:LEU:HA	1.81	0.42
1:G:390:ASN:OD1	1:G:688:LYS:HD3	2.20	0.42
1:H:678:PRO:O	1:H:683:ARG:HD3	2.20	0.42
1:A:732:VAL:HG23	1:A:733:ALA:N	2.34	0.42
1:C:277:ASP:C	1:C:279:GLN:H	2.22	0.42
1:C:488:LEU:HD22	1:C:528:PHE:HE1	1.84	0.42
1:C:658:GLY:O	1:C:659:LYS:C	2.58	0.42
1:C:757:LEU:C	1:C:757:LEU:CD2	2.87	0.42
1:E:678:PRO:O	1:E:683:ARG:HD3	2.19	0.42
1:F:556:LEU:HD13	1:F:590:LEU:HD23	2.02	0.42
1:H:431:SER:O	1:H:435:VAL:HG23	2.19	0.42
1:A:255:LYS:HZ2	1:A:399:ILE:HA	1.84	0.42
1:B:245:GLU:OE2	1:B:245:GLU:HA	2.18	0.42
1:B:637:ARG:NH2	1:B:646:THR:HA	2.34	0.42
1:D:128:ASP:HA	1:D:178:PHE:CD1	2.54	0.42
1:D:337:THR:HB	1:D:338:PRO:CD	2.49	0.42
1:E:337:THR:HB	1:E:338:PRO:CD	2.49	0.42
1:E:724:LYS:HD2	1:E:724:LYS:N	2.25	0.42
1:F:419:GLY:HA2	1:F:510:GLU:CG	2.40	0.42
1:F:645:TYR:CZ	1:G:656:GLU:HG2	2.54	0.42
1:G:556:LEU:HD13	1:G:590:LEU:HD23	2.02	0.42
1:E:757:LEU:C	1:E:757:LEU:CD2	2.88	0.42
1:F:430:ARG:HD2	1:F:466:VAL:O	2.20	0.42
1:G:108:LEU:HG	1:G:144:LEU:HD22	2.01	0.42
1:A:719:VAL:O	1:A:719:VAL:HG12	2.18	0.42
1:B:108:LEU:HG	1:B:144:LEU:HD22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ILE:HG12	1:C:417:ASN:N	2.35	0.42
1:D:17:LEU:HD21	1:D:49:MET:HE1	2.02	0.42
1:D:108:LEU:HG	1:D:144:LEU:HD22	2.01	0.42
1:D:284:THR:HG23	1:D:287:LYS:CB	2.50	0.42
1:D:416:ILE:HG12	1:D:417:ASN:N	2.35	0.42
1:E:289:LYS:O	1:E:293:VAL:HG23	2.20	0.42
1:E:710:LYS:HB3	1:E:711:PHE:H	1.60	0.42
1:F:217:MET:HA	1:F:273:GLU:HG3	2.02	0.42
1:G:59:PHE:CD2	1:G:93:ILE:HD11	2.54	0.42
1:H:168:VAL:HA	1:H:343:CYS:O	2.20	0.42
1:A:108:LEU:HG	1:A:144:LEU:HD22	2.01	0.42
1:C:250:GLU:CD	1:C:250:GLU:H	2.23	0.42
1:E:277:ASP:C	1:E:279:GLN:H	2.23	0.42
1:G:307:HIS:CE1	1:H:303:THR:HG23	2.55	0.42
1:G:355:LEU:HD12	1:G:355:LEU:N	2.35	0.42
1:G:619:VAL:HG11	1:G:657:GLU:HB2	2.02	0.42
1:A:153:GLN:HE21	1:A:153:GLN:HB2	1.54	0.41
1:B:556:LEU:HD13	1:B:590:LEU:HD23	2.02	0.41
1:D:100:ALA:O	1:D:106:GLY:HA3	2.20	0.41
1:D:516:LEU:HA	1:D:516:LEU:HD23	1.85	0.41
1:D:658:GLY:O	1:D:661:VAL:HG12	2.20	0.41
1:E:501:ASN:O	1:E:530:VAL:HB	2.20	0.41
1:F:495:MET:HA	1:F:500:ILE:HD12	2.01	0.41
1:F:732:VAL:HG23	1:F:733:ALA:N	2.34	0.41
1:G:478:GLY:HA3	1:H:572:GLY:HA3	2.02	0.41
1:H:153:GLN:HE21	1:H:153:GLN:HB2	1.53	0.41
1:H:368:GLN:OE1	1:H:368:GLN:HA	2.20	0.41
1:H:533:VAL:HG23	1:H:697:ILE:HD11	2.02	0.41
1:A:168:VAL:HG12	1:A:333:LEU:HD13	1.98	0.41
1:A:590:LEU:HD23	1:A:590:LEU:HA	1.92	0.41
1:C:303:THR:HG21	1:D:307:HIS:HE1	1.82	0.41
1:C:527:GLU:CD	1:C:527:GLU:H	2.22	0.41
1:D:93:ILE:HD13	1:D:93:ILE:HA	1.78	0.41
1:E:37:GLN:HB3	1:E:314:PRO:HB3	2.01	0.41
1:E:100:ALA:O	1:E:106:GLY:HA3	2.20	0.41
1:F:337:THR:HB	1:F:338:PRO:CD	2.49	0.41
1:F:736:LYS:HA	1:F:739:THR:CG2	2.50	0.41
1:H:187:THR:HG21	1:H:223:TYR:CE2	2.49	0.41
1:H:231:ALA:HA	1:H:684:ASN:HD21	1.84	0.41
1:H:662:PHE:CD1	1:H:662:PHE:C	2.94	0.41
1:A:140:GLU:O	1:A:144:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ILE:HD11	1:B:449:GLY:C	2.41	0.41
1:B:678:PRO:O	1:B:683:ARG:HD3	2.19	0.41
1:C:430:ARG:HD2	1:C:466:VAL:O	2.20	0.41
1:C:622:LEU:O	1:C:626:MET:HG2	2.20	0.41
1:D:237:VAL:HG23	1:D:394:TYR:CE2	2.56	0.41
1:D:315:SER:O	1:D:319:ARG:HG3	2.20	0.41
1:D:459:LYS:HG2	1:D:460:GLU:N	2.35	0.41
1:D:750:TRP:CG	1:D:751:TRP:N	2.87	0.41
1:E:256:LEU:HD21	1:E:269:ILE:HD11	2.02	0.41
1:F:237:VAL:HG23	1:F:394:TYR:CE2	2.55	0.41
1:G:533:VAL:HG22	1:G:696:TRP:CZ3	2.55	0.41
1:G:630:ILE:HG22	1:G:631:GLN:N	2.34	0.41
1:H:44:ARG:HA	1:H:82:VAL:HB	2.02	0.41
1:H:139:LYS:HE3	1:H:139:LYS:HB3	1.86	0.41
1:H:277:ASP:C	1:H:279:GLN:H	2.23	0.41
1:H:693:ALA:HB2	1:H:720:LEU:HD23	2.01	0.41
1:A:337:THR:HB	1:A:338:PRO:CD	2.49	0.41
1:C:262:ARG:HG2	1:C:262:ARG:NH1	2.33	0.41
1:D:515:LEU:HD11	1:D:534:MET:HB2	2.02	0.41
1:E:333:LEU:HD12	1:E:333:LEU:HA	1.82	0.41
1:E:662:PHE:CD1	1:E:662:PHE:C	2.93	0.41
1:F:59:PHE:CD2	1:F:93:ILE:HD11	2.55	0.41
1:F:168:VAL:HG11	1:F:333:LEU:HD13	2.00	0.41
1:F:195:ILE:HD11	1:F:231:ALA:HB3	2.02	0.41
1:F:518:LEU:HD13	1:F:532:MET:HE2	2.00	0.41
1:G:487:TYR:O	1:G:491:ILE:HG13	2.20	0.41
1:G:550:ILE:CD1	1:G:686:GLY:HA2	2.51	0.41
1:H:155:ASP:HB3	1:H:158:ALA:HB2	2.02	0.41
1:H:230:LEU:H	1:H:230:LEU:CD2	2.32	0.41
1:A:237:VAL:HG23	1:A:394:TYR:CE2	2.56	0.41
1:A:249:GLU:CG	1:A:291:LEU:HD21	2.50	0.41
1:C:140:GLU:O	1:C:144:LEU:HG	2.21	0.41
1:C:619:VAL:HG11	1:C:657:GLU:HB2	2.02	0.41
1:C:732:VAL:HG23	1:C:733:ALA:N	2.36	0.41
1:E:258:GLU:O	1:E:262:ARG:HG3	2.21	0.41
1:E:416:ILE:HG12	1:E:417:ASN:N	2.36	0.41
1:F:513:LEU:HD23	1:F:513:LEU:HA	1.76	0.41
1:G:65:GLN:HA	1:G:98:CYS:SG	2.60	0.41
1:G:128:ASP:N	1:G:128:ASP:OD2	2.52	0.41
1:H:556:LEU:HD13	1:H:590:LEU:HD23	2.03	0.41
1:H:622:LEU:O	1:H:626:MET:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:O	1:A:279:GLN:N	2.53	0.41
1:A:510:GLU:CD	1:A:510:GLU:H	2.24	0.41
1:A:662:PHE:CD1	1:A:662:PHE:C	2.93	0.41
1:B:484:PRO:HG2	1:B:517:GLU:OE1	2.20	0.41
1:D:136:LEU:C	1:D:136:LEU:HD23	2.41	0.41
1:D:508:GLY:HA3	1:D:538:THR:HG23	2.02	0.41
1:E:50:GLY:O	1:E:53:VAL:HG22	2.21	0.41
1:E:136:LEU:C	1:E:136:LEU:HD23	2.41	0.41
1:E:459:LYS:HG2	1:E:460:GLU:N	2.36	0.41
1:E:655:SER:OG	1:E:664:CYS:HB2	2.21	0.41
1:F:277:ASP:C	1:F:279:GLN:H	2.22	0.41
1:F:689:ILE:HG13	1:F:689:ILE:H	1.64	0.41
1:G:49:MET:HG3	1:G:327:VAL:HA	2.01	0.41
1:G:187:THR:HG21	1:G:223:TYR:CE2	2.50	0.41
1:G:340:THR:HG23	1:G:340:THR:O	2.20	0.41
1:G:673:GLN:N	1:G:673:GLN:CD	2.74	0.41
1:G:757:LEU:C	1:G:757:LEU:HD23	2.41	0.41
1:H:337:THR:HB	1:H:338:PRO:CD	2.50	0.41
1:A:128:ASP:HA	1:A:178:PHE:CD1	2.55	0.41
1:A:412:ASN:HB2	1:A:499:SER:O	2.21	0.41
1:A:615:LEU:HD12	1:A:615:LEU:HA	1.91	0.41
1:B:736:LYS:HA	1:B:739:THR:CG2	2.51	0.41
1:C:136:LEU:C	1:C:136:LEU:HD23	2.41	0.41
1:C:212:PHE:CE1	1:C:303:THR:CG2	2.94	0.41
1:D:509:PHE:HE2	1:D:513:LEU:HD21	1.85	0.41
1:D:683:ARG:HG2	1:D:683:ARG:H	1.47	0.41
1:E:481:ARG:HH11	1:E:481:ARG:CB	2.32	0.41
1:H:519:SER:HB2	1:H:717:ILE:HD12	2.01	0.41
1:H:618:ASN:N	1:H:618:ASN:ND2	2.68	0.41
1:H:750:TRP:CG	1:H:751:TRP:N	2.89	0.41
1:A:100:ALA:O	1:A:106:GLY:HA3	2.21	0.41
1:A:416:ILE:HG12	1:A:417:ASN:N	2.36	0.41
1:A:666:LYS:HB3	1:A:666:LYS:HE2	1.86	0.41
1:A:750:TRP:CG	1:A:751:TRP:N	2.89	0.41
1:D:59:PHE:CD2	1:D:93:ILE:HD11	2.56	0.41
1:D:183:MET:SD	1:D:187:THR:HB	2.61	0.41
1:D:718:CYS:HB3	1:D:719:VAL:H	1.74	0.41
1:F:423:ALA:HB1	1:F:678:PRO:HA	2.03	0.41
1:F:519:SER:HB2	1:F:717:ILE:CD1	2.50	0.41
1:G:445:ALA:HB1	1:G:477:LEU:HD11	2.03	0.41
1:G:469:TRP:CD2	1:G:476:ILE:HD12	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:702:LYS:HE2	1:G:702:LYS:HB3	1.67	0.41
1:H:430:ARG:HD2	1:H:466:VAL:O	2.20	0.41
1:A:349:GLY:O	1:A:350:ASN:HB3	2.21	0.41
1:A:496:ARG:HG2	1:A:496:ARG:NH2	2.36	0.41
1:B:556:LEU:HD12	1:B:556:LEU:HA	1.90	0.41
1:C:230:LEU:H	1:C:230:LEU:CD2	2.33	0.41
1:C:258:GLU:O	1:C:262:ARG:HG3	2.21	0.41
1:C:337:THR:HB	1:C:338:PRO:CD	2.50	0.41
1:C:662:PHE:CD1	1:C:662:PHE:C	2.94	0.41
1:D:32:SER:HB3	1:D:130:SER:OG	2.20	0.41
1:D:65:GLN:HA	1:D:98:CYS:SG	2.60	0.41
1:D:224:LEU:HD23	1:D:224:LEU:HA	1.86	0.41
1:D:480:LYS:HB3	1:D:482:VAL:HG23	2.03	0.41
1:D:509:PHE:CE2	1:D:513:LEU:HD21	2.56	0.41
1:D:515:LEU:O	1:D:519:SER:HB2	2.21	0.41
1:D:750:TRP:CD2	1:D:751:TRP:N	2.89	0.41
1:E:567:LYS:HG2	1:E:632:ARG:HG2	2.03	0.41
1:E:580:ILE:HB	1:E:636:LEU:HD22	2.03	0.41
1:F:493:THR:O	1:F:497:THR:HG23	2.20	0.41
1:F:496:ARG:HG2	1:F:496:ARG:HH21	1.86	0.41
1:F:720:LEU:HD22	1:F:729:PHE:CZ	2.56	0.41
1:G:416:ILE:HD11	1:G:449:GLY:C	2.41	0.41
1:G:662:PHE:CD1	1:G:662:PHE:C	2.94	0.41
1:H:45:ALA:O	1:H:49:MET:HB2	2.21	0.41
1:H:732:VAL:HG23	1:H:733:ALA:N	2.36	0.41
1:A:136:LEU:HD23	1:A:136:LEU:C	2.40	0.41
1:A:580:ILE:HB	1:A:636:LEU:HD22	2.03	0.41
1:B:486:LYS:HB2	1:B:487:TYR:CD2	2.56	0.41
1:B:534:MET:HE1	1:B:543:VAL:HG11	2.03	0.41
1:B:630:ILE:HG22	1:B:631:GLN:N	2.35	0.41
1:C:44:ARG:HA	1:C:82:VAL:HG11	2.03	0.41
1:D:171:VAL:HG21	1:D:181:THR:HG21	2.03	0.41
1:D:296:LEU:HD13	1:D:298:TYR:CE2	2.55	0.41
1:D:519:SER:O	1:D:521:ALA:N	2.54	0.41
1:D:610:PHE:CD1	1:D:610:PHE:N	2.89	0.41
1:F:611:ASP:OD2	1:F:611:ASP:C	2.59	0.41
1:F:646:THR:HG23	1:G:652:GLN:NE2	2.36	0.41
1:H:93:ILE:HD13	1:H:93:ILE:HA	1.80	0.41
1:B:142:SER:O	1:B:146:GLU:HG2	2.20	0.40
1:B:262:ARG:HG2	1:B:262:ARG:NH1	2.34	0.40
1:B:721:GLY:O	1:B:727:VAL:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:SER:HB3	1:D:62:GLU:OE2	2.21	0.40
1:C:370:ALA:HA	1:C:375:ARG:NH1	2.37	0.40
1:C:416:ILE:HD11	1:C:449:GLY:C	2.41	0.40
1:E:445:ALA:HB1	1:E:477:LEU:HD11	2.02	0.40
1:G:217:MET:HG3	1:G:309:GLN:HE22	1.84	0.40
1:H:333:LEU:HD12	1:H:333:LEU:HA	1.85	0.40
1:A:59:PHE:CD2	1:A:93:ILE:HD11	2.56	0.40
1:A:151:ASN:HD22	1:A:151:ASN:N	2.19	0.40
1:A:678:PRO:O	1:A:683:ARG:HD3	2.22	0.40
1:B:212:PHE:CE1	1:B:303:THR:CG2	2.99	0.40
1:C:128:ASP:HB3	1:C:177:ASP:O	2.20	0.40
1:D:673:GLN:CD	1:D:673:GLN:N	2.74	0.40
1:D:757:LEU:CD2	1:D:757:LEU:C	2.90	0.40
1:E:153:GLN:HE21	1:E:153:GLN:HB2	1.51	0.40
1:E:215:GLU:OE1	1:E:304:ILE:HG23	2.22	0.40
1:F:630:ILE:HG22	1:F:631:GLN:N	2.35	0.40
1:F:678:PRO:O	1:F:683:ARG:HD3	2.21	0.40
1:G:430:ARG:HD2	1:G:466:VAL:O	2.21	0.40
1:G:503:LEU:HD12	1:G:504:LEU:H	1.86	0.40
1:G:637:ARG:NH2	1:G:646:THR:HA	2.36	0.40
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.82	0.40
1:A:673:GLN:N	1:A:673:GLN:CD	2.75	0.40
1:B:155:ASP:OD2	1:B:156:LYS:N	2.55	0.40
1:D:64:TYR:OH	1:D:134:ALA:HB2	2.22	0.40
1:D:170:MET:CE	1:D:325:MET:HB3	2.51	0.40
1:D:550:ILE:CD1	1:D:686:GLY:HA2	2.51	0.40
1:F:481:ARG:HG2	1:F:510:GLU:HG3	2.03	0.40
1:G:140:GLU:O	1:G:144:LEU:HG	2.21	0.40
1:G:689:ILE:HG22	1:G:720:LEU:CD2	2.52	0.40
1:A:195:ILE:HD13	1:A:195:ILE:HA	1.93	0.40
1:A:307:HIS:ND1	1:A:307:HIS:N	2.69	0.40
1:B:93:ILE:HD13	1:B:93:ILE:HA	1.78	0.40
1:B:136:LEU:C	1:B:136:LEU:HD23	2.42	0.40
1:B:237:VAL:HG23	1:B:394:TYR:CE2	2.57	0.40
1:B:702:LYS:HB3	1:B:702:LYS:HE2	1.88	0.40
1:C:44:ARG:HA	1:C:82:VAL:CB	2.52	0.40
1:C:44:ARG:HH12	1:C:761:LEU:HD13	1.86	0.40
1:C:529:CYS:O	1:C:711:PHE:HB2	2.22	0.40
1:E:129:GLY:O	1:E:130:SER:C	2.59	0.40
1:E:349:GLY:O	1:E:350:ASN:HB3	2.21	0.40
1:F:166:ASN:OD1	1:F:336:ALA:CB	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:356:PRO:HG2	1:G:359:GLU:HB2	2.04	0.40
1:G:755:ARG:HG3	1:G:755:ARG:NH1	2.36	0.40
1:H:450:PHE:CD1	1:H:484:PRO:HD3	2.55	0.40
1:H:615:LEU:HD12	1:H:615:LEU:HA	1.94	0.40
1:H:757:LEU:HD23	1:H:757:LEU:C	2.41	0.40
1:A:551:GLY:H	1:A:682:ASP:CG	2.24	0.40
1:B:59:PHE:CD2	1:B:93:ILE:HD11	2.57	0.40
1:B:194:ILE:HG12	1:B:305:LEU:HD23	2.04	0.40
1:B:431:SER:O	1:B:435:VAL:HG23	2.21	0.40
1:C:139:LYS:HE3	1:C:139:LYS:HB3	1.86	0.40
1:C:239:LEU:HA	1:C:240:PRO:HD3	1.95	0.40
1:D:16:PHE:CD1	1:D:769:ASP:HA	2.49	0.40
1:D:490:GLU:OE1	1:D:490:GLU:N	2.47	0.40
1:D:503:LEU:HD23	1:D:532:MET:HE2	2.04	0.40
1:D:630:ILE:HG22	1:D:631:GLN:N	2.36	0.40
1:E:99:GLN:HA	1:E:99:GLN:HE21	1.85	0.40
1:E:139:LYS:HE3	1:E:139:LYS:HB3	1.88	0.40
1:E:262:ARG:HG2	1:E:262:ARG:NH1	2.33	0.40
1:F:215:GLU:OE1	1:F:304:ILE:HG23	2.22	0.40
1:F:550:ILE:CD1	1:F:686:GLY:HA2	2.51	0.40
1:F:608:GLU:CD	1:F:755:ARG:HE	2.24	0.40
1:G:99:GLN:HA	1:G:99:GLN:HE21	1.85	0.40
1:G:509:PHE:HE2	1:G:513:LEU:HD21	1.87	0.40
1:G:757:LEU:HD23	1:G:757:LEU:O	2.22	0.40
1:H:505:ILE:O	1:H:534:MET:HA	2.21	0.40
1:H:750:TRP:CD2	1:H:751:TRP:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	766/812 (94%)	706 (92%)	57 (7%)	3 (0%)	34	69
1	B	766/812 (94%)	699 (91%)	60 (8%)	7 (1%)	17	52
1	C	756/812 (93%)	686 (91%)	62 (8%)	8 (1%)	14	46
1	D	757/812 (93%)	694 (92%)	57 (8%)	6 (1%)	19	54
1	E	761/812 (94%)	697 (92%)	58 (8%)	6 (1%)	19	54
1	F	757/812 (93%)	691 (91%)	60 (8%)	6 (1%)	19	54
1	G	756/812 (93%)	693 (92%)	58 (8%)	5 (1%)	22	57
1	H	735/812 (90%)	672 (91%)	59 (8%)	4 (0%)	29	64
All	All	6054/6496 (93%)	5538 (92%)	471 (8%)	45 (1%)	22	57

