



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:09 AM UTC

PDB ID : 4XYJ / pdb_00004xyj
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:

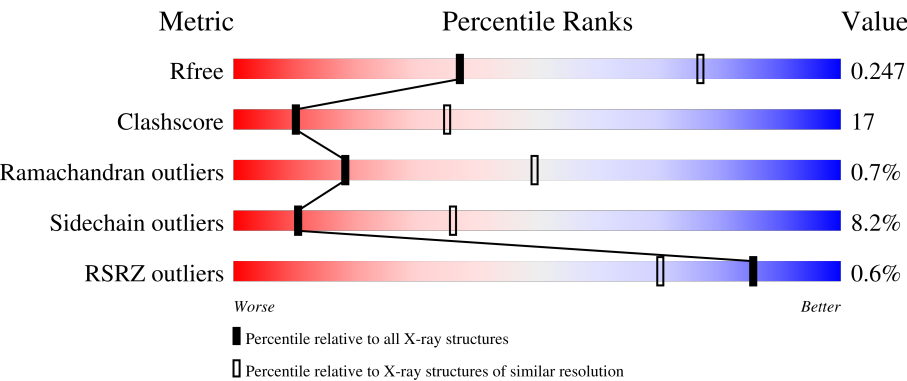
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	812	61%29%5%
1	B	812	% 61%29%5%
1	C	812	% 60%30%6%
1	D	812	59%30%5%6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	812	58%31%5%6%
1	F	812	60%29%5%6%
1	G	812	% 59%31%•6%
1	H	812	57%30%•9%

2 Entry composition

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...

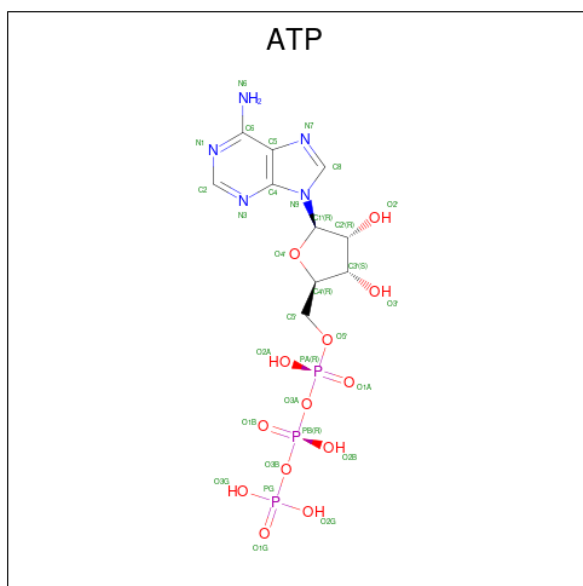
Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	ILE	-	expression tag	UNP Q01813
G	-13	PRO	-	expression tag	UNP Q01813
G	-12	THR	-	expression tag	UNP Q01813
G	-11	THR	-	expression tag	UNP Q01813
G	-10	GLU	-	expression tag	UNP Q01813
G	-9	ASN	-	expression tag	UNP Q01813
G	-8	LEU	-	expression tag	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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

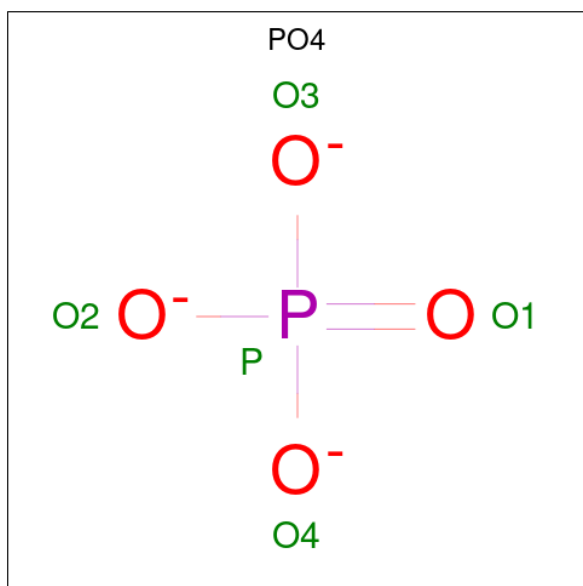
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is COBALT (II) ION (CCD ID: CO) (formula: Co).

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

- Molecule 6 is water.

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

Continued on next page...

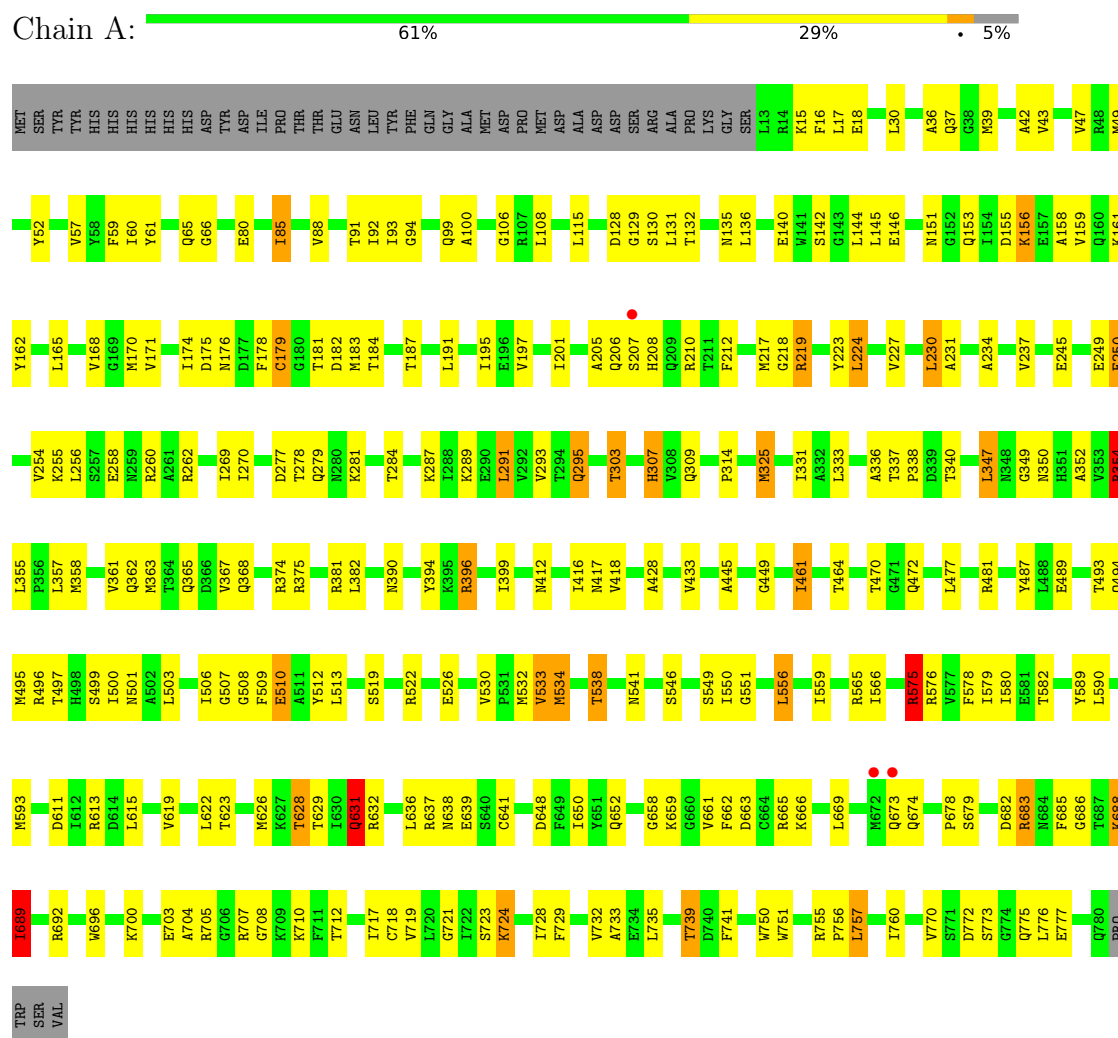
Continued from previous page...

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

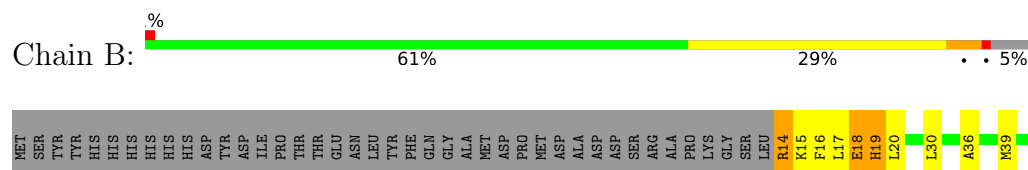
3 Residue-property plots

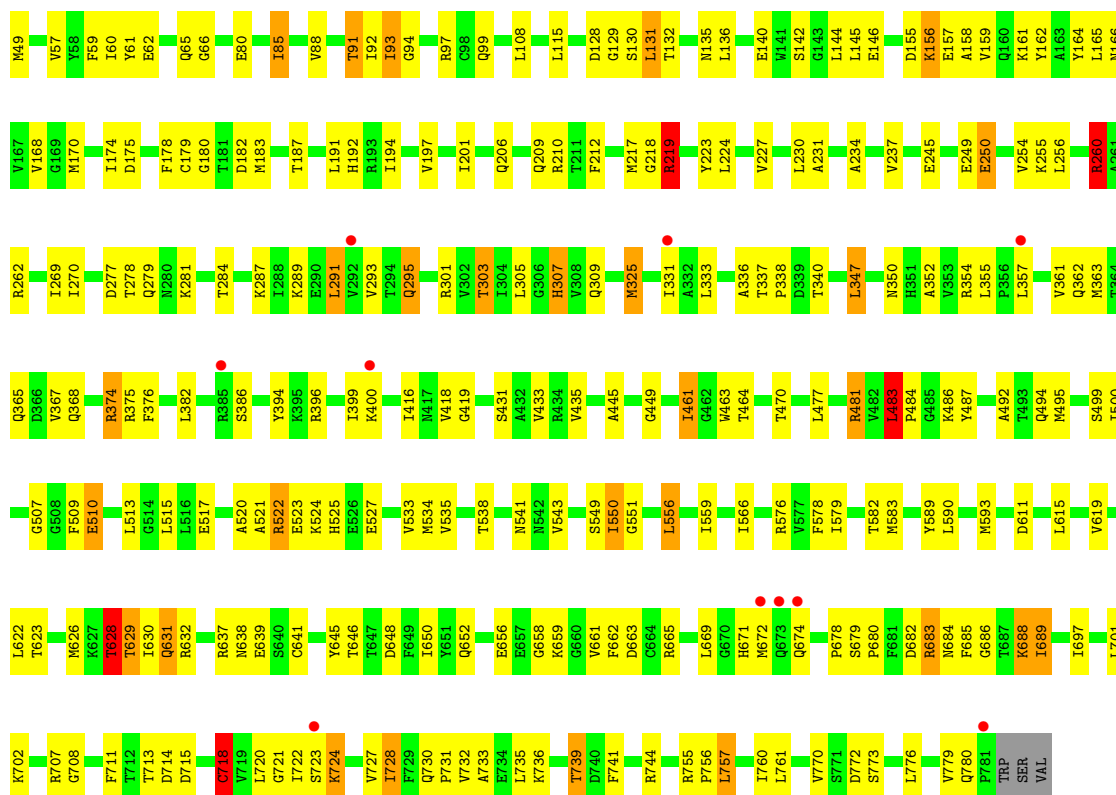
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