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	486	LYS
1	H	713	THR
1	A	278	THR
1	A	724	LYS
1	B	278	THR
1	B	708	GLY
1	B	724	LYS
1	C	182	ASP
1	C	278	THR
1	C	485	GLY
1	C	724	LYS
1	D	278	THR
1	D	485	GLY
1	D	724	LYS
1	E	278	THR
1	E	485	GLY
1	E	724	LYS
1	F	278	THR
1	F	724	LYS
1	G	278	THR
1	G	499	SER
1	G	724	LYS
1	H	278	THR
1	H	724	LYS
1	B	713	THR
1	D	520	ALA
1	E	717	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	219	ARG
1	A	219	ARG
1	B	18	GLU
1	B	219	ARG
1	C	219	ARG
1	C	528	PHE
1	D	219	ARG
1	E	219	ARG
1	F	219	ARG
1	F	499	SER
1	F	715	ASP
1	G	219	ARG
1	B	15	LYS
1	C	527	GLU
1	E	180	GLY
1	G	516	LEU
1	F	527	GLU
1	C	180	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	619/658 (94%)	573 (93%)	46 (7%)	13	42
1	B	619/658 (94%)	567 (92%)	52 (8%)	11	38
1	C	614/658 (93%)	568 (92%)	46 (8%)	13	42
1	D	614/658 (93%)	564 (92%)	50 (8%)	11	39
1	E	617/658 (94%)	570 (92%)	47 (8%)	13	41
1	F	614/658 (93%)	563 (92%)	51 (8%)	11	38
1	G	614/658 (93%)	568 (92%)	46 (8%)	13	42
1	H	594/658 (90%)	549 (92%)	45 (8%)	13	41
All	All	4905/5264 (93%)	4522 (92%)	383 (8%)	12	40

All (383) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	43	VAL
1	A	69	ASP
1	A	80	GLU
1	A	91	THR
1	A	107	ARG
1	A	115	LEU
1	A	131	LEU
1	A	156	LYS
1	A	165	LEU
1	A	176	ASN
1	A	179	CYS
1	A	182	ASP
1	A	183	MET
1	A	191	LEU
1	A	224	LEU
1	A	230	LEU
1	A	250	GLU
1	A	260	ARG
1	A	295	GLN
1	A	301	ARG
1	A	303	THR
1	A	325	MET
1	A	362	GLN
1	A	368	GLN
1	A	396	ARG
1	A	453	PHE
1	A	461	ILE
1	A	470	THR
1	A	472	GLN
1	A	533	VAL
1	A	534	MET
1	A	538	THR
1	A	575	ARG
1	A	628	THR
1	A	631	GLN
1	A	632	ARG
1	A	683	ARG
1	A	689	ILE
1	A	705	ARG
1	A	712	THR
1	A	739	THR
1	A	757	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	772	ASP
1	A	776	LEU
1	A	780	GLN
1	B	14	ARG
1	B	20	LEU
1	B	43	VAL
1	B	80	GLU
1	B	91	THR
1	B	107	ARG
1	B	115	LEU
1	B	131	LEU
1	B	156	LYS
1	B	157	GLU
1	B	165	LEU
1	B	176	ASN
1	B	182	ASP
1	B	183	MET
1	B	191	LEU
1	B	224	LEU
1	B	230	LEU
1	B	250	GLU
1	B	260	ARG
1	B	295	GLN
1	B	301	ARG
1	B	303	THR
1	B	325	MET
1	B	362	GLN
1	B	374	ARG
1	B	386	SER
1	B	396	ARG
1	B	453	PHE
1	B	461	ILE
1	B	470	THR
1	B	481	ARG
1	B	483	LEU
1	B	494	GLN
1	B	499	SER
1	B	524	LYS
1	B	533	VAL
1	B	538	THR
1	B	575	ARG
1	B	628	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	631	GLN
1	B	632	ARG
1	B	683	ARG
1	B	689	ILE
1	B	707	ARG
1	B	714	ASP
1	B	718	CYS
1	B	722	ILE
1	B	728	ILE
1	B	739	THR
1	B	757	LEU
1	B	772	ASP
1	B	776	LEU
1	C	14	ARG
1	C	17	LEU
1	C	43	VAL
1	C	69	ASP
1	C	80	GLU
1	C	105	GLU
1	C	115	LEU
1	C	131	LEU
1	C	156	LYS
1	C	157	GLU
1	C	165	LEU
1	C	176	ASN
1	C	183	MET
1	C	191	LEU
1	C	224	LEU
1	C	230	LEU
1	C	250	GLU
1	C	260	ARG
1	C	295	GLN
1	C	301	ARG
1	C	303	THR
1	C	325	MET
1	C	362	GLN
1	C	368	GLN
1	C	396	ARG
1	C	453	PHE
1	C	461	ILE
1	C	470	THR
1	C	481	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	494	GLN
1	C	510	GLU
1	C	530	VAL
1	C	533	VAL
1	C	538	THR
1	C	575	ARG
1	C	628	THR
1	C	631	GLN
1	C	632	ARG
1	C	683	ARG
1	C	688	LYS
1	C	689	ILE
1	C	714	ASP
1	C	739	THR
1	C	757	LEU
1	C	772	ASP
1	C	776	LEU
1	D	14	ARG
1	D	43	VAL
1	D	69	ASP
1	D	80	GLU
1	D	91	THR
1	D	115	LEU
1	D	131	LEU
1	D	156	LYS
1	D	160	GLN
1	D	165	LEU
1	D	176	ASN
1	D	183	MET
1	D	191	LEU
1	D	224	LEU
1	D	230	LEU
1	D	235	ASP
1	D	254	VAL
1	D	255	LYS
1	D	260	ARG
1	D	295	GLN
1	D	301	ARG
1	D	303	THR
1	D	325	MET
1	D	362	GLN
1	D	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	374	ARG
1	D	396	ARG
1	D	453	PHE
1	D	461	ILE
1	D	470	THR
1	D	472	GLN
1	D	494	GLN
1	D	495	MET
1	D	522	ARG
1	D	533	VAL
1	D	538	THR
1	D	568	GLN
1	D	575	ARG
1	D	628	THR
1	D	631	GLN
1	D	632	ARG
1	D	683	ARG
1	D	688	LYS
1	D	689	ILE
1	D	692	ARG
1	D	714	ASP
1	D	739	THR
1	D	757	LEU
1	D	772	ASP
1	D	780	GLN
1	E	14	ARG
1	E	17	LEU
1	E	20	LEU
1	E	43	VAL
1	E	80	GLU
1	E	107	ARG
1	E	115	LEU
1	E	156	LYS
1	E	157	GLU
1	E	165	LEU
1	E	176	ASN
1	E	183	MET
1	E	191	LEU
1	E	224	LEU
1	E	230	LEU
1	E	260	ARG
1	E	295	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	301	ARG
1	E	303	THR
1	E	325	MET
1	E	362	GLN
1	E	368	GLN
1	E	396	ARG
1	E	453	PHE
1	E	461	ILE
1	E	470	THR
1	E	472	GLN
1	E	481	ARG
1	E	487	TYR
1	E	510	GLU
1	E	519	SER
1	E	533	VAL
1	E	534	MET
1	E	538	THR
1	E	575	ARG
1	E	628	THR
1	E	631	GLN
1	E	632	ARG
1	E	683	ARG
1	E	689	ILE
1	E	714	ASP
1	E	715	ASP
1	E	739	THR
1	E	757	LEU
1	E	768	TYR
1	E	772	ASP
1	E	780	GLN
1	F	43	VAL
1	F	69	ASP
1	F	80	GLU
1	F	115	LEU
1	F	156	LYS
1	F	165	LEU
1	F	166	ASN
1	F	176	ASN
1	F	191	LEU
1	F	224	LEU
1	F	230	LEU
1	F	250	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	260	ARG
1	F	295	GLN
1	F	301	ARG
1	F	303	THR
1	F	325	MET
1	F	358	MET
1	F	362	GLN
1	F	368	GLN
1	F	374	ARG
1	F	396	ARG
1	F	404	ASP
1	F	431	SER
1	F	453	PHE
1	F	461	ILE
1	F	470	THR
1	F	481	ARG
1	F	501	ASN
1	F	510	GLU
1	F	522	ARG
1	F	524	LYS
1	F	525	HIS
1	F	533	VAL
1	F	538	THR
1	F	568	GLN
1	F	575	ARG
1	F	628	THR
1	F	631	GLN
1	F	632	ARG
1	F	683	ARG
1	F	689	ILE
1	F	710	LYS
1	F	715	ASP
1	F	724	LYS
1	F	739	THR
1	F	748	GLU
1	F	757	LEU
1	F	760	ILE
1	F	772	ASP
1	F	776	LEU
1	G	14	ARG
1	G	15	LYS
1	G	43	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	69	ASP
1	G	80	GLU
1	G	115	LEU
1	G	131	LEU
1	G	160	GLN
1	G	165	LEU
1	G	166	ASN
1	G	176	ASN
1	G	191	LEU
1	G	224	LEU
1	G	230	LEU
1	G	250	GLU
1	G	260	ARG
1	G	295	GLN
1	G	301	ARG
1	G	325	MET
1	G	358	MET
1	G	359	GLU
1	G	369	LYS
1	G	385	ARG
1	G	396	ARG
1	G	453	PHE
1	G	461	ILE
1	G	470	THR
1	G	526	GLU
1	G	533	VAL
1	G	538	THR
1	G	574	LYS
1	G	575	ARG
1	G	628	THR
1	G	631	GLN
1	G	632	ARG
1	G	648	ASP
1	G	683	ARG
1	G	689	ILE
1	G	703	GLU
1	G	713	THR
1	G	714	ASP
1	G	739	THR
1	G	748	GLU
1	G	757	LEU
1	G	772	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	779	VAL
1	H	43	VAL
1	H	49	MET
1	H	69	ASP
1	H	80	GLU
1	H	87	GLN
1	H	115	LEU
1	H	131	LEU
1	H	156	LYS
1	H	160	GLN
1	H	165	LEU
1	H	176	ASN
1	H	191	LEU
1	H	224	LEU
1	H	230	LEU
1	H	245	GLU
1	H	250	GLU
1	H	260	ARG
1	H	295	GLN
1	H	301	ARG
1	H	325	MET
1	H	362	GLN
1	H	368	GLN
1	H	385	ARG
1	H	396	ARG
1	H	453	PHE
1	H	461	ILE
1	H	470	THR
1	H	472	GLN
1	H	482	VAL
1	H	487	TYR
1	H	533	VAL
1	H	534	MET
1	H	538	THR
1	H	575	ARG
1	H	621	HIS
1	H	625	LYS
1	H	628	THR
1	H	632	ARG
1	H	643	GLU
1	H	683	ARG
1	H	689	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	715	ASP
1	H	739	THR
1	H	757	LEU
1	H	761	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	116	GLN
1	A	151	ASN
1	A	153	GLN
1	A	176	ASN
1	A	307	HIS
1	A	309	GLN
1	A	377	GLN
1	A	417	ASN
1	A	616	GLN
1	A	618	ASN
1	A	652	GLN
1	A	674	GLN
1	A	684	ASN
1	B	99	GLN
1	B	116	GLN
1	B	153	GLN
1	B	176	ASN
1	B	309	GLN
1	B	417	ASN
1	B	568	GLN
1	B	616	GLN
1	B	618	ASN
1	B	671	HIS
1	B	674	GLN
1	B	684	ASN
1	C	19	HIS
1	C	99	GLN
1	C	116	GLN
1	C	151	ASN
1	C	176	ASN
1	C	417	ASN
1	C	457	GLN
1	C	568	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	652	GLN
1	C	674	GLN
1	C	684	ASN
1	D	19	HIS
1	D	99	GLN
1	D	116	GLN
1	D	151	ASN
1	D	153	GLN
1	D	176	ASN
1	D	307	HIS
1	D	309	GLN
1	D	417	ASN
1	D	525	HIS
1	D	568	GLN
1	D	618	ASN
1	D	673	GLN
1	D	684	ASN
1	D	780	GLN
1	E	99	GLN
1	E	116	GLN
1	E	151	ASN
1	E	153	GLN
1	E	176	ASN
1	E	307	HIS
1	E	309	GLN
1	E	417	ASN
1	E	494	GLN
1	E	498	HIS
1	E	568	GLN
1	E	616	GLN
1	E	673	GLN
1	E	674	GLN
1	E	684	ASN
1	F	99	GLN
1	F	151	ASN
1	F	153	GLN
1	F	307	HIS
1	F	309	GLN
1	F	417	ASN
1	F	494	GLN
1	F	498	HIS
1	F	674	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	684	ASN
1	F	749	GLN
1	G	19	HIS
1	G	65	GLN
1	G	99	GLN
1	G	116	GLN
1	G	151	ASN
1	G	153	GLN
1	G	160	GLN
1	G	176	ASN
1	G	192	HIS
1	G	309	GLN
1	G	417	ASN
1	G	568	GLN
1	G	616	GLN
1	G	618	ASN
1	G	684	ASN
1	H	87	GLN
1	H	99	GLN
1	H	116	GLN
1	H	151	ASN
1	H	153	GLN
1	H	176	ASN
1	H	309	GLN
1	H	417	ASN
1	H	498	HIS
1	H	568	GLN
1	H	618	ASN
1	H	673	GLN
1	H	674	GLN
1	H	684	ASN