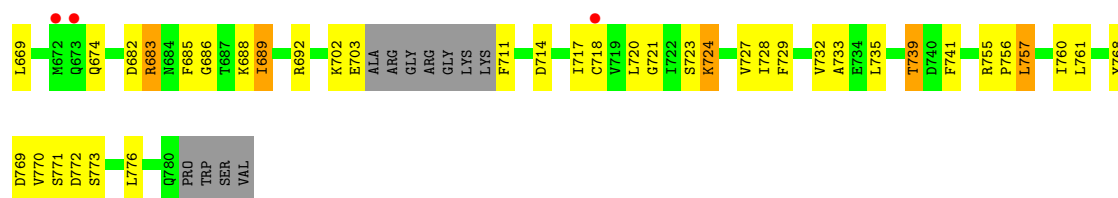
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



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

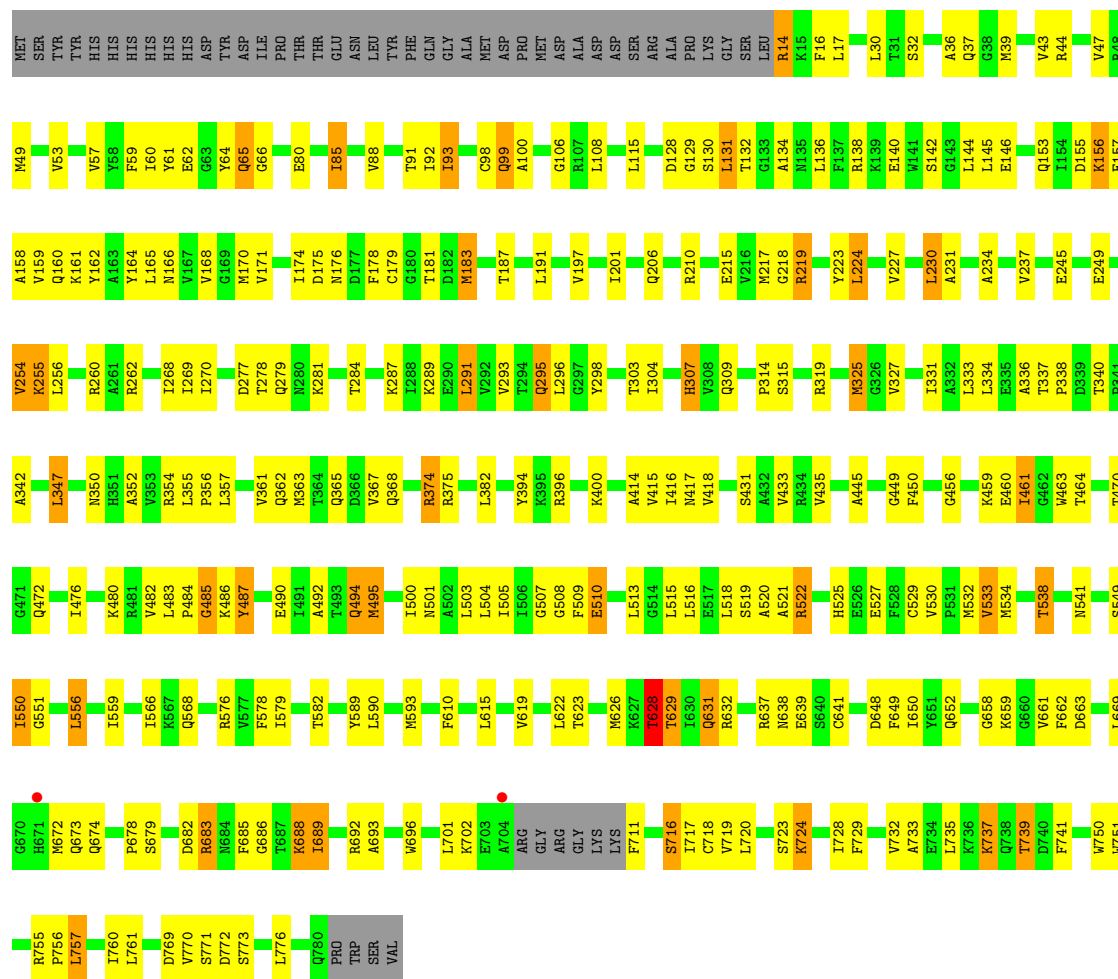






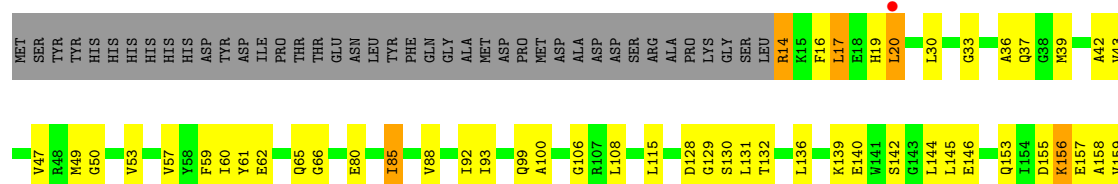
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

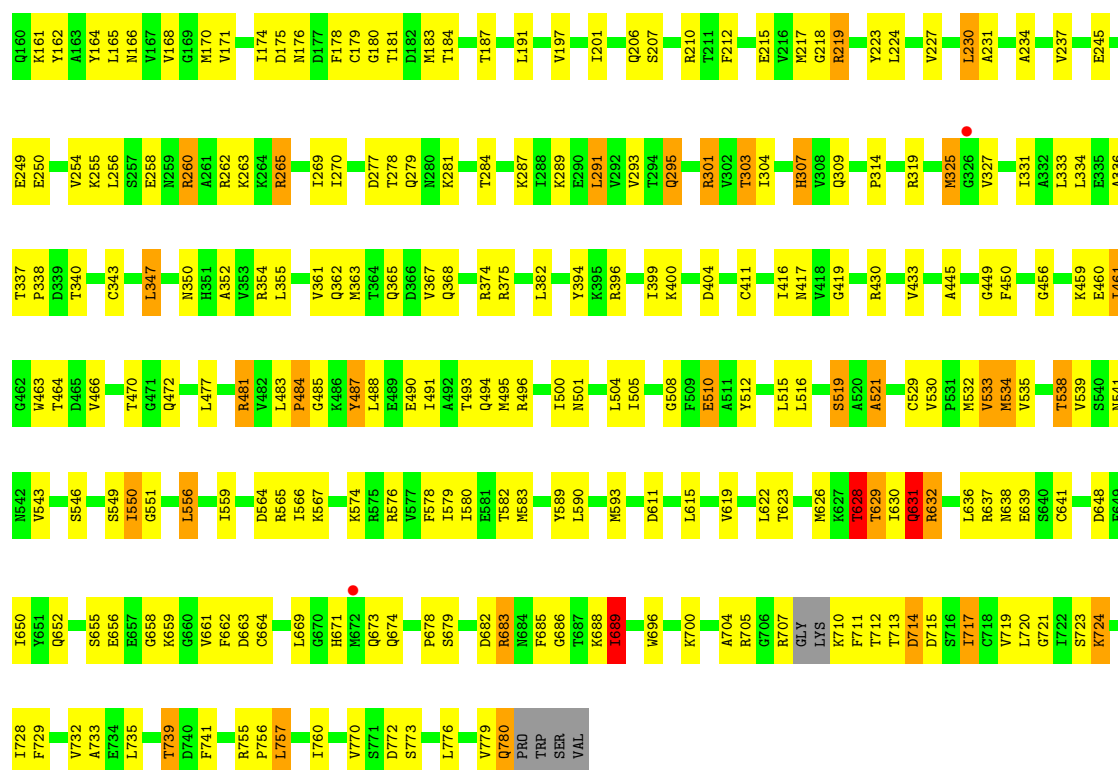
Chain D: 59% 30% 5% 6%



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

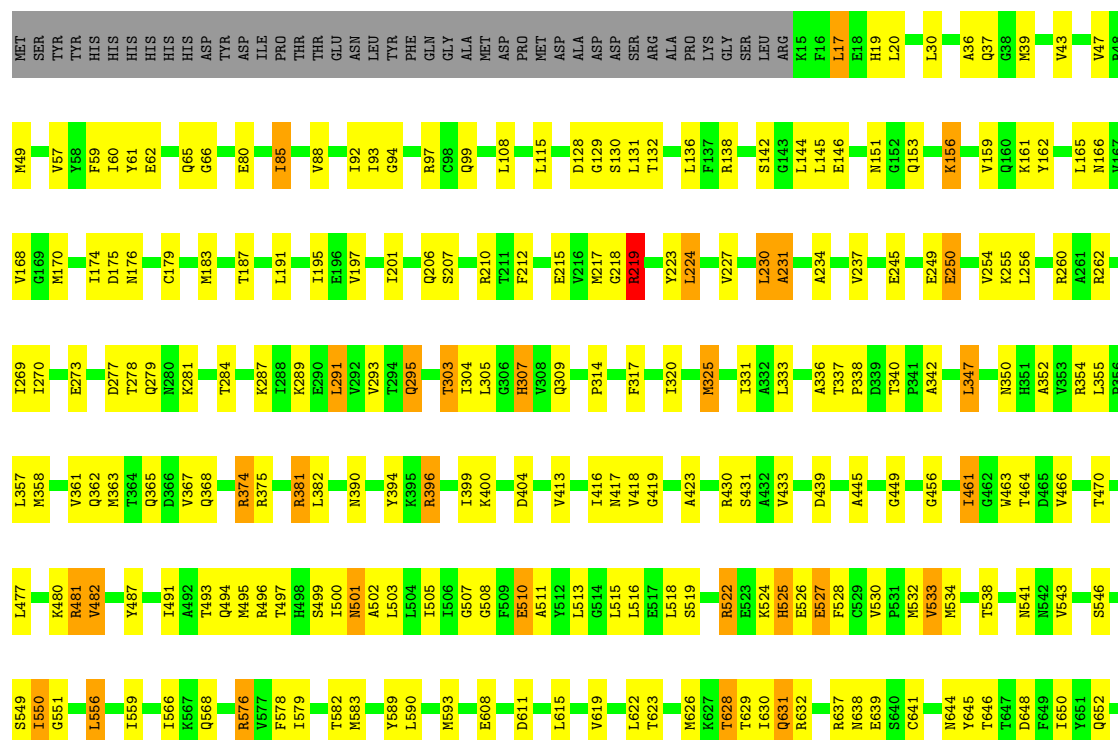
Chain E: 58% 31% 5% 6%

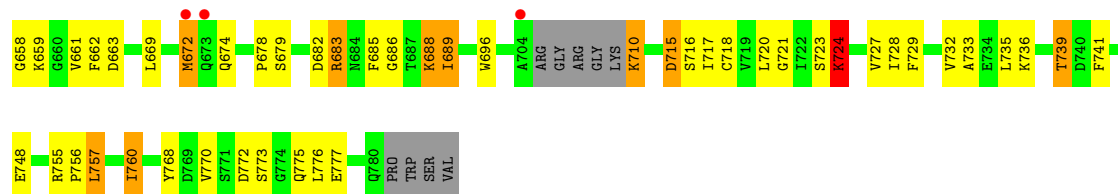




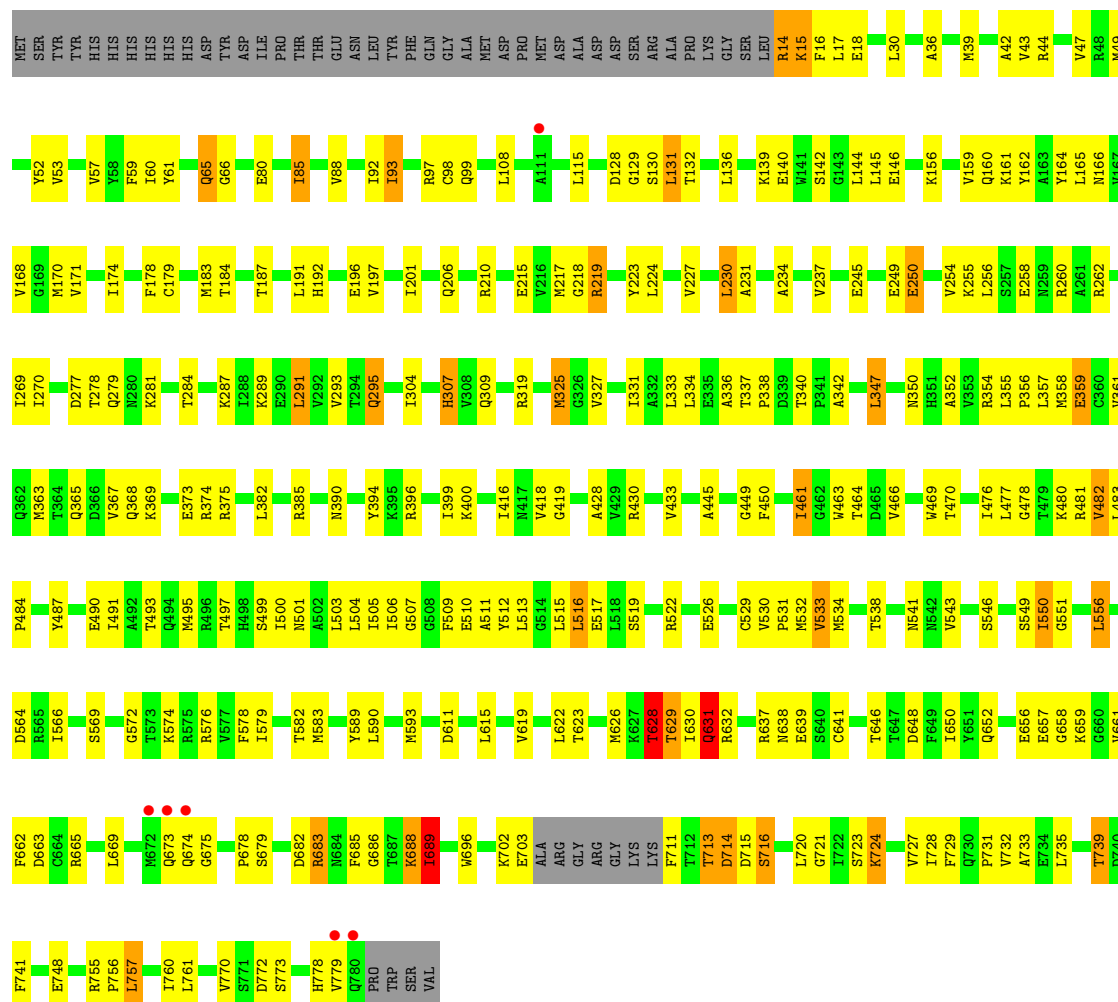
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain F: 60% 29% 5% 6%

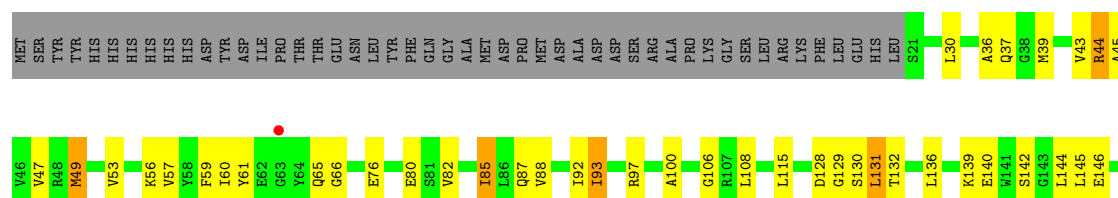




- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



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



F741	F661	S569	L477	S346	E249	Q153
W750	F662	G572	V482	L347	E250	I154
W751	L669	T573	L483			D155
		K574	P484	N350	V254	K156
R755	M672	R575	G485	H351	K255	A157
P756	Q673	R576	K486	A352	L256	V159
L757	Q674	V577	Y487	V353		Q160
W758	Q675	F578		R354	R260	
W759	P678	I579	I491	L355	A261	Y164
I760	S679				K262	L165
L761	P680	T582	M495	M358	K263	N166
A762	F681	Y589	I500	E359		V167
K763	D682	L590	L503	C360	I269	V168
TYR	R683		L504	V361	I270	M170
LYS	N684	M593	I505	Q362	E273	I174
ALA	F685	D601	G508	Q363		D175
SER	G686	D611	F509	T364	D277	N176
TYR	T687	L615	E510	Q365	T278	D177
ASP	K688	Q616	A511	D366	Q279	F178
VAL	L689	S617	L515	V367		
ASP	A693	N618	L516	Q368	T284	
SER		V619	E517	R374	K287	T181
GLY	L697	E620	L518	R375	L288	
GLN		H621	S519	R381	T289	T187
LEU	E703	A622	A520	L382	E290	
GLU	A704	L622	A521		L291	L191
HIS	R705	T623	E522	R385	V292	H192
VAL	GLY	ARG	E524	N390	V293	I195
GLN	GLY	K625	E523		T294	E196
PRO	GLY	M626		R396	Q295	V197
TRP	LYS	R627	E526		L296	
SER	K710	F711	T628	I416	G297	I201
VAL	T712	T629	V530		Y298	
	T713	I630	P531	R430	T303	Q206
	D714	Q631	M532	S431	I304	Q209
	D715	R632	V533	A432		R210
	S716		M534	V433	H307	E215
	I717	N637	T538	R434	Q309	V216
	L720	R638		V435		N217
	G721	E639	N541	A445	P314	G218
	I722	C641	N542			R219
	S723	S642	V543	G449	M325	H220
	K724	E643		F450	G326	C221
		N644	F548		V327	G222
	V727	Y645	S549	I461		Y223
	I728	I550	I550		L333	L224
	F729	D648	G551	T464	L334	
		F649	L556	D465	E335	V227
	V732	I650		V466	A336	
	A733	Y651			T337	L230
	E734	Q652	I559	T470	P338	A231
	L735		I566	G471	D339	
		G658	K567	Q472	T340	A234
	T739	K659	Q568			E245
	D740	G660		I476	C343	

4 Data and refinement statistics

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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.0 (49.69-3.10) 85.0 (49.69-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.07Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.221 , 0.246 0.221 , 0.247	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 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.59	0/5977	1.15	43/8067 (0.5%)
1	B	0.58	1/5977 (0.0%)	0.99	29/8068 (0.4%)
1	C	0.49	2/5915 (0.0%)	0.97	25/7986 (0.3%)
1	D	0.51	0/5920	0.99	22/7993 (0.3%)
1	E	0.51	0/5955	1.01	30/8037 (0.4%)
1	F	0.52	2/5918 (0.0%)	1.00	25/7990 (0.3%)
1	G	0.49	1/5915 (0.0%)	0.97	22/7986 (0.3%)
1	H	0.51	0/5734	1.02	30/7741 (0.4%)
All	All	0.53	6/47311 (0.0%)	1.01	226/63868 (0.4%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	583	MET	SD-CE	6.21	1.95	1.79
1	B	583	MET	SD-CE	5.89	1.94	1.79
1	C	683	ARG	CD-NE	-5.78	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	583	MET	SD-CE	5.50	1.93	1.79
1	C	583	MET	SD-CE	5.27	1.92	1.79
1	F	138	ARG	CD-NE	-5.20	1.39	1.46