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 37 ligands modelled in this entry, 17 are monoatomic - leaving 20 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	PO4	E	804	-	4,4,4	1.64	0	6,6,6	0.43	0
4	PO4	B	805	-	4,4,4	1.62	0	6,6,6	0.43	0
4	PO4	H	804	-	4,4,4	1.64	1 (25%)	6,6,6	0.41	0
4	PO4	G	805	-	4,4,4	1.61	0	6,6,6	0.44	0
2	ATP	E	801	3	26,33,33	1.38	3 (11%)	31,52,52	1.46	3 (9%)
4	PO4	D	803	-	4,4,4	1.68	0	6,6,6	0.40	0
2	ATP	C	801	3	26,33,33	1.12	2 (7%)	31,52,52	1.42	3 (9%)
2	ATP	A	801	3	26,33,33	1.42	3 (11%)	31,52,52	1.61	5 (16%)
2	ATP	H	801	3	26,33,33	1.39	2 (7%)	31,52,52	1.58	6 (19%)
4	PO4	B	804	-	4,4,4	1.60	1 (25%)	6,6,6	0.43	0
4	PO4	G	804	-	4,4,4	1.55	0	6,6,6	0.43	0
2	ATP	G	801	3	26,33,33	1.39	3 (11%)	31,52,52	1.50	3 (9%)
4	PO4	F	804	-	4,4,4	1.57	0	6,6,6	0.43	0
2	ATP	D	801	3	26,33,33	1.47	4 (15%)	31,52,52	1.49	4 (12%)
2	ATP	F	801	3	26,33,33	1.23	2 (7%)	31,52,52	1.45	4 (12%)
4	PO4	C	804	-	4,4,4	1.62	0	6,6,6	0.46	0
4	PO4	A	804	-	4,4,4	1.60	0	6,6,6	0.46	0
4	PO4	F	805	-	4,4,4	1.62	0	6,6,6	0.43	0
4	PO4	A	805	-	4,4,4	1.63	0	6,6,6	0.44	0
2	ATP	B	801	3	26,33,33	1.40	4 (15%)	31,52,52	1.48	4 (12%)

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
2	ATP	G	801	3	-	3/18/38/38	0/3/3/3
2	ATP	H	801	3	-	1/18/38/38	0/3/3/3
2	ATP	D	801	3	-	2/18/38/38	0/3/3/3
2	ATP	F	801	3	-	1/18/38/38	0/3/3/3
2	ATP	E	801	3	-	2/18/38/38	0/3/3/3
2	ATP	C	801	3	-	2/18/38/38	0/3/3/3
2	ATP	A	801	3	-	0/18/38/38	0/3/3/3
2	ATP	B	801	3	-	0/18/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	801	ATP	O4'-C1'	4.50	1.47	1.41
2	A	801	ATP	O4'-C1'	4.22	1.47	1.41
2	D	801	ATP	O4'-C1'	3.87	1.46	1.41
2	B	801	ATP	O4'-C1'	3.75	1.46	1.41
2	E	801	ATP	O4'-C1'	3.53	1.46	1.41
2	A	801	ATP	PG-O1G	3.39	1.61	1.50
2	F	801	ATP	PG-O1G	3.36	1.61	1.50
2	H	801	ATP	PG-O1G	3.29	1.61	1.50
2	G	801	ATP	O4'-C1'	3.21	1.45	1.41
2	D	801	ATP	PA-O1A	3.08	1.61	1.50
2	B	801	ATP	PB-O1B	3.06	1.61	1.50
2	G	801	ATP	PB-O1B	3.00	1.61	1.50
2	B	801	ATP	PA-O1A	2.98	1.61	1.50
2	G	801	ATP	PA-O1A	2.98	1.61	1.50
2	C	801	ATP	O4'-C1'	2.96	1.45	1.41
2	E	801	ATP	PB-O1B	2.91	1.61	1.50
2	E	801	ATP	PA-O1A	2.82	1.60	1.50
2	D	801	ATP	PB-O1B	2.75	1.60	1.50
2	F	801	ATP	O4'-C1'	2.59	1.44	1.41
2	A	801	ATP	PG-O3G	2.36	1.63	1.54
4	B	804	PO4	P-O3	-2.10	1.48	1.54
2	C	801	ATP	PG-O3G	2.09	1.62	1.54
2	D	801	ATP	PG-O2G	2.07	1.62	1.54
2	B	801	ATP	PG-O3G	2.05	1.62	1.54
4	H	804	PO4	P-O4	-2.00	1.48	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	801	ATP	N3-C2-N1	-5.31	120.38	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	801	ATP	N3-C2-N1	-5.16	120.61	128.68
2	H	801	ATP	N3-C2-N1	-5.09	120.72	128.68
2	C	801	ATP	N3-C2-N1	-5.01	120.85	128.68
2	A	801	ATP	N3-C2-N1	-5.00	120.87	128.68
2	D	801	ATP	N3-C2-N1	-4.97	120.91	128.68
2	E	801	ATP	N3-C2-N1	-4.96	120.93	128.68
2	B	801	ATP	N3-C2-N1	-4.94	120.96	128.68
2	E	801	ATP	PB-O3B-PG	-4.27	118.16	132.83
2	D	801	ATP	PB-O3B-PG	-3.91	119.41	132.83
2	C	801	ATP	PB-O3B-PG	-3.83	119.70	132.83
2	A	801	ATP	PB-O3B-PG	-3.71	120.11	132.83
2	G	801	ATP	PA-O3A-PB	-3.70	120.14	132.83
2	B	801	ATP	PB-O3B-PG	-3.68	120.21	132.83
2	H	801	ATP	PB-O3B-PG	-3.60	120.46	132.83
2	G	801	ATP	PB-O3B-PG	-3.39	121.19	132.83
2	C	801	ATP	PA-O3A-PB	-3.11	122.15	132.83
2	A	801	ATP	PA-O3A-PB	-2.97	122.63	132.83
2	D	801	ATP	PA-O3A-PB	-2.79	123.27	132.83
2	H	801	ATP	PA-O3A-PB	-2.74	123.42	132.83
2	A	801	ATP	O2G-PG-O3B	2.64	113.50	104.64
2	B	801	ATP	O4'-C1'-C2'	-2.62	103.10	106.93
2	F	801	ATP	PB-O3B-PG	-2.55	124.09	132.83
2	E	801	ATP	PA-O3A-PB	-2.54	124.10	132.83
2	F	801	ATP	PA-O3A-PB	-2.50	124.26	132.83
2	H	801	ATP	O4'-C1'-C2'	-2.48	103.31	106.93
2	B	801	ATP	PA-O3A-PB	-2.42	124.50	132.83
2	D	801	ATP	O4'-C1'-C2'	-2.40	103.42	106.93
2	F	801	ATP	O2G-PG-O3B	2.32	112.41	104.64
2	H	801	ATP	O3G-PG-O3B	2.23	112.11	104.64
2	A	801	ATP	C2'-C3'-C4'	-2.09	98.57	102.64
2	H	801	ATP	C2'-C3'-C4'	-2.04	98.67	102.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	801	ATP	O4'-C4'-C5'-O5'
2	G	801	ATP	C3'-C4'-C5'-O5'
2	C	801	ATP	O4'-C4'-C5'-O5'
2	C	801	ATP	C3'-C4'-C5'-O5'
2	G	801	ATP	C4'-C5'-O5'-PA
2	D	801	ATP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	801	ATP	O4'-C4'-C5'-O5'
2	H	801	ATP	O4'-C4'-C5'-O5'
2	F	801	ATP	C5'-O5'-PA-O1A
2	D	801	ATP	C3'-C4'-C5'-O5'
2	E	801	ATP	C3'-C4'-C5'-O5'

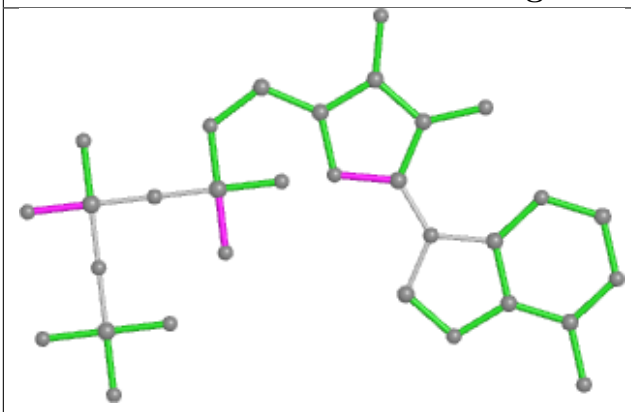
There are no ring outliers.

1 monomer is involved in 1 short contact:

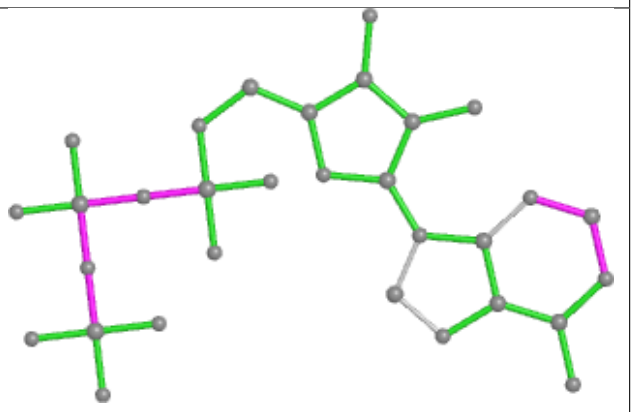
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	ATP	1	0

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.