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	219	ARG	NE-CZ-NH2	15.31	132.98	119.20
1	A	613	ARG	NE-CZ-NH2	15.03	132.73	119.20
1	H	219	ARG	NE-CZ-NH1	-14.29	107.21	121.50
1	A	396	ARG	NE-CZ-NH2	-14.26	106.36	119.20
1	A	613	ARG	NE-CZ-NH1	-14.26	107.24	121.50
1	A	575	ARG	NE-CZ-NH2	-13.72	106.85	119.20
1	A	381	ARG	NE-CZ-NH2	13.71	131.53	119.20
1	F	138	ARG	NE-CZ-NH2	-13.27	107.26	119.20
1	A	396	ARG	CD-NE-CZ	13.15	142.80	124.40
1	H	219	ARG	CD-NE-CZ	12.60	142.04	124.40
1	A	354	ARG	NE-CZ-NH2	12.43	130.39	119.20
1	A	381	ARG	NE-CZ-NH1	-12.37	109.14	121.50
1	A	692	ARG	NE-CZ-NH2	-12.30	108.12	119.20
1	A	565	ARG	NE-CZ-NH2	12.20	130.18	119.20
1	A	396	ARG	NE-CZ-NH1	11.83	133.33	121.50
1	A	565	ARG	NE-CZ-NH1	-11.81	109.69	121.50
1	A	613	ARG	CD-NE-CZ	11.81	140.93	124.40
1	A	575	ARG	CD-NE-CZ	11.80	140.93	124.40
1	E	565	ARG	NE-CZ-NH2	11.64	129.68	119.20
1	E	565	ARG	NE-CZ-NH1	-11.62	109.88	121.50
1	A	575	ARG	NE-CZ-NH1	11.59	133.09	121.50
1	A	354	ARG	NE-CZ-NH1	-11.46	110.04	121.50
1	F	138	ARG	CD-NE-CZ	11.43	140.40	124.40
1	F	138	ARG	NE-CZ-NH1	11.26	132.76	121.50
1	C	683	ARG	NE-CZ-NH1	-11.24	110.26	121.50
1	C	683	ARG	NE-CZ-NH2	11.15	129.24	119.20
1	E	260	ARG	NE-CZ-NH2	-11.05	109.25	119.20
1	A	381	ARG	CD-NE-CZ	11.01	139.81	124.40
1	A	692	ARG	NE-CZ-NH1	10.03	131.53	121.50
1	A	704	ALA	N-CA-C	-9.75	99.50	111.40
1	A	692	ARG	CD-NE-CZ	9.71	138.00	124.40
1	E	260	ARG	CD-NE-CZ	9.55	137.76	124.40
1	A	565	ARG	CD-NE-CZ	9.45	137.63	124.40
1	E	565	ARG	CD-NE-CZ	9.40	137.57	124.40
1	E	260	ARG	NE-CZ-NH1	9.30	130.81	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ARG	NE-CZ-NH2	8.65	126.99	119.20
1	D	375	ARG	NE-CZ-NH2	8.60	126.94	119.20
1	H	375	ARG	NE-CZ-NH2	8.47	126.83	119.20
1	F	374	ARG	NE-CZ-NH2	-8.37	111.66	119.20
1	G	375	ARG	NE-CZ-NH2	8.29	126.66	119.20
1	B	374	ARG	NE-CZ-NH2	-8.27	111.76	119.20
1	H	375	ARG	NE-CZ-NH1	-8.23	113.27	121.50
1	F	374	ARG	CD-NE-CZ	8.19	135.87	124.40
1	D	375	ARG	NE-CZ-NH1	-8.14	113.36	121.50
1	D	374	ARG	NE-CZ-NH2	-8.01	111.99	119.20
1	B	374	ARG	CD-NE-CZ	8.00	135.60	124.40
1	H	704	ALA	N-CA-C	-7.94	104.56	112.97
1	A	354	ARG	CD-NE-CZ	7.90	135.46	124.40
1	D	374	ARG	CD-NE-CZ	7.88	135.43	124.40
1	G	375	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	G	15	LYS	N-CA-C	7.66	121.53	109.81
1	E	483	LEU	CA-C-N	7.64	127.53	119.05
1	E	483	LEU	C-N-CA	7.64	127.53	119.05
1	A	375	ARG	NE-CZ-NH1	-7.56	113.94	121.50
1	F	374	ARG	NE-CZ-NH1	7.32	128.82	121.50
1	A	396	ARG	CG-CD-NE	-7.18	96.21	112.00
1	A	629	THR	N-CA-C	7.15	119.74	111.02
1	C	492	ALA	N-CA-C	-7.15	103.10	111.03
1	G	629	THR	N-CA-C	7.13	119.72	111.02
1	D	530	VAL	CA-C-N	-7.13	112.97	120.03
1	D	530	VAL	C-N-CA	-7.13	112.97	120.03
1	F	85	ILE	N-CA-C	-7.12	106.36	113.20
1	C	683	ARG	CD-NE-CZ	7.12	134.37	124.40
1	D	629	THR	N-CA-C	7.08	119.66	111.02
1	B	374	ARG	NE-CZ-NH1	7.08	128.58	121.50
1	B	688	LYS	N-CA-C	7.04	118.61	111.07
1	E	629	THR	N-CA-C	7.04	119.60	111.02
1	B	513	LEU	N-CA-C	-7.00	103.70	111.82
1	D	688	LYS	N-CA-C	6.99	118.54	111.07
1	C	629	THR	N-CA-C	6.92	119.46	111.02
1	E	231	ALA	N-CA-C	-6.87	105.05	113.50
1	B	483	LEU	CA-C-N	6.85	128.40	119.84
1	B	483	LEU	C-N-CA	6.85	128.40	119.84
1	G	231	ALA	N-CA-C	-6.83	105.10	113.50
1	A	85	ILE	N-CA-C	-6.81	106.66	113.20
1	H	688	LYS	N-CA-C	6.81	118.36	111.07
1	H	231	ALA	N-CA-C	-6.79	105.15	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	ALA	N-CA-C	-6.78	105.16	113.50
1	D	374	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	B	629	THR	N-CA-C	6.78	119.29	111.02
1	H	716	SER	N-CA-C	-6.76	104.65	113.17
1	G	688	LYS	N-CA-C	6.71	118.25	111.07
1	E	688	LYS	N-CA-C	6.67	118.21	111.07
1	H	629	THR	N-CA-C	6.65	119.14	111.02
1	H	85	ILE	N-CA-C	-6.64	106.83	113.20
1	C	85	ILE	N-CA-C	-6.63	106.84	113.20
1	E	375	ARG	NE-CZ-NH2	-6.62	113.24	119.20
1	C	231	ALA	N-CA-C	-6.59	105.40	113.50
1	G	374	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	C	374	ARG	NE-CZ-NH1	-6.55	114.95	121.50
1	F	17	LEU	N-CA-C	6.53	118.19	111.14
1	A	688	LYS	N-CA-C	6.52	118.04	111.07
1	C	375	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	C	688	LYS	N-CA-C	6.50	118.03	111.07
1	C	374	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	F	629	THR	N-CA-C	6.49	118.93	111.02
1	F	688	LYS	N-CA-C	6.46	117.98	111.07
1	B	718	CYS	N-CA-C	6.44	117.94	108.86
1	E	484	PRO	N-CA-C	6.43	122.47	113.53
1	E	374	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	G	674	GLN	N-CA-C	-6.36	104.98	114.64
1	A	231	ALA	N-CA-C	-6.34	105.70	113.50
1	A	375	ARG	CD-NE-CZ	6.30	133.22	124.40
1	F	231	ALA	N-CA-C	-6.29	105.76	113.50
1	G	374	ARG	NE-CZ-NH1	-6.27	115.23	121.50
1	G	375	ARG	CD-NE-CZ	6.24	133.14	124.40
1	H	674	GLN	N-CA-C	-6.24	105.16	114.64
1	E	85	ILE	N-CA-C	-6.22	107.23	113.20
1	A	374	ARG	NE-CZ-NH1	-6.22	115.28	121.50
1	H	374	ARG	NE-CZ-NH2	6.22	124.79	119.20
1	H	88	VAL	N-CA-C	6.21	116.87	108.17
1	B	85	ILE	N-CA-C	-6.21	107.23	113.20
1	E	375	ARG	CD-NE-CZ	6.20	133.08	124.40
1	F	375	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	A	374	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	B	375	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	D	88	VAL	N-CA-C	6.18	116.82	108.17
1	F	674	GLN	N-CA-C	-6.17	105.27	114.64
1	H	374	ARG	NE-CZ-NH1	-6.15	115.35	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	375	ARG	CD-NE-CZ	6.15	133.00	124.40
1	D	85	ILE	N-CA-C	-6.14	107.31	113.20
1	E	374	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	B	375	ARG	CD-NE-CZ	6.08	132.91	124.40
1	H	375	ARG	CD-NE-CZ	6.07	132.90	124.40
1	F	375	ARG	CD-NE-CZ	6.04	132.85	124.40
1	H	508	GLY	N-CA-C	6.03	120.21	112.13
1	F	718	CYS	N-CA-C	6.01	117.33	108.86
1	C	375	ARG	CD-NE-CZ	6.01	132.81	124.40
1	G	550	ILE	N-CA-C	-6.00	100.97	108.89
1	A	88	VAL	N-CA-C	5.97	116.52	108.17
1	B	88	VAL	N-CA-C	5.96	116.52	108.17
1	B	295	GLN	N-CA-C	5.95	117.57	111.14
1	A	674	GLN	N-CA-C	-5.95	105.60	114.64
1	F	307	HIS	N-CA-C	-5.93	105.89	113.01
1	G	85	ILE	N-CA-C	-5.91	107.52	113.20
1	C	674	GLN	N-CA-C	-5.90	105.67	114.64
1	D	674	GLN	N-CA-C	-5.88	105.71	114.64
1	D	702	LYS	N-CA-C	-5.88	106.15	113.38
1	H	721	GLY	N-CA-C	5.83	119.60	111.10
1	C	683	ARG	CB-CG-CD	-5.82	97.91	111.30
1	E	674	GLN	N-CA-C	-5.81	105.81	114.64
1	B	550	ILE	N-CA-C	-5.79	101.25	108.89
1	B	231	ALA	N-CA-C	-5.78	106.40	113.50
1	B	180	GLY	N-CA-C	-5.77	107.61	114.48
1	F	88	VAL	N-CA-C	5.75	116.22	108.17
1	C	88	VAL	N-CA-C	5.73	116.19	108.17
1	F	295	GLN	N-CA-C	5.73	117.60	111.36
1	C	295	GLN	N-CA-C	5.72	117.59	111.36
1	G	295	GLN	N-CA-C	5.70	117.57	111.36
1	B	628	THR	O-C-N	5.68	125.03	120.83
1	E	88	VAL	N-CA-C	5.67	116.12	108.17
1	D	307	HIS	N-CA-C	-5.65	106.23	113.01
1	B	19	HIS	N-CA-C	-5.65	103.76	111.56
1	C	307	HIS	N-CA-C	-5.63	106.26	113.01
1	G	483	LEU	CA-C-N	5.63	125.30	119.56
1	G	483	LEU	C-N-CA	5.63	125.30	119.56
1	A	295	GLN	N-CA-C	5.62	117.48	111.36
1	G	88	VAL	N-CA-C	5.56	115.96	108.17
1	B	674	GLN	N-CA-C	-5.56	106.19	114.64
1	D	628	THR	O-C-N	5.56	124.94	120.83
1	E	521	ALA	N-CA-C	5.54	118.08	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	550	ILE	N-CA-C	-5.53	101.58	108.89
1	G	716	SER	N-CA-C	-5.48	106.76	113.50
1	H	307	HIS	N-CA-C	-5.48	106.44	113.01
1	E	307	HIS	N-CA-C	-5.42	106.51	113.01
1	C	628	THR	N-CA-C	5.40	116.72	108.30
1	D	295	GLN	N-CA-C	5.39	117.24	111.36
1	F	550	ILE	N-CA-C	-5.39	101.78	108.89
1	B	535	VAL	CA-C-N	5.37	126.55	119.84
1	B	535	VAL	C-N-CA	5.37	126.55	119.84
1	D	716	SER	N-CA-C	-5.35	106.26	112.89
1	H	518	LEU	N-CA-C	5.34	117.18	111.36
1	G	714	ASP	N-CA-C	-5.33	106.82	113.38
1	C	520	ALA	N-CA-C	-5.32	106.84	113.38
1	A	689	ILE	CB-CA-C	-5.31	104.89	112.22
1	B	520	ALA	N-CA-C	-5.30	105.09	112.45
1	E	631	GLN	N-CA-C	-5.29	107.48	114.31
1	B	522	ARG	N-CA-C	-5.29	106.07	113.37
1	E	628	THR	O-C-N	5.29	124.74	120.83
1	D	550	ILE	N-CA-C	-5.29	101.91	108.89
1	D	628	THR	N-CA-C	5.28	116.54	108.30
1	H	689	ILE	CB-CA-C	-5.28	104.93	112.22
1	E	535	VAL	CA-C-N	5.26	126.41	119.84
1	E	535	VAL	C-N-CA	5.26	126.41	119.84
1	E	375	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	C	375	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	D	631	GLN	N-CA-C	-5.25	107.53	114.31
1	F	138	ARG	CG-CD-NE	-5.25	100.45	112.00
1	H	511	ALA	N-CA-C	-5.24	104.82	111.11
1	B	720	LEU	N-CA-C	-5.24	100.64	108.96
1	H	295	GLN	N-CA-C	5.24	117.07	111.36
1	F	628	THR	N-CA-C	5.23	116.45	108.30
1	F	375	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	A	628	THR	O-C-N	5.22	124.69	120.83
1	B	307	HIS	N-CA-C	-5.21	106.76	113.01
1	C	535	VAL	CA-C-N	5.21	126.35	119.84
1	C	535	VAL	C-N-CA	5.21	126.35	119.84
1	B	628	THR	N-CA-C	5.20	116.40	108.30
1	F	716	SER	N-CA-C	-5.19	106.97	113.72
1	H	628	THR	N-CA-C	5.17	116.37	108.30
1	A	628	THR	N-CA-C	5.17	116.37	108.30
1	A	307	HIS	N-CA-C	-5.17	106.80	113.01
1	G	307	HIS	N-CA-C	-5.16	106.82	113.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	522	ARG	N-CA-C	-5.16	106.74	112.57
1	H	550	ILE	N-CA-C	-5.16	102.08	108.89
1	E	550	ILE	N-CA-C	-5.15	102.09	108.89
1	B	376	PHE	N-CA-C	5.15	117.56	111.33
1	E	628	THR	N-CA-C	5.15	116.33	108.30
1	G	689	ILE	CB-CA-C	-5.15	105.12	112.22
1	A	179	CYS	N-CA-C	5.12	117.65	110.23
1	H	631	GLN	N-CA-C	-5.11	107.72	114.31
1	E	295	GLN	N-CA-C	5.10	116.92	111.36
1	A	718	CYS	N-CA-C	5.10	117.61	109.81
1	F	628	THR	O-C-N	5.10	124.60	120.83
1	A	631	GLN	N-CA-C	-5.09	107.74	114.31
1	G	631	GLN	N-CA-C	-5.09	107.74	114.31
1	C	628	THR	CB-CA-C	-5.07	105.12	115.27
1	H	486	LYS	N-CA-C	5.07	116.81	111.28
1	G	628	THR	O-C-N	5.06	124.57	120.83
1	H	762	ALA	N-CA-C	-5.06	106.80	113.12
1	H	219	ARG	CG-CD-NE	-5.05	100.88	112.00
1	C	628	THR	O-C-N	5.03	124.55	120.83
1	H	628	THR	O-C-N	5.03	124.55	120.83
1	E	689	ILE	CB-CA-C	-5.01	105.31	112.22
1	A	354	ARG	CG-CD-NE	5.01	123.02	112.00
1	B	525	HIS	N-CA-C	5.01	116.57	108.26