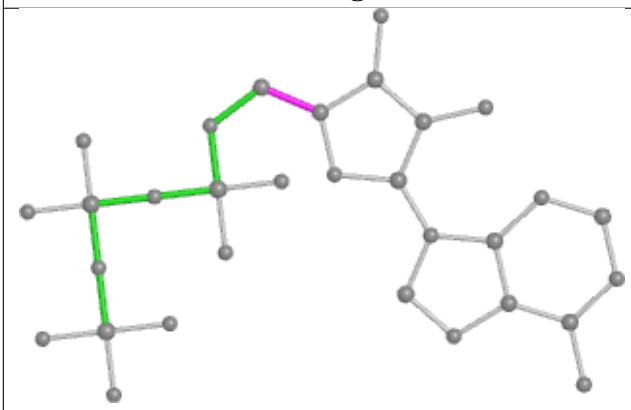
Ligand ATP E 801



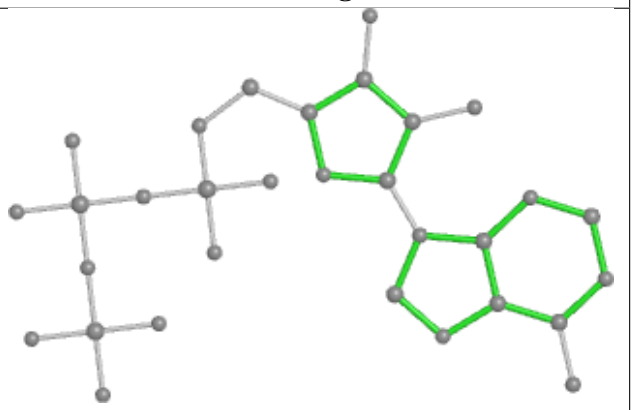
Bond lengths



Bond angles

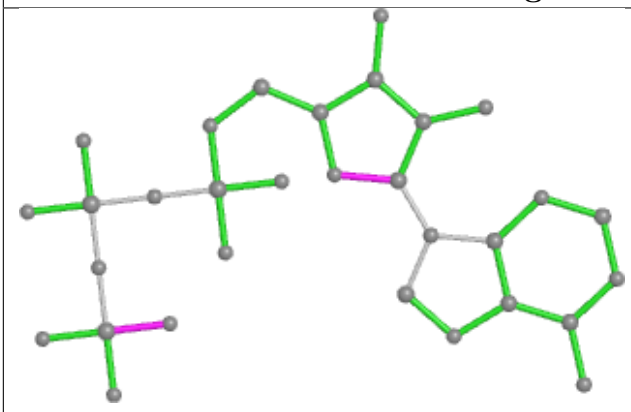


Torsions

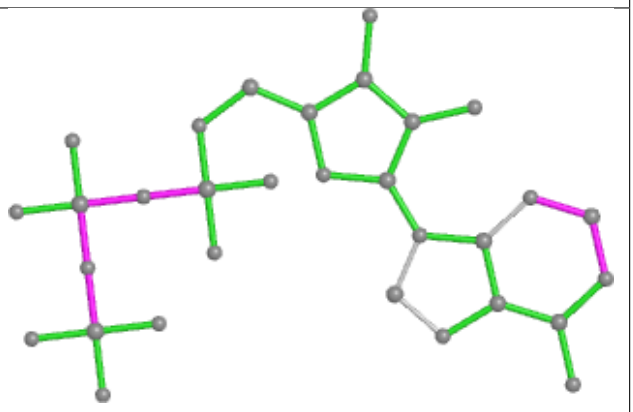


Rings

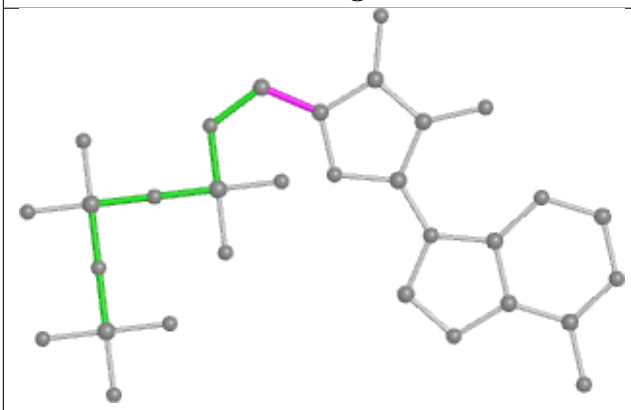
Ligand ATP C 801



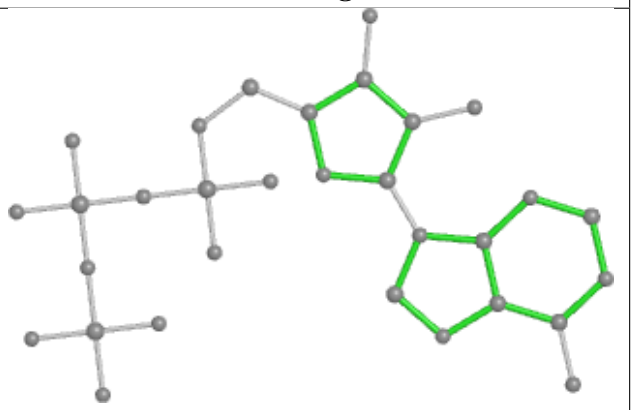
Bond lengths



Bond angles

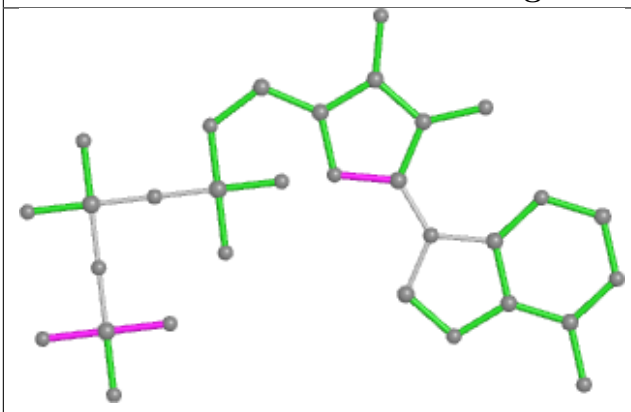


Torsions

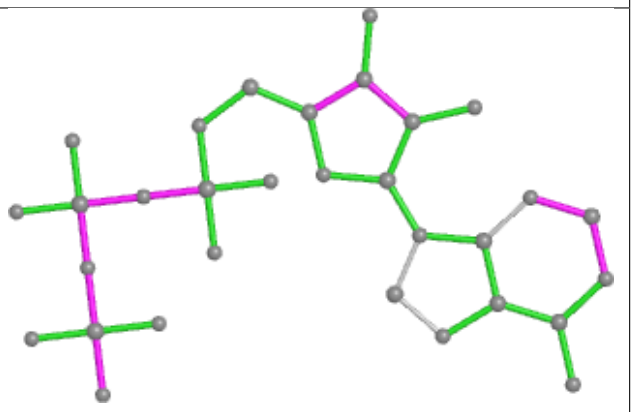


Rings

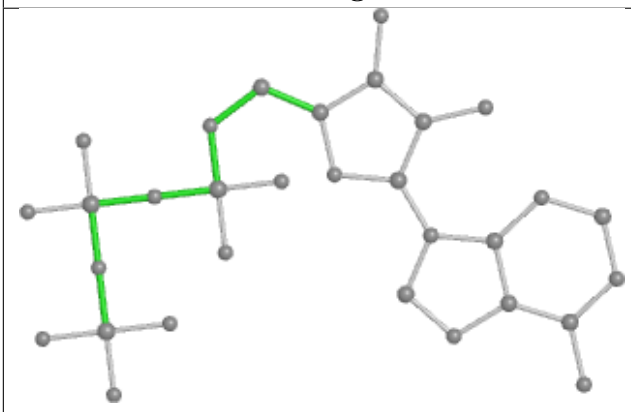
Ligand ATP A 801



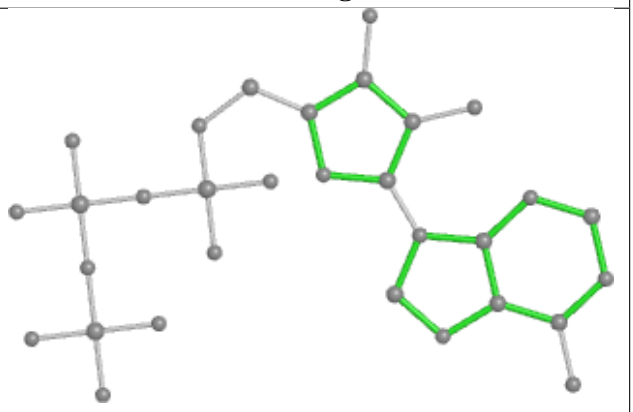
Bond lengths



Bond angles

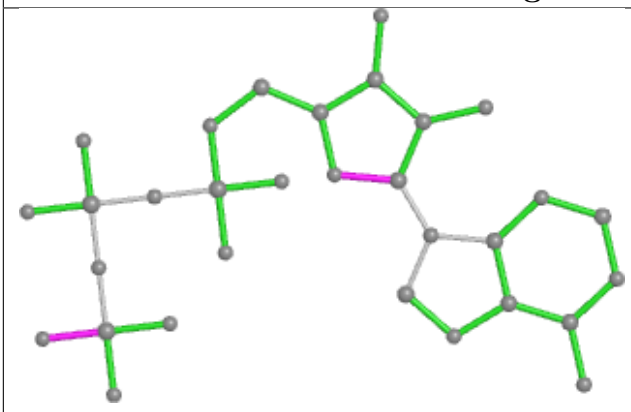


Torsions

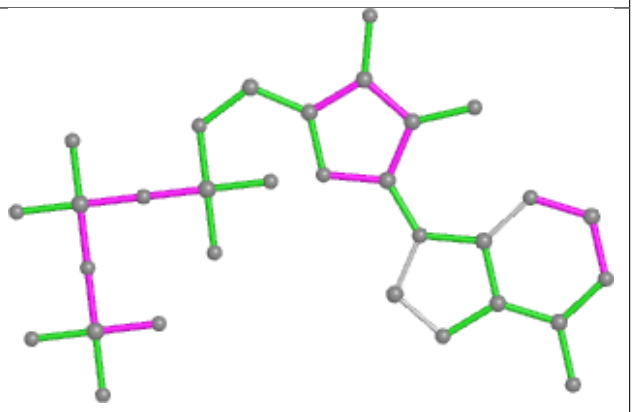


Rings

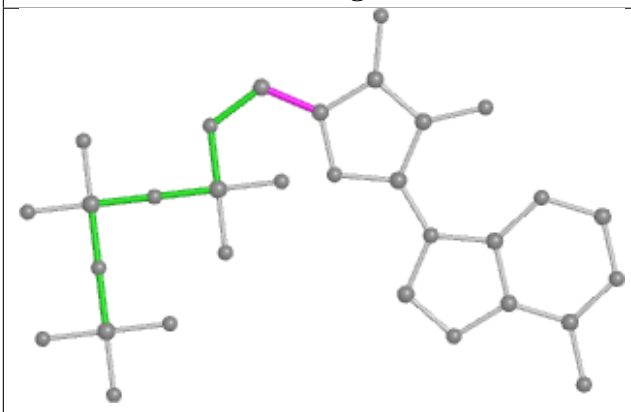
Ligand ATP H 801



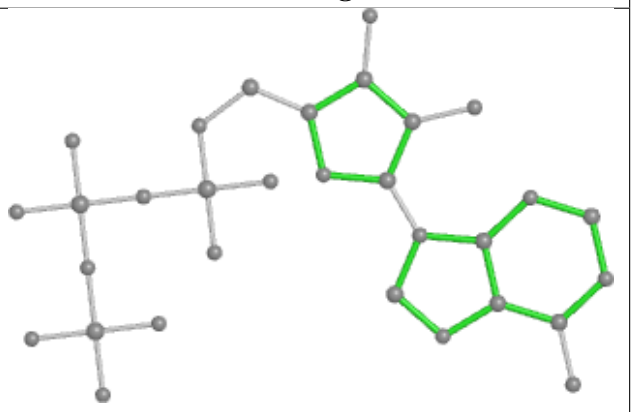
Bond lengths



Bond angles

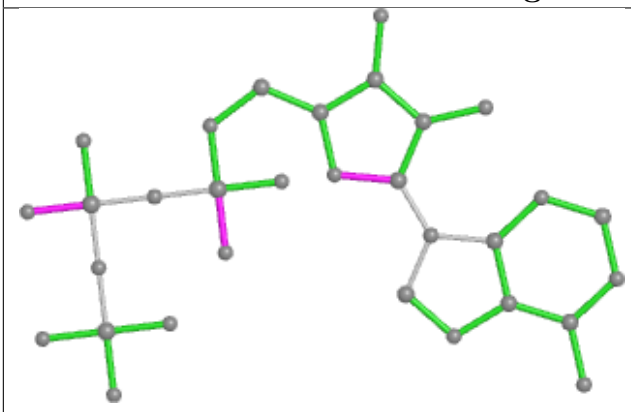


Torsions

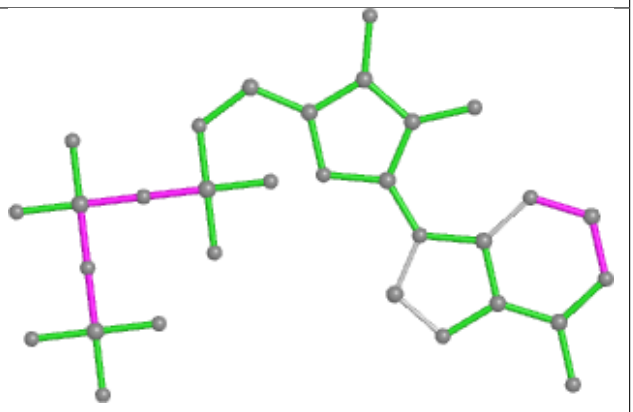


Rings

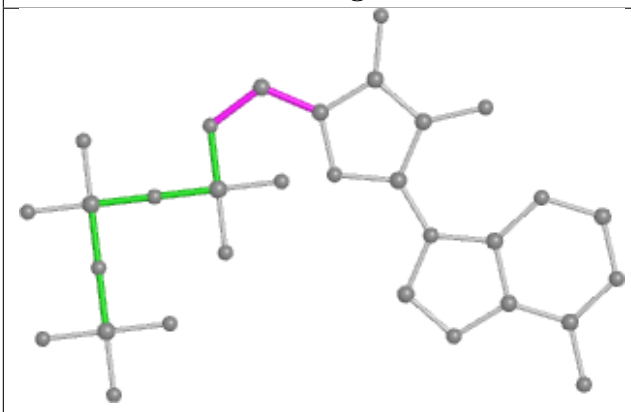
Ligand ATP G 801



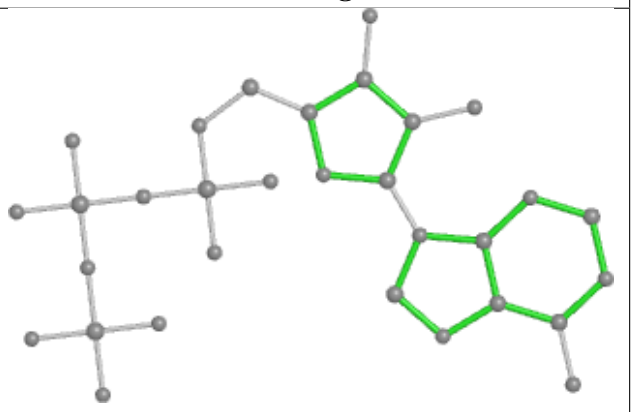
Bond lengths



Bond angles

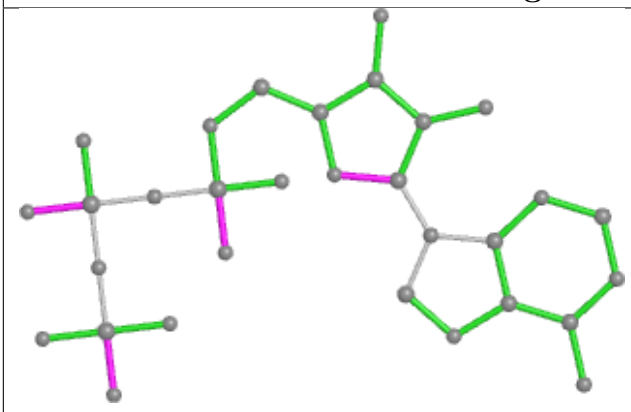


Torsions

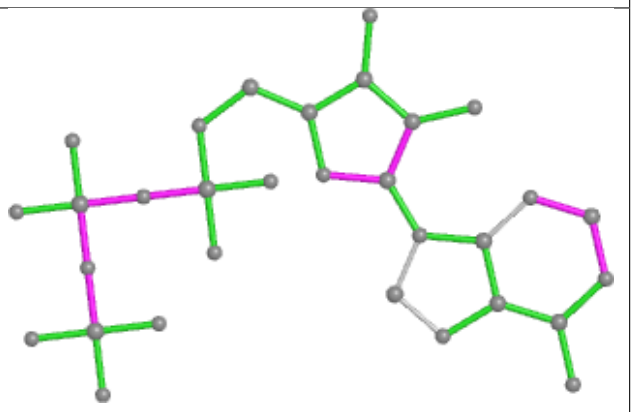


Rings

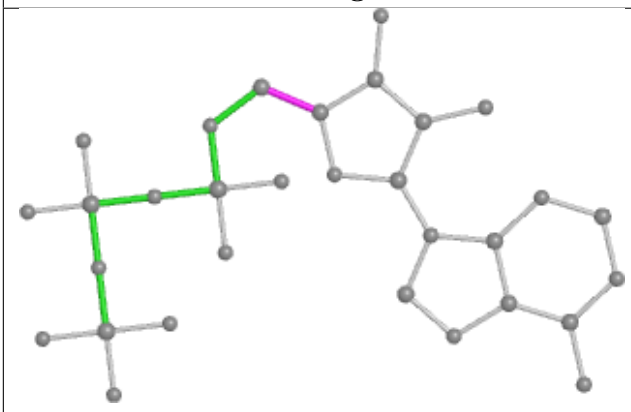
Ligand ATP D 801



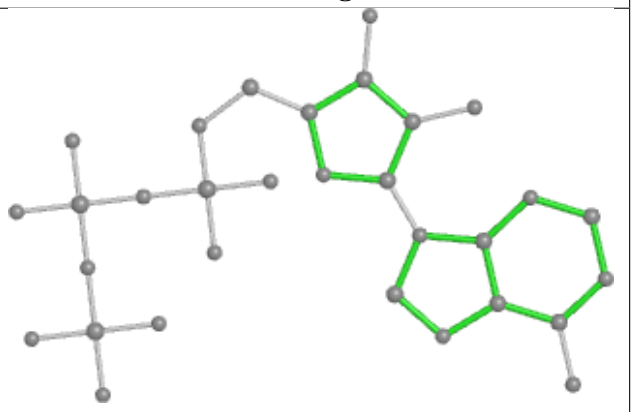
Bond lengths



Bond angles

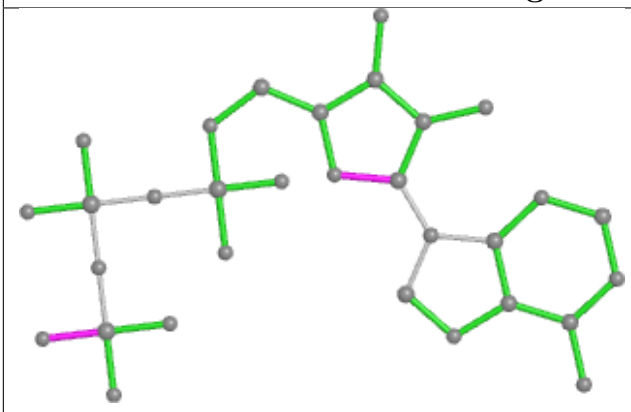


Torsions

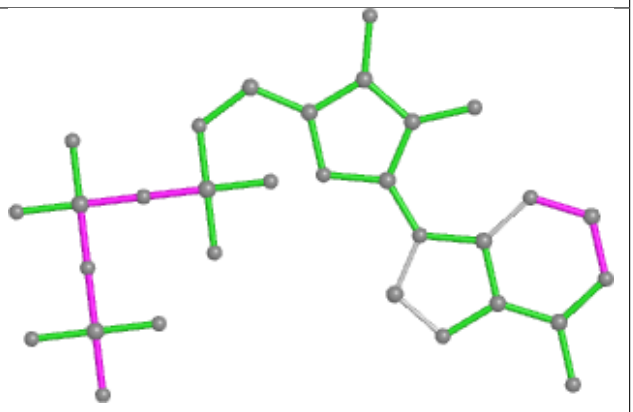


Rings

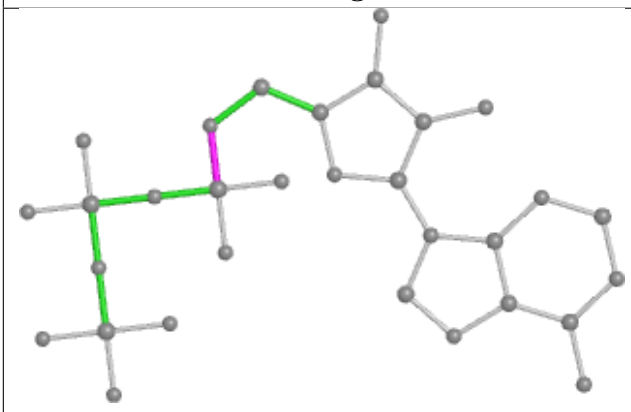
Ligand ATP F 801



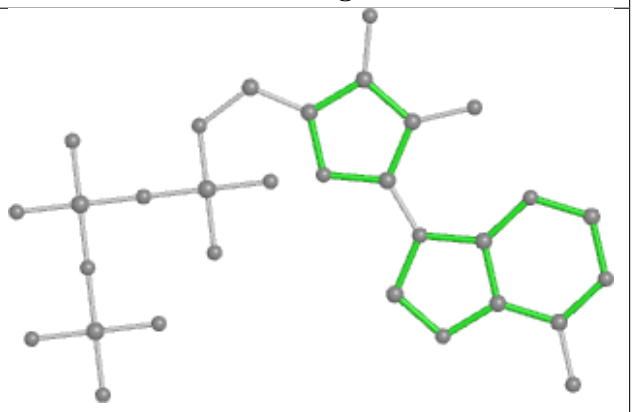
Bond lengths



Bond angles

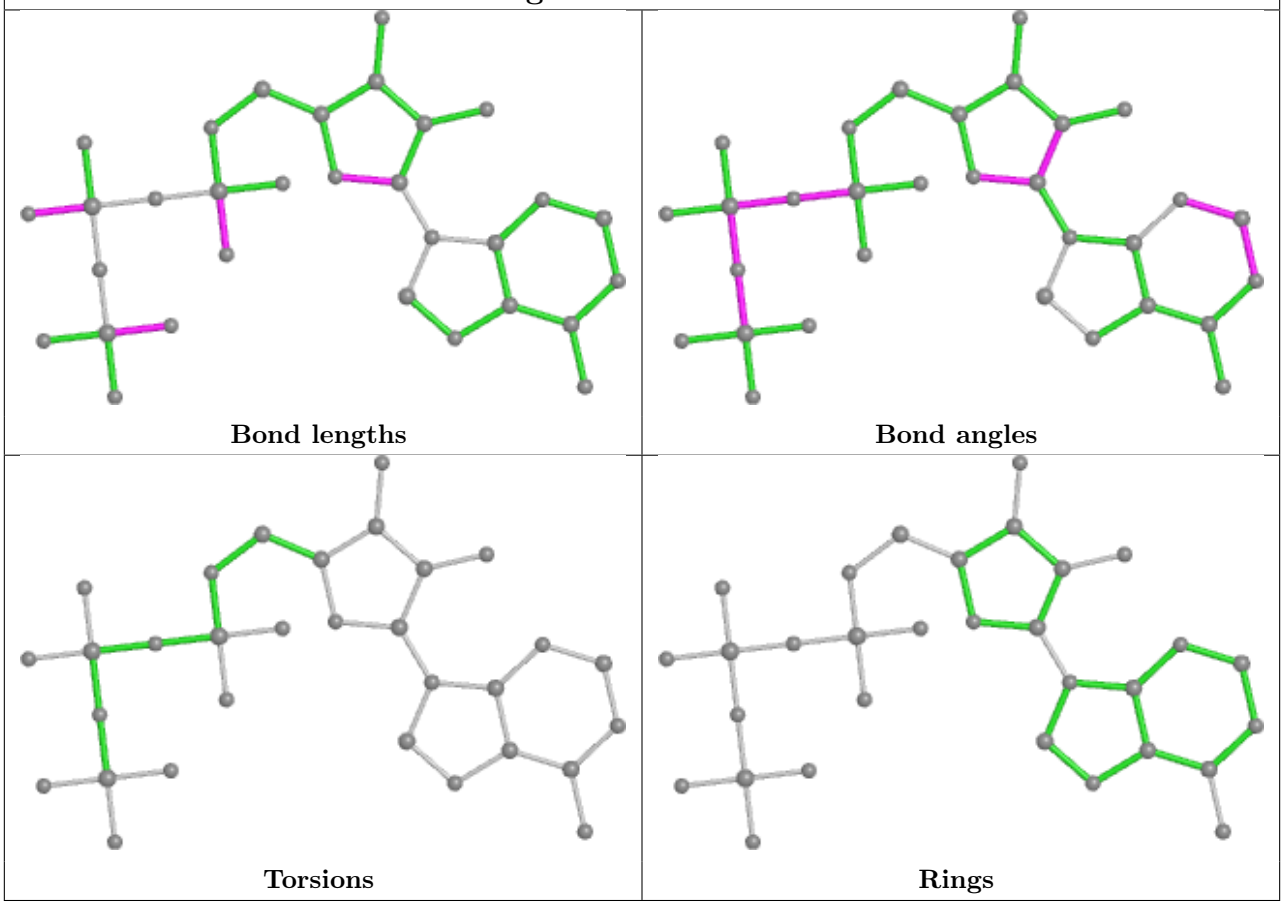


Torsions



Rings