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	210	0
1	B	5880	0	5908	201	0
1	C	5820	0	5837	197	0
1	D	5825	0	5842	209	0
1	E	5860	0	5884	226	0
1	F	5823	0	5842	206	0
1	G	5820	0	5837	215	0
1	H	5644	0	5678	192	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1602	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 17.

All (1602) 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:G:17:LEU:HD21	1:G:49:MET:HE1	1.55	0.88
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:503:LEU:HD23	1:F:532:MET:HE2	1.59	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: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
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:B:534:MET:HE1	1:B:543:VAL:HG11	1.61	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:F:518:LEU:HD13	1:F:532:MET:HE1	1.61	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:G:17:LEU:CD2	1:G:49:MET:HE1	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:495:MET:HE3	1:D:500:ILE:HB	1.69	0.74
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:E:17:LEU:HD21	1:E:49:MET:HE1	1.70	0.74
1:B:170:MET:HE3	1:B:325:MET:HB3	1.70	0.73
1:D:170:MET:HE3	1:D:325:MET:HB3	1.69	0.73
1:G:217:MET:HG3	1:G:309:GLN:NE2	2.03	0.73
1:B:534:MET:HE1	1:B:543:VAL:CG1	2.18	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
1:F:325:MET:HE3	1:F:325:MET:HA	1.70	0.73
1:G:325:MET:HA	1:G:325:MET:HE3	1.70	0.73
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:D:325:MET:HE3	1:D:325:MET:HA	1.71	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:MET:HG3	1:D:309:GLN:NE2	2.06	0.70
1:E:780:GLN:H	1:E:780:GLN:CD	1.99	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:E:170:MET:HE3	1:E:325:MET:HB3	1.74	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:325:MET:HA	1:E:325:MET:HE3	1.73	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:H:170:MET:HE3	1:H:325:MET:HB3	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:H:325:MET:HE3	1:H:325:MET:HA	1.73	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
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:B:521:ALA:C	1:B:523:GLU:H	1.98	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:C:325:MET:HE3	1:C:325:MET:HA	1.74	0.68
1:E:179:CYS:C	1:E:181:THR:H	2.02	0.68
1:H:757:LEU:HD23	1:H:761:LEU:HG	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:MET:HE3	1:B:325:MET:HA	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:H:503:LEU:HD23	1:H:532:MET:HE2	1.75	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:A:325:MET:HE3	1:A:325:MET:HA	1.75	0.67
1:C:433:VAL:HG22	1:C:461:ILE:HD12	1.75	0.67
1:B:17:LEU:HD21	1:B:49:MET:HE1	1.74	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
1:B:718:CYS:HB3	1:B:730:GLN:C	2.20	0.66
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:G:665:ARG:HD2	1:H:672:MET:HE1	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:170:MET:HE3	1:F:325:MET:HB3	1.79	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
1:G:187:THR:HG21	1:G:223:TYR:HE2	1.63	0.63
1:A:170:MET:HE3	1:A:325:MET:HB3	1.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:MET:HE3	1:C:325:MET:HB3	1.79	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:18:GLU:H	1:A:18:GLU:CD	2.08	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: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
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:601:ASP:CG	1:H:622:LEU:HD13	2.24	0.61
1:H:363:MET:O	1:H:367:VAL:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:17:LEU:HD21	1:B:49:MET:CE	2.31	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:17:LEU:HD21	1:A:49:MET:HE1	1.84	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:17:LEU:HD21	1:E:49:MET:CE	2.32	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:D:519:SER:C	1:D:521:ALA:H	2.10	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:E:534:MET:HE1	1:E:543:VAL:HG11	1.84	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
1:A:99:GLN:HA	1:A:99:GLN:NE2	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:170:MET:HE3	1:G:325:MET:HB3	1.87	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
1:D:756:PRO:O	1:D:760:ILE:HG23	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:530:VAL:HG22	1:E:532:MET:HE2	1.87	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:G:534:MET:HE1	1:G:543:VAL:CG1	2.35	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:49:MET:HE2	1:G:327:VAL:HG13	1.87	0.56
1:B:521:ALA:C	1:B:523:GLU:N	2.60	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:D:518:LEU:HD13	1:D:532:MET:HE1	1.87	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:ARG:HH12	1:D:716:SER:HB2	1.70	0.55
1:E:49:MET:HE2	1:E:327:VAL:HG13	1.88	0.55
1:E:168:VAL:CG1	1:E:333:LEU:HD13	2.36	0.55
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:F:183:MET:HE3	1:F:317:PHE:CE2	2.41	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:A:17:LEU:CD2	1:A:49:MET:HE1	2.36	0.55
1:C:428:ALA:CB	1:C:506:ILE:HD13	2.36	0.55
1:E:19:HIS:O	1:E:20:LEU:C	2.50	0.55
1:F:648:ASP:O	1:F:652:GLN:HG3	2.07	0.55
1:A:723:SER:O	1:A:724:LYS:C	2.50	0.55
1:B:209:GLN:OE1	1:B:260:ARG:HD2	2.07	0.55
1:F:723:SER:O	1:F:724:LYS:C	2.50	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:723:SER:O	1:E:724:LYS:C	2.51	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: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:C:723:SER:O	1:C:724:LYS:C	2.51	0.53
1:H:685:PHE:O	1:H:689:ILE:HG13	2.08	0.53
1:D:723:SER:O	1:D:724:LYS:C	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:HIS:HA	1:H:680:PRO:HG2	1.90	0.53
1:B:723:SER:O	1:B:724:LYS:C	2.52	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:B:354:ARG:C	1:B:355:LEU:HD12	2.33	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
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:G:723:SER:O	1:G:724:LYS:C	2.52	0.53
1:B:179:CYS:SG	1:B:363:MET:HE2	2.49	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:527:GLU:CD	1:D:527:GLU:H	2.17	0.53
1:B:17:LEU:CD2	1:B:49:MET:HE1	2.39	0.52
1:C:354:ARG:C	1:C:355:LEU:HD12	2.34	0.52
1:D:354:ARG:C	1:D:355:LEU:HD12	2.34	0.52
1:D:576:ARG:HG2	1:D:578:PHE:CE1	2.43	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:354:ARG:C	1:E:355:LEU:HD12	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:672:MET:HA	1:F:672:MET:HE2	1.90	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:C:495:MET:HE3	1:C:500:ILE:HB	1.90	0.52
1:E:207:SER:HB2	1:F:94:GLY:HA3	1.92	0.52
1:E:776:LEU:HD13	1:E:776:LEU:C	2.34	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
1:C:433:VAL:HG21	1:C:461:ILE:HD12	1.91	0.52
1:E:255:LYS:HZ2	1:E:399:ILE:HA	1.75	0.52
1:G:534:MET:HE1	1:G:543:VAL:HG11	1.91	0.52
1:H:679:SER:O	1:H:683:ARG:HG2	2.10	0.52
1:H:723:SER:O	1:H:724:LYS:C	2.52	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:E:658:GLY:O	1:E:659:LYS:C	2.52	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:G:354:ARG:C	1:G:355:LEU:HD12	2.35	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:D:518:LEU:CD1	1:D:532:MET:HE1	2.40	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:658:GLY:O	1:F:659:LYS:C	2.53	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:61:TYR:O	1:A:66:GLY:HA3	2.10	0.51
1:A:658:GLY:O	1:A:659:LYS:C	2.53	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
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:H:354:ARG:C	1:H:355:LEU:HD12	2.35	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:A:17:LEU:HD21	1:A:49:MET:CE	2.41	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:277:ASP:C	1:A:279:GLN:H	2.19	0.50
1:A:708:GLY:C	1:A:710:LYS:H	2.20	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:C:521:ALA:C	1:C:523:GLU:H	2.20	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:B:658:GLY:O	1:B:659:LYS:C	2.55	0.50
1:C:665:ARG:HD2	1:D:672:MET:HE1	1.94	0.50
1:E:227:VAL:HA	1:E:230:LEU:HD21	1.94	0.50
1:G:757:LEU:C	1:G:757:LEU:CD2	2.85	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
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:495:MET:HE3	1:B:500:ILE:HB	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:757:LEU:CD2	1:H:757:LEU:C	2.85	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:17:LEU:C	1:B:19:HIS:H	2.20	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:H:136:LEU:C	1:H:136:LEU:HD23	2.38	0.49
1:H:658:GLY:O	1:H:659:LYS:C	2.55	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:D:688:LYS:C	1:D:688:LYS:HD2	2.36	0.49
1:F:354:ARG:C	1:F:355:LEU:HD12	2.37	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:H:534:MET:HE1	1:H:543:VAL:CG1	2.42	0.49
1:C:14:ARG:NH1	1:C:771:SER:CB	2.75	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:A:250:GLU:CD	1:A:250:GLU:H	2.19	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:H:49:MET:HE2	1:H:327:VAL:HG13	1.95	0.49
1:B:206:GLN:HG3	1:B:210:ARG:HD3	1.94	0.49
1:E:17:LEU:CD2	1:E:49:MET:HE1	2.39	0.49
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:181:THR:O	1:C:182:ASP:C	2.56	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:703:GLU:HB3	1:E:404:ASP:CG	2.38	0.48
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: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:527:GLU:C	1:C:529:CYS:H	2.22	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:277:ASP:C	1:G:279:GLN:H	2.21	0.48
1:G:331:ILE:CD1	1:G:773:SER:HB2	2.42	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
1:A:679:SER:O	1:A:683:ARG:HG2	2.14	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:MET:HE2	1:E:500:ILE:HB	1.94	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:18:GLU:CD	1:G:18:GLU:H	2.22	0.48
1:B:551:GLY:H	1:B:682:ASP:CG	2.20	0.48
1:D:142:SER:O	1:D:146:GLU:HG2	2.14	0.48
1:E:539:VAL:HG21	1:E:583:MET:HE3	1.96	0.48
1:F:161:LYS:HE3	1:F:162:TYR:CZ	2.49	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:704:ALA:O	1:E:705:ARG:C	2.57	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:H:534:MET:HE1	1:H:543:VAL:HG11	1.95	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:D:658:GLY:O	1:D:659:LYS:C	2.56	0.48
1:F:227:VAL:HA	1:F:230:LEU:CD2	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:B:757:LEU:C	1:B:757:LEU:CD2	2.87	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:582:THR:O	1:D:639:GLU:HG3	2.13	0.48
1:G:136:LEU:C	1:G:136:LEU:HD23	2.39	0.48
1:H:579:ILE:N	1:H:579:ILE:HD12	2.29	0.48
1:H:703:GLU:C	1:H:705:ARG:H	2.21	0.48
1:A:354:ARG:C	1:A:355:LEU:HD12	2.39	0.48
1:A:652:GLN:NE2	1:D:649:PHE:HB2	2.28	0.48
1:C:495:MET:HE1	1:C:530:VAL:HG21	1.96	0.48
1:C:720:LEU:CD1	1:C:727:VAL:HG12	2.44	0.48
1:D:728:ILE:HD12	1:D:729:PHE:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:277:ASP:C	1:B:279:GLN:H	2.22	0.48
1:D:331:ILE:HD11	1:D:773:SER:HB2	1.96	0.48
1:G:724:LYS:H	1:G:724:LYS:CD	2.27	0.48
1:A:255:LYS:HZ2	1:A:399:ILE:HA	1.77	0.47
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:D:485:GLY:C	1:D:487:TYR:H	2.22	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:F:757:LEU:C	1:F:757:LEU:CD2	2.87	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:A:757:LEU:C	1:A:757:LEU:CD2	2.87	0.47
1:B:155:ASP:HB3	1:B:158:ALA:HB2	1.96	0.47
1:C:456:GLY:HA2	1:C:494:GLN:HG2	1.96	0.47
1:C:527:GLU:CD	1:C:527:GLU:H	2.22	0.47
1:D:256:LEU:HD21	1:D:269:ILE:HD11	1.96	0.47
1:D:277:ASP:C	1:D:279:GLN:H	2.22	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:G:658:GLY:O	1:G:659:LYS:C	2.57	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:250:GLU:CD	1:H:250:GLU:H	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:673:GLN:N	1:E:673:GLN:CD	2.72	0.47
1:F:17:LEU:C	1:F:19:HIS:H	2.22	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
1:F:615:LEU:O	1:F:619:VAL:HG23	2.15	0.47
1:F:760:ILE:C	1:F:760:ILE:HD12	2.39	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:H:521:ALA:C	1:H:523:GLU:H	2.21	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: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:277:ASP:C	1:C:279:GLN:H	2.22	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:F:136:LEU:HD23	1:F:136:LEU:C	2.40	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:416:ILE:HD11	1:H:449:GLY:C	2.40	0.47
1:H:551:GLY:H	1:H:682:ASP:CG	2.22	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:C:658:GLY:O	1:C:659:LYS:C	2.58	0.47
1:C:757:LEU:C	1:C:757:LEU:CD2	2.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:757:LEU:C	1:E:757:LEU:CD2	2.88	0.47
1:F:230:LEU:H	1:F:230:LEU:CD2	2.27	0.47
1:F:526:GLU:C	1:F:528:PHE:N	2.70	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: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: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:E:168:VAL:HG12	1:E:333:LEU:HD13	1.97	0.46
1:E:277:ASP:C	1:E:279:GLN:H	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:250:GLU:CD	1:C:250:GLU:H	2.23	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:G:546:SER:HB2	1:G:721:GLY:HA3	1.96	0.46
1:H:662:PHE:CD1	1:H:662:PHE:C	2.94	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
1:H:277:ASP:C	1:H:279:GLN:H	2.23	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:E:662:PHE:CD1	1:E:662:PHE:C	2.93	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:C:42:ALA:HB1	1:C:170:MET:HE1	1.98	0.46
1:D:140:GLU:O	1:D:144:LEU:HG	2.16	0.46
1:F:183:MET:HE3	1:F:317:PHE:CZ	2.50	0.46
1:F:277:ASP:C	1:F:279:GLN:H	2.22	0.46
1:F:496:ARG:HB2	1:F:527:GLU:CG	2.44	0.46
1:G:416:ILE:HD11	1:G:449:GLY:C	2.41	0.46
1:A:510:GLU:CD	1:A:510:GLU:H	2.24	0.46
1:A:662:PHE:CD1	1:A:662:PHE:C	2.93	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:D:673:GLN:CD	1:D:673:GLN:N	2.74	0.46
1:E:136:LEU:C	1:E:136:LEU:HD23	2.41	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:G:673:GLN:N	1:G:673:GLN:CD	2.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ALA:HB2	1:C:461:ILE:CD1	2.46	0.46
1:D:49:MET:HE2	1:D:327:VAL:HG13	1.96	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:136:LEU:HD23	1:A:136:LEU:C	2.40	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:C:136:LEU:C	1:C:136:LEU:HD23	2.41	0.46
1:D:136:LEU:C	1:D:136:LEU:HD23	2.41	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: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:G:662:PHE:CD1	1:G:662:PHE:C	2.94	0.45
1:A:576:ARG:HG2	1:A:578:PHE:CZ	2.52	0.45
1:C:662:PHE:CD1	1:C:662:PHE:C	2.94	0.45
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:B:337:THR:HB	1:B:338:PRO:CD	2.46	0.45
1:B:416:ILE:HD11	1:B:449:GLY:C	2.41	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:611:ASP:OD2	1:F:611:ASP:C	2.59	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:C:416:ILE:HD11	1:C:449:GLY:C	2.41	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:D:757:LEU:C	1:D:757:LEU:CD2	2.90	0.45
1:F:608:GLU:CD	1:F:755:ARG:HE	2.24	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:A:673:GLN:CD	1:A:673:GLN:N	2.75	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:G:757:LEU:C	1:G:757:LEU:HD23	2.41	0.45
1:H:559:ILE:HG12	1:H:669:LEU:HD11	1.99	0.45
1:H:757:LEU:HD23	1:H:757:LEU:C	2.41	0.45
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.78	0.45
1:A:551:GLY:H	1:A:682:ASP:CG	2.24	0.45
1:B:136:LEU:C	1:B:136:LEU:HD23	2.42	0.45
1:B:262:ARG:HB3	1:B:464:THR:HG21	1.99	0.45
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:A:156:LYS:HE2	1:A:156:LYS:HA	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:LEU:HD12	1:C:504:LEU:C	2.42	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: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: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:G:319:ARG:HH22	1:G:564:ASP:CG	2.24	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:30:LEU:C	1:A:30:LEU:HD12	2.42	0.45
1:A:428:ALA:CB	1:A:506:ILE:HD13	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: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
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:F:505:ILE:HD12	1:F:515:LEU:CD2	2.47	0.44
1:F:662:PHE:CD1	1:F:662:PHE:C	2.95	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:H:164:TYR:OH	1:H:166:ASN:CG	2.60	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:D:416:ILE:HD11	1:D:449:GLY:C	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:129:GLY:O	1:B:130:SER:C	2.61	0.44
1:B:250:GLU:CD	1:B:250:GLU:H	2.25	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:B:662:PHE:CD1	1:B:662:PHE:C	2.96	0.44
1:D:589:TYR:CE1	1:D:593:MET:HG3	2.52	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:503:LEU:O	1:D:532:MET:HA	2.18	0.44
1:E:129:GLY:O	1:E:130:SER:C	2.59	0.44
1:E:533:VAL:HG13	1:E:696:TRP:CZ3	2.52	0.44
1:F:416:ILE:HD11	1:F:449:GLY:C	2.42	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:416:ILE:HD11	1:A:449:GLY:C	2.42	0.44
1:A:757:LEU:C	1:A:757:LEU:HD23	2.43	0.44
1:B:18:GLU:CD	1:B:18:GLU:H	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:757:LEU:C	1:C:757:LEU:HD23	2.43	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:551:GLY:H	1:G:682:ASP:CG	2.26	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:B:757:LEU:C	1:B:757:LEU:HD23	2.43	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:F:551:GLY:H	1:F:682:ASP:CG	2.26	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:A:611:ASP:OD2	1:A:611:ASP:C	2.61	0.43
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:C:484:PRO:O	1:C:485:GLY:C	2.60	0.43
1:D:519:SER:C	1:D:521:ALA:N	2.76	0.43
1:D:662:PHE:CD1	1:D:662:PHE:C	2.95	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:218:GLY:O	1:F:219:ARG:C	2.59	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:H:166:ASN:CG	1:H:336:ALA:CB	2.91	0.43
1:H:601:ASP:OD2	1:H:622:LEU:HD13	2.17	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:495:MET:HE2	1:B:495:MET:HB3	1.65	0.43