Ligand ATP B 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	768/812 (94%)	-0.24	0 100 100	25, 56, 83, 113	0
1	B	768/812 (94%)	-0.22	2 (0%) 94 88	26, 55, 83, 114	0
1	C	760/812 (93%)	-0.15	2 (0%) 94 88	36, 62, 93, 114	0
1	D	761/812 (93%)	-0.27	0 100 100	36, 59, 86, 113	0
1	E	765/812 (94%)	-0.20	0 100 100	37, 59, 86, 114	0
1	F	761/812 (93%)	-0.25	0 100 100	36, 60, 86, 114	0
1	G	760/812 (93%)	-0.16	5 (0%) 87 75	36, 62, 89, 113	0
1	H	739/812 (91%)	-0.13	4 (0%) 91 81	38, 61, 87, 114	0
All	All	6082/6496 (93%)	-0.20	13 (0%) 95 90	25, 60, 87, 114	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	155	ASP	3.1
1	H	629	THR	3.0
1	H	67	MET	2.6
1	H	148	LEU	2.6
1	B	157	GLU	2.3
1	G	703	GLU	2.3
1	B	156	LYS	2.2
1	C	502	ALA	2.2
1	H	149	ALA	2.2
1	G	253	CYS	2.1
1	G	701	LEU	2.0
1	C	164	TYR	2.0
1	G	156	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	H	803	1/1	0.75	0.18	67,67,67,67	0
3	MG	A	802	1/1	0.79	0.16	43,43,43,43	0
3	MG	H	802	1/1	0.80	0.15	47,47,47,47	0
3	MG	F	802	1/1	0.80	0.20	54,54,54,54	0
4	PO4	B	805	5/5	0.82	0.28	120,120,121,121	0
3	MG	G	803	1/1	0.85	0.14	40,40,40,40	0
3	MG	G	802	1/1	0.85	0.12	36,36,36,36	0
4	PO4	C	804	5/5	0.86	0.21	113,113,114,114	0
3	MG	D	802	1/1	0.89	0.20	37,37,37,37	0
4	PO4	F	804	5/5	0.89	0.26	104,105,105,105	0
4	PO4	A	805	5/5	0.91	0.18	103,103,103,104	0
4	PO4	G	804	5/5	0.91	0.20	90,91,91,92	0
3	MG	C	803	1/1	0.92	0.09	34,34,34,34	0
2	ATP	E	801	31/31	0.92	0.20	79,88,95,95	0
3	MG	C	802	1/1	0.92	0.12	60,60,60,60	0
2	ATP	H	801	31/31	0.93	0.17	74,83,85,86	0
3	MG	E	803	1/1	0.93	0.12	40,40,40,40	0
4	PO4	F	805	5/5	0.93	0.13	90,91,91,91	0
2	ATP	C	801	31/31	0.93	0.17	78,86,92,93	0
4	PO4	G	805	5/5	0.93	0.15	113,113,114,114	0