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:129:GLY:O	1:F:130:SER:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:VAL:O	1:F:507:GLY:HA3	2.18	0.43
1:A:42:ALA:HB1	1:A:170:MET:HE1	2.00	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: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:G:42:ALA:HB1	1:G:170:MET:HE1	1.99	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:340:THR:O	1:D:340:THR:HG23	2.18	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: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: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:757:LEU:C	1:E:757:LEU:HD23	2.44	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:129:GLY:O	1:A:130:SER:C	2.61	0.43
1:A:622:LEU:O	1:A:626:MET:HG2	2.18	0.43
1:B:510:GLU:CD	1:B:510:GLU:H	2.27	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:O	1:C:506:ILE:HG22	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:289:LYS:O	1:G:293:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:505:ILE:CG2	1:G:511:ALA:HB1	2.46	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:176:ASN:C	1:D:176:ASN:HD22	2.27	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:700:LYS:O	1:A:703:GLU:HG2	2.18	0.43
1:B:732:VAL:HG23	1:B:733:ALA:N	2.34	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: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: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:325:MET:HA	1:A:325:MET:CE	2.48	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: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
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:350:ASN:O	1:G:350:ASN:CG	2.61	0.43
1:G:400:LYS:HB2	1:G:463:TRP:CZ2	2.53	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:611:ASP:C	1:E:611:ASP:OD2	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:630:ILE:HG22	1:E:631:GLN:N	2.33	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: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:C:551:GLY:H	1:C:682:ASP:CG	2.26	0.42
1:D:17:LEU:HD21	1:D:49:MET:HE2	2.01	0.42
1:D:325:MET:HA	1:D:325:MET:CE	2.45	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:G:515:LEU:HA	1:G:515:LEU:HD23	1.71	0.42
1:G:515:LEU:C	1:G:517:GLU:N	2.77	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:526:GLU:O	1:F:527:GLU:C	2.61	0.42
1:F:590:LEU:HD23	1:F:590:LEU:HA	1.87	0.42
1:H:129:GLY:O	1:H:130:SER:C	2.62	0.42
1:A:739:THR:HG23	1:A:741:PHE:CE1	2.53	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:129:GLY:O	1:D:130:SER:C	2.61	0.42
1:D:342:ALA:O	1:D:357:LEU:HB2	2.19	0.42
1:E:551:GLY:H	1:E:682:ASP:CG	2.26	0.42
1:F:350:ASN:CG	1:F:350:ASN:O	2.62	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:A:218:GLY:O	1:A:219:ARG:C	2.63	0.42
1:A:303:THR:CG2	1:B:307:HIS:CE1	2.96	0.42
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:C:350:ASN:CG	1:C:350:ASN:O	2.62	0.42
1:D:431:SER:O	1:D:435:VAL:HG23	2.20	0.42
1:D:495:MET:HB3	1:D:495:MET:HE2	1.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:503:LEU:O	1:H:532:MET:HA	2.19	0.42
1:H:611:ASP:OD2	1:H:611:ASP:C	2.61	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:218:GLY:O	1:C:219:ARG:C	2.63	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: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:350:ASN:O	1:A:350:ASN:CG	2.63	0.42
1:A:732:VAL:HG23	1:A:733:ALA:N	2.34	0.42
1:C:488:LEU:HD22	1:C:528:PHE:HE1	1.84	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:F:757:LEU:C	1:F:757:LEU:HD23	2.44	0.42
1:H:218:GLY:O	1:H:219:ARG:C	2.63	0.42
1:H:431:SER:O	1:H:435:VAL:HG23	2.19	0.42
1:H:519:SER:O	1:H:520:ALA:C	2.62	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:D:551:GLY:H	1:D:682:ASP:CG	2.27	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:A:250:GLU:CD	1:A:250:GLU:N	2.77	0.42
1:C:129:GLY:O	1:C:130:SER:C	2.63	0.42
1:F:430:ARG:HD2	1:F:466:VAL:O	2.20	0.42
1:F:534:MET:HE1	1:F:543:VAL:HG11	2.01	0.42
1:G:108:LEU:HG	1:G:144:LEU:HD22	2.01	0.42
1:G:325:MET:HA	1:G:325:MET:CE	2.45	0.42
1:G:611:ASP:OD2	1:G:611:ASP:C	2.62	0.42
1:A:719:VAL:O	1:A:719:VAL:HG12	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:HG	1:B:144:LEU:HD22	2.01	0.42
1:B:218:GLY:O	1:B:219:ARG:C	2.62	0.42
1:C:416:ILE:HG12	1:C:417:ASN:N	2.35	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:179:CYS:C	1:E:181:THR:N	2.67	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:F:320:ILE:HD13	1:F:593:MET:HE3	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: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:218:GLY:O	1:D:219:ARG:C	2.63	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:218:GLY:O	1:E:219:ARG:C	2.63	0.41
1:E:319:ARG:HH22	1:E:564:ASP:CG	2.28	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:363:MET:HE2	1:G:363:MET:HB3	1.95	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:140:GLU:O	1:A:144:LEU:HG	2.20	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:515:LEU:O	1:G:516:LEU:C	2.63	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: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:A:665:ARG:HD2	1:B:672:MET:HE1	2.02	0.41
1:B:30:LEU:HD12	1:B:30:LEU:C	2.46	0.41
1:C:262:ARG:HG2	1:C:262:ARG:NH1	2.33	0.41
1:D:350:ASN:CG	1:D:350:ASN:O	2.62	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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:350:ASN:CG	1:H:350:ASN:O	2.63	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
1:A:277:ASP:O	1:A:279:GLN:N	2.53	0.41
1:B:350:ASN:O	1:B:350:ASN:CG	2.63	0.41
1:B:484:PRO:HG2	1:B:517:GLU:OE1	2.20	0.41
1:C:363:MET:HE2	1:C:363:MET:HB3	1.96	0.41
1:C:732:VAL:HG23	1:C:733:ALA:N	2.36	0.41
1:D:30:LEU:C	1:D:30:LEU:HD12	2.46	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: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: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: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:495:MET:HE2	1:A:495:MET:HB3	1.94	0.41
1:A:615:LEU:HD12	1:A:615:LEU:HA	1.91	0.41
1:B:611:ASP:OD2	1:B:611:ASP:C	2.62	0.41
1:B:736:LYS:HA	1:B:739:THR:CG2	2.51	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:334:LEU:C	1:E:336:ALA:H	2.28	0.41
1:E:481:ARG:HH11	1:E:481:ARG:CB	2.32	0.41
1:F:30:LEU:C	1:F:30:LEU:HD12	2.45	0.41
1:H:519:SER:HB2	1:H:717:ILE:HD12	2.01	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:E:416:ILE:HD11	1:E:449:GLY:C	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:534:MET:HE1	1:G:543:VAL:HG13	2.02	0.41
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:255:LYS:HZ2	1:B:399:ILE:HA	1.86	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: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:42:ALA:HB1	1:E:170:MET:HE1	2.02	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:495:MET:HE3	1:G:500:ILE:HB	2.03	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: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: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:646:THR:HG23	1:G:652:GLN:NE2	2.36	0.41
1:G:218:GLY:O	1:G:219:ARG:C	2.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:GLY:O	1:B:727:VAL:HA	2.22	0.40
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: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:277:ASP:C	1:A:279:GLN:N	2.79	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: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:E:350:ASN:O	1:E:350:ASN:CG	2.63	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:H:30:LEU:C	1:H:30:LEU:HD12	2.46	0.40
1:H:250:GLU:CD	1:H:250:GLU:N	2.79	0.40
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.82	0.40
1:B:155:ASP:OD2	1:B:156:LYS:N	2.55	0.40
1:C:702:LYS:C	1:C:703:GLU:OE2	2.65	0.40
1:D:64:TYR:OH	1:D:134:ALA:HB2	2.22	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:129:GLY:O	1:G:130:SER:C	2.63	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:H:750:TRP:CG	1:H:751:TRP:N	2.89	0.40
1:A:195:ILE:HD13	1:A:195:ILE:HA	1.93	0.40
1:A:255:LYS:HZ1	1:A:399:ILE:HA	1.87	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ASN:C	1:E:176:ASN:HD22	2.29	0.40
1:F:166:ASN:OD1	1:F:336:ALA:CB	2.69	0.40
1:F:304:ILE:O	1:F:305:LEU:C	2.65	0.40
1:G:30:LEU:HD12	1:G:30:LEU:C	2.46	0.40
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: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:484:PRO:O	1:D:485:GLY:C	2.65	0.40
1:D:490:GLU:OE1	1:D:490:GLU:N	2.47	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: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%)	30	61
1	B	766/812 (94%)	699 (91%)	60 (8%)	7 (1%)	14	44
1	C	756/812 (93%)	686 (91%)	62 (8%)	8 (1%)	11	39
1	D	757/812 (93%)	694 (92%)	57 (8%)	6 (1%)	16	47
1	E	761/812 (94%)	697 (92%)	58 (8%)	6 (1%)	16	47
1	F	757/812 (93%)	691 (91%)	60 (8%)	6 (1%)	16	47
1	G	756/812 (93%)	693 (92%)	58 (8%)	5 (1%)	18	49
1	H	735/812 (90%)	672 (91%)	59 (8%)	4 (0%)	24	57
All	All	6054/6496 (93%)	5538 (92%)	471 (8%)	45 (1%)	18	49