4	PO4	H	804	5/5	0.93	0.17	75,75,76,76	0
3	MG	F	803	1/1	0.94	0.09	32,32,32,32	0
4	PO4	A	804	5/5	0.94	0.19	65,66,67,67	0
4	PO4	D	803	5/5	0.94	0.18	83,83,84,84	0
2	ATP	F	801	31/31	0.94	0.20	45,54,62,62	0
3	MG	E	802	1/1	0.95	0.18	39,39,39,39	0
2	ATP	G	801	31/31	0.95	0.16	72,75,78,78	0

Continued on next page...

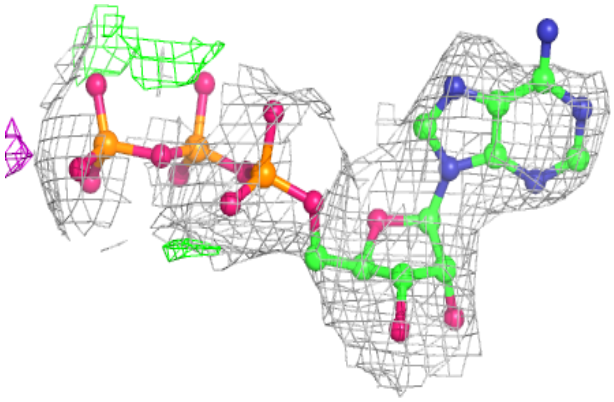
Continued from previous page...

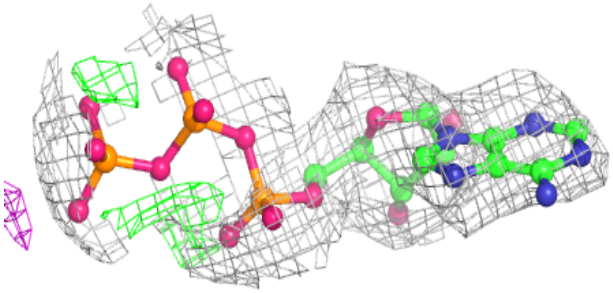
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ATP	D	801	31/31	0.95	0.17	55,69,82,83	0
2	ATP	A	801	31/31	0.96	0.14	46,50,53,54	0
4	PO4	B	804	5/5	0.97	0.17	66,67,67,69	0
3	MG	B	802	1/1	0.97	0.26	13,13,13,13	0
2	ATP	B	801	31/31	0.97	0.15	36,45,53,53	0
4	PO4	E	804	5/5	0.98	0.27	77,78,78,78	0
3	MG	B	803	1/1	0.98	0.07	13,13,13,13	0
3	MG	A	803	1/1	0.98	0.13	18,18,18,18	0
5	CO	B	806	1/1	0.98	0.12	48,48,48,48	0
5	CO	F	806	1/1	0.98	0.03	71,71,71,71	1

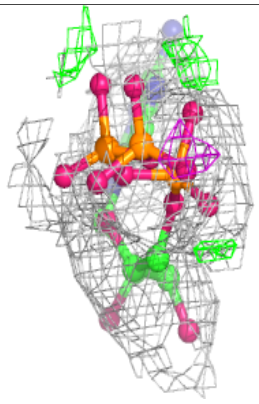
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP E 801:

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

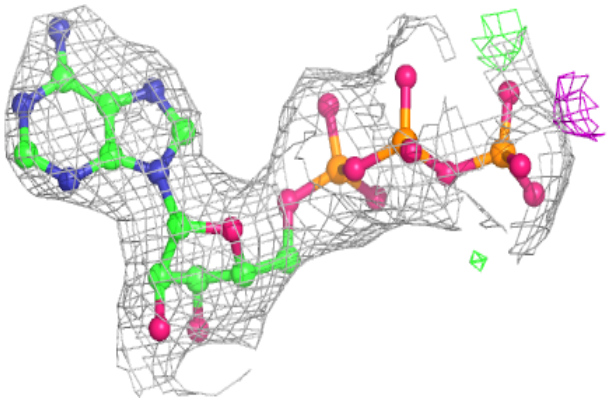


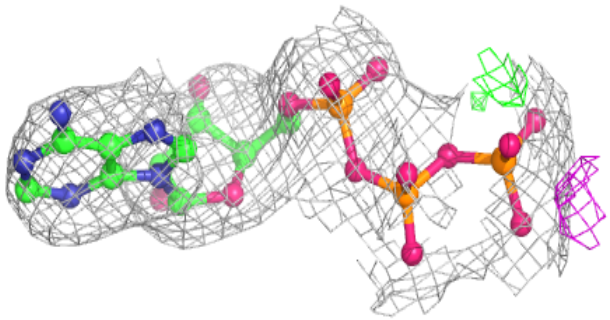


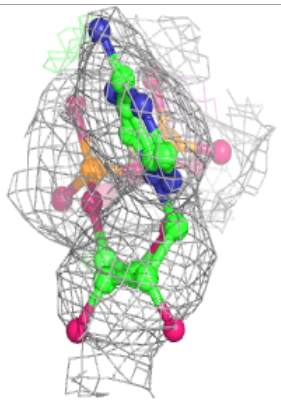


Electron density around ATP H 801:

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

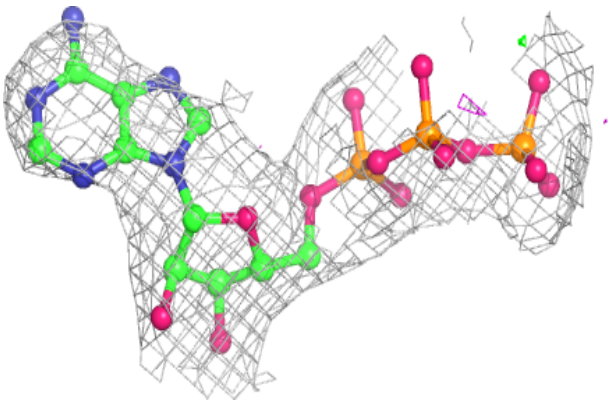


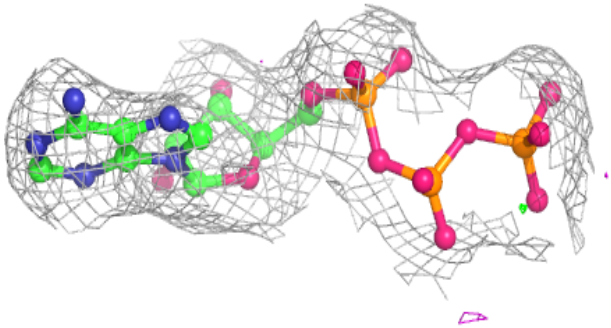


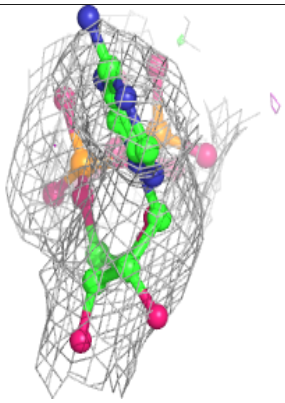


Electron density around ATP C 801:

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

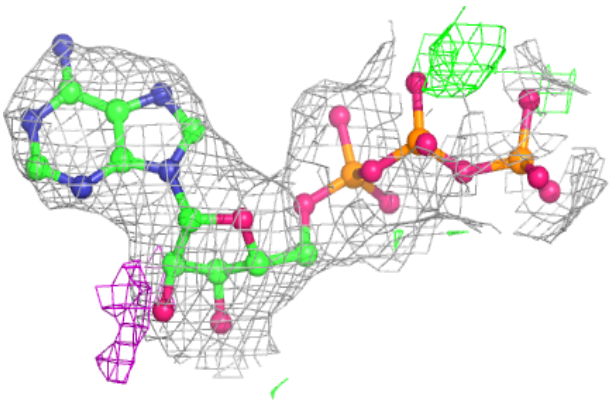


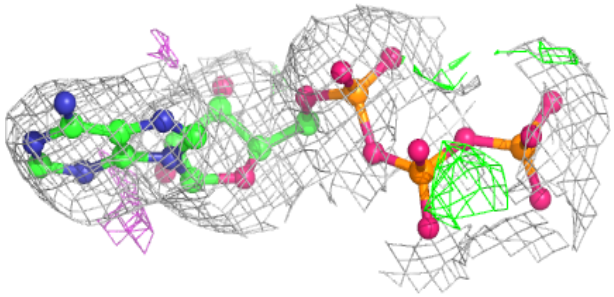


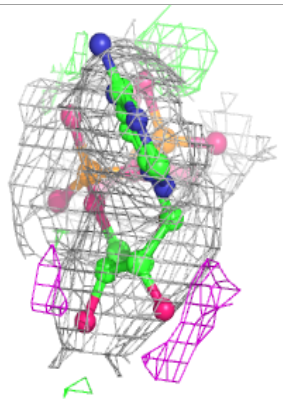


Electron density around ATP F 801:

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

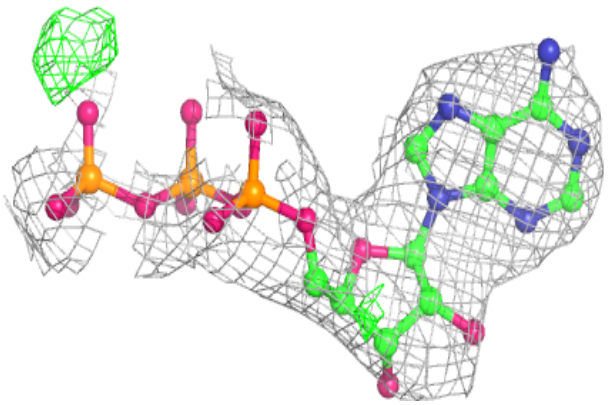


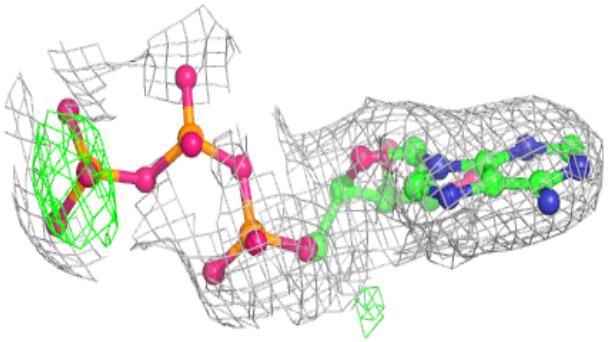


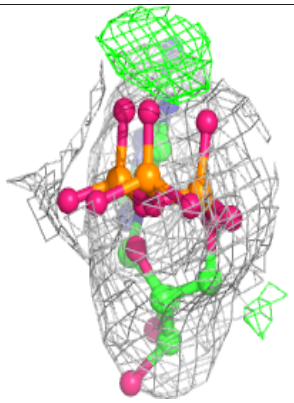


Electron density around ATP G 801:

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

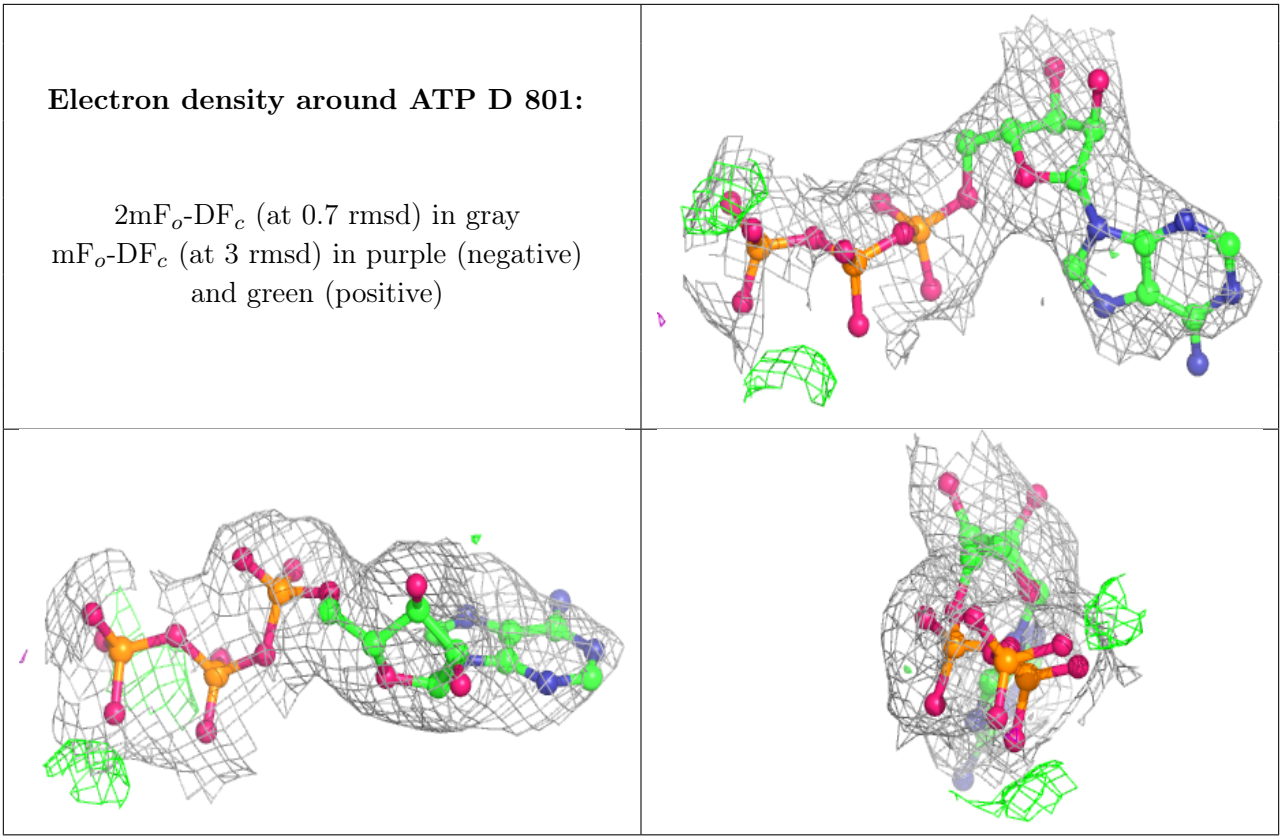






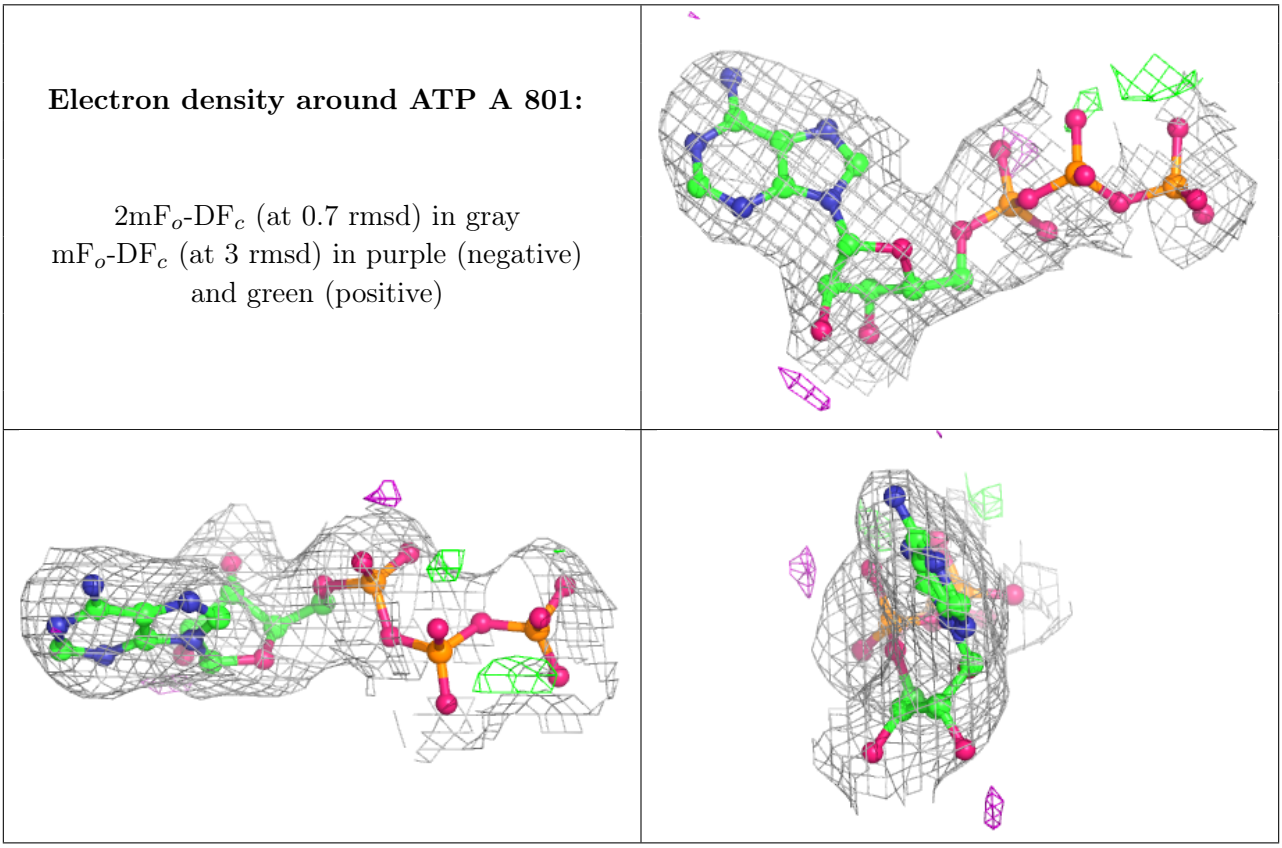
Electron density around ATP D 801:

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



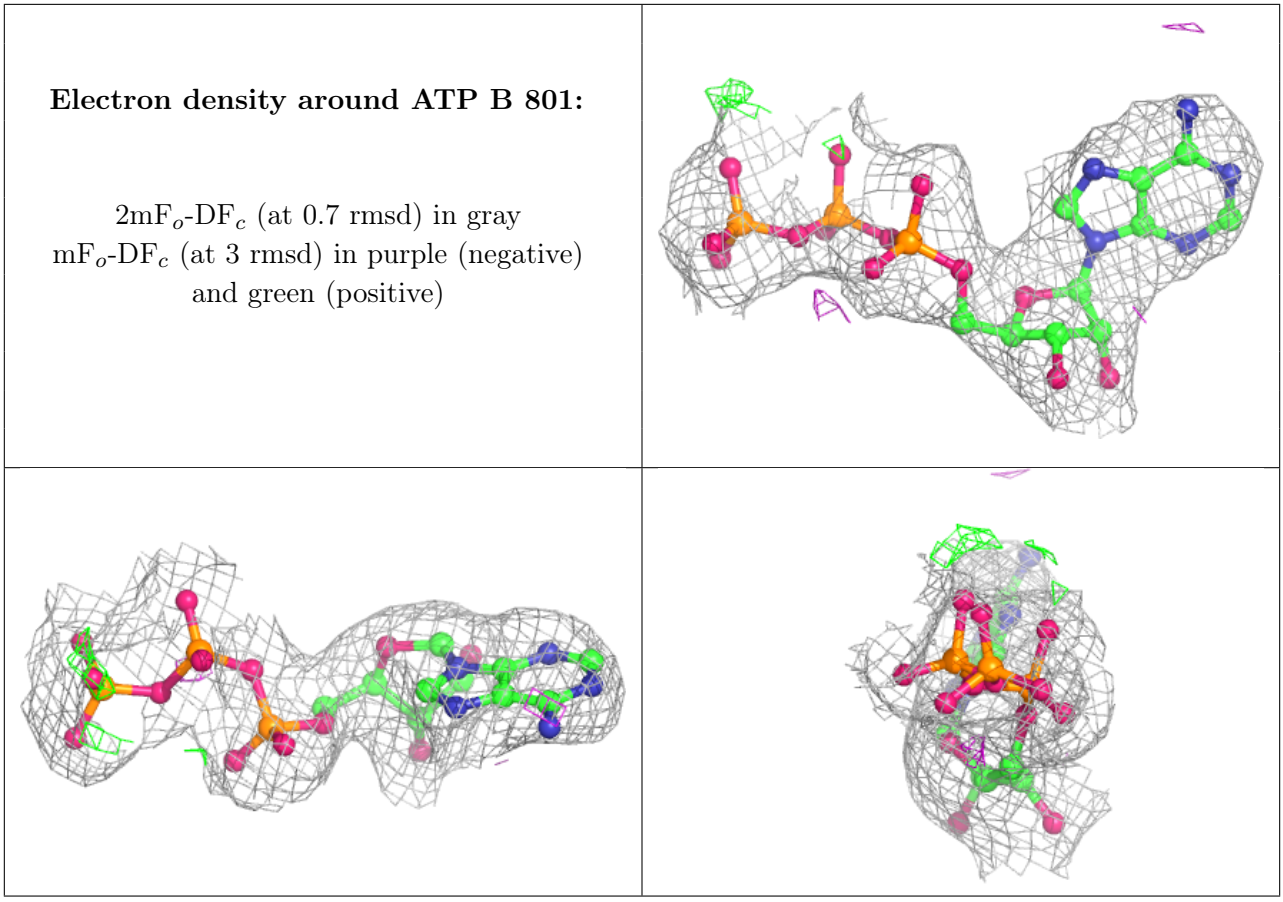
Electron density around ATP A 801:

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



Electron density around ATP B 801:

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



6.5 Other polymers

There are no such residues in this entry.