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 ⓘ

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%)	569 (92%)	50 (8%)	11	36
1	B	619/658 (94%)	564 (91%)	55 (9%)	9	33
1	C	614/658 (93%)	569 (93%)	45 (7%)	13	40
1	D	614/658 (93%)	563 (92%)	51 (8%)	10	35
1	E	617/658 (94%)	567 (92%)	50 (8%)	11	36
1	F	614/658 (93%)	560 (91%)	54 (9%)	9	33
1	G	614/658 (93%)	563 (92%)	51 (8%)	10	35
1	H	594/658 (90%)	546 (92%)	48 (8%)	11	36
All	All	4905/5264 (93%)	4501 (92%)	404 (8%)	10	36

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	43	VAL
1	A	65	GLN
1	A	80	GLU
1	A	91	THR
1	A	115	LEU
1	A	131	LEU
1	A	156	LYS
1	A	165	LEU
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	291	LEU
1	A	295	GLN
1	A	303	THR
1	A	325	MET
1	A	347	LEU
1	A	354	ARG
1	A	362	GLN
1	A	368	GLN
1	A	396	ARG
1	A	461	ILE
1	A	470	THR
1	A	472	GLN
1	A	489	GLU
1	A	494	GLN
1	A	510	GLU
1	A	526	GLU
1	A	533	VAL
1	A	534	MET
1	A	538	THR
1	A	556	LEU
1	A	566	ILE
1	A	575	ARG
1	A	628	THR
1	A	631	GLN
1	A	632	ARG
1	A	683	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	689	ILE
1	A	705	ARG
1	A	712	THR
1	A	739	THR
1	A	757	LEU
1	A	772	ASP
1	A	776	LEU
1	B	14	ARG
1	B	20	LEU
1	B	43	VAL
1	B	65	GLN
1	B	80	GLU
1	B	91	THR
1	B	93	ILE
1	B	115	LEU
1	B	131	LEU
1	B	156	LYS
1	B	157	GLU
1	B	165	LEU
1	B	182	ASP
1	B	183	MET
1	B	191	LEU
1	B	224	LEU
1	B	250	GLU
1	B	260	ARG
1	B	291	LEU
1	B	295	GLN
1	B	303	THR
1	B	325	MET
1	B	347	LEU
1	B	362	GLN
1	B	368	GLN
1	B	374	ARG
1	B	386	SER
1	B	396	ARG
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	510	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	524	LYS
1	B	533	VAL
1	B	538	THR
1	B	556	LEU
1	B	566	ILE
1	B	628	THR
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	B	780	GLN
1	C	14	ARG
1	C	17	LEU
1	C	43	VAL
1	C	65	GLN
1	C	80	GLU
1	C	105	GLU
1	C	115	LEU
1	C	131	LEU
1	C	136	LEU
1	C	156	LYS
1	C	157	GLU
1	C	165	LEU
1	C	183	MET
1	C	191	LEU
1	C	224	LEU
1	C	245	GLU
1	C	250	GLU
1	C	260	ARG
1	C	291	LEU
1	C	295	GLN
1	C	303	THR
1	C	325	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	347	LEU
1	C	362	GLN
1	C	368	GLN
1	C	461	ILE
1	C	470	THR
1	C	481	ARG
1	C	494	GLN
1	C	510	GLU
1	C	530	VAL
1	C	533	VAL
1	C	538	THR
1	C	556	LEU
1	C	566	ILE
1	C	628	THR
1	C	631	GLN
1	C	632	ARG
1	C	683	ARG
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	65	GLN
1	D	80	GLU
1	D	91	THR
1	D	93	ILE
1	D	99	GLN
1	D	115	LEU
1	D	131	LEU
1	D	156	LYS
1	D	160	GLN
1	D	165	LEU
1	D	183	MET
1	D	191	LEU
1	D	224	LEU
1	D	230	LEU
1	D	254	VAL
1	D	255	LYS
1	D	260	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	268	ILE
1	D	291	LEU
1	D	295	GLN
1	D	303	THR
1	D	325	MET
1	D	347	LEU
1	D	362	GLN
1	D	368	GLN
1	D	374	ARG
1	D	396	ARG
1	D	461	ILE
1	D	470	THR
1	D	472	GLN
1	D	494	GLN
1	D	495	MET
1	D	510	GLU
1	D	522	ARG
1	D	533	VAL
1	D	538	THR
1	D	556	LEU
1	D	566	ILE
1	D	568	GLN
1	D	628	THR
1	D	631	GLN
1	D	632	ARG
1	D	683	ARG
1	D	689	ILE
1	D	692	ARG
1	D	737	LYS
1	D	739	THR
1	D	757	LEU
1	D	772	ASP
1	E	14	ARG
1	E	17	LEU
1	E	20	LEU
1	E	43	VAL
1	E	65	GLN
1	E	80	GLU
1	E	115	LEU
1	E	131	LEU
1	E	156	LYS
1	E	157	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	165	LEU
1	E	183	MET
1	E	191	LEU
1	E	224	LEU
1	E	230	LEU
1	E	260	ARG
1	E	291	LEU
1	E	295	GLN
1	E	301	ARG
1	E	303	THR
1	E	325	MET
1	E	347	LEU
1	E	362	GLN
1	E	368	GLN
1	E	396	ARG
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	556	LEU
1	E	566	ILE
1	E	574	LYS
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	719	VAL
1	E	739	THR
1	E	757	LEU
1	E	772	ASP
1	E	780	GLN
1	F	20	LEU
1	F	43	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	65	GLN
1	F	80	GLU
1	F	115	LEU
1	F	131	LEU
1	F	156	LYS
1	F	165	LEU
1	F	176	ASN
1	F	191	LEU
1	F	224	LEU
1	F	230	LEU
1	F	250	GLU
1	F	260	ARG
1	F	291	LEU
1	F	295	GLN
1	F	303	THR
1	F	325	MET
1	F	347	LEU
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	461	ILE
1	F	470	THR
1	F	481	ARG
1	F	482	VAL
1	F	501	ASN
1	F	510	GLU
1	F	524	LYS
1	F	525	HIS
1	F	533	VAL
1	F	538	THR
1	F	556	LEU
1	F	566	ILE
1	F	568	GLN
1	F	628	THR
1	F	631	GLN
1	F	632	ARG
1	F	672	MET
1	F	683	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	43	VAL
1	G	65	GLN
1	G	80	GLU
1	G	93	ILE
1	G	115	LEU
1	G	131	LEU
1	G	139	LYS
1	G	160	GLN
1	G	165	LEU
1	G	183	MET
1	G	191	LEU
1	G	224	LEU
1	G	230	LEU
1	G	250	GLU
1	G	260	ARG
1	G	291	LEU
1	G	295	GLN
1	G	325	MET
1	G	347	LEU
1	G	358	MET
1	G	359	GLU
1	G	368	GLN
1	G	369	LYS
1	G	373	GLU
1	G	385	ARG
1	G	396	ARG
1	G	461	ILE
1	G	470	THR
1	G	482	VAL
1	G	526	GLU
1	G	533	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	538	THR
1	G	556	LEU
1	G	566	ILE
1	G	574	LYS
1	G	628	THR
1	G	631	GLN
1	G	632	ARG
1	G	669	LEU
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
1	G	778	HIS
1	G	779	VAL
1	H	43	VAL
1	H	49	MET
1	H	65	GLN
1	H	80	GLU
1	H	87	GLN
1	H	93	ILE
1	H	115	LEU
1	H	131	LEU
1	H	156	LYS
1	H	160	GLN
1	H	165	LEU
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	291	LEU
1	H	295	GLN
1	H	325	MET
1	H	347	LEU
1	H	362	GLN
1	H	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	385	ARG
1	H	396	ARG
1	H	461	ILE
1	H	470	THR
1	H	472	GLN
1	H	482	VAL
1	H	487	TYR
1	H	495	MET
1	H	510	GLU
1	H	533	VAL
1	H	538	THR
1	H	556	LEU
1	H	566	ILE
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
1	H	712	THR
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 (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	99	GLN
1	A	116	GLN
1	A	151	ASN
1	A	153	GLN
1	A	176	ASN
1	A	192	HIS
1	A	307	HIS
1	A	377	GLN
1	A	417	ASN
1	A	494	GLN
1	A	498	HIS
1	A	616	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	618	ASN
1	A	652	GLN
1	A	671	HIS
1	A	674	GLN
1	A	684	ASN
1	A	778	HIS
1	B	65	GLN
1	B	99	GLN
1	B	116	GLN
1	B	135	ASN
1	B	153	GLN
1	B	176	ASN
1	B	192	HIS
1	B	390	ASN
1	B	417	ASN
1	B	494	GLN
1	B	498	HIS
1	B	568	GLN
1	B	616	GLN
1	B	618	ASN
1	B	652	GLN
1	B	671	HIS
1	B	674	GLN
1	B	684	ASN
1	C	19	HIS
1	C	65	GLN
1	C	99	GLN
1	C	116	GLN
1	C	135	ASN
1	C	151	ASN
1	C	176	ASN
1	C	192	HIS
1	C	417	ASN
1	C	525	HIS
1	C	568	GLN
1	C	618	ASN
1	C	652	GLN
1	C	671	HIS
1	C	674	GLN
1	C	684	ASN
1	C	778	HIS
1	D	19	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	65	GLN
1	D	99	GLN
1	D	116	GLN
1	D	135	ASN
1	D	151	ASN
1	D	153	GLN
1	D	176	ASN
1	D	192	HIS
1	D	208	HIS
1	D	307	HIS
1	D	348	ASN
1	D	417	ASN
1	D	494	GLN
1	D	525	HIS
1	D	568	GLN
1	D	618	ASN
1	D	644	ASN
1	D	652	GLN
1	D	673	GLN
1	D	684	ASN
1	D	780	GLN
1	E	65	GLN
1	E	99	GLN
1	E	116	GLN
1	E	135	ASN
1	E	151	ASN
1	E	153	GLN
1	E	176	ASN
1	E	192	HIS
1	E	307	HIS
1	E	348	ASN
1	E	410	ASN
1	E	417	ASN
1	E	494	GLN
1	E	498	HIS
1	E	568	GLN
1	E	616	GLN
1	E	652	GLN
1	E	673	GLN
1	E	674	GLN
1	E	684	ASN
1	F	65	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	99	GLN
1	F	151	ASN
1	F	153	GLN
1	F	192	HIS
1	F	220	HIS
1	F	307	HIS
1	F	417	ASN
1	F	472	GLN
1	F	494	GLN
1	F	498	HIS
1	F	568	GLN
1	F	652	GLN
1	F	674	GLN
1	F	684	ASN
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	176	ASN
1	G	192	HIS
1	G	368	GLN
1	G	417	ASN
1	G	494	GLN
1	G	498	HIS
1	G	568	GLN
1	G	616	GLN
1	G	618	ASN
1	G	684	ASN
1	H	65	GLN
1	H	87	GLN
1	H	99	GLN
1	H	116	GLN
1	H	135	ASN
1	H	151	ASN
1	H	153	GLN
1	H	176	ASN
1	H	192	HIS
1	H	417	ASN
1	H	498	HIS
1	H	568	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	618	ASN
1	H	652	GLN
1	H	673	GLN
1	H	674	GLN
1	H	684	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	ATP	E	801	3	32,33,33	1.40	3 (9%)	48,52,52	1.69	7 (14%)
4	PO4	C	804	-	4,4,4	1.67	0	6,6,6	0.49	0
4	PO4	G	804	-	4,4,4	1.61	0	6,6,6	0.46	0
4	PO4	D	803	-	4,4,4	1.74	2 (50%)	6,6,6	0.43	0
4	PO4	G	805	-	4,4,4	1.67	0	6,6,6	0.47	0
4	PO4	A	805	-	4,4,4	1.69	0	6,6,6	0.47	0
2	ATP	F	801	3	32,33,33	1.85	4 (12%)	48,52,52	1.69	10 (20%)
4	PO4	A	804	-	4,4,4	1.65	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	G	801	3	32,33,33	1.60	5 (15%)	48,52,52	1.66	7 (14%)
4	PO4	F	805	-	4,4,4	1.67	0	6,6,6	0.47	0
4	PO4	F	804	-	4,4,4	1.63	0	6,6,6	0.46	0
2	ATP	A	801	3	32,33,33	1.30	4 (12%)	48,52,52	1.75	13 (27%)
4	PO4	H	804	-	4,4,4	1.70	1 (25%)	6,6,6	0.44	0
4	PO4	B	804	-	4,4,4	1.65	1 (25%)	6,6,6	0.46	0
4	PO4	B	805	-	4,4,4	1.67	1 (25%)	6,6,6	0.46	0
4	PO4	E	804	-	4,4,4	1.70	2 (50%)	6,6,6	0.46	0
2	ATP	H	801	3	32,33,33	1.48	5 (15%)	48,52,52	1.71	9 (18%)
2	ATP	C	801	3	32,33,33	1.20	3 (9%)	48,52,52	1.62	7 (14%)
2	ATP	B	801	3	32,33,33	1.48	6 (18%)	48,52,52	1.77	9 (18%)
2	ATP	D	801	3	32,33,33	1.46	5 (15%)	48,52,52	1.73	8 (16%)

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	E	801	3	-	1/22/38/38	0/3/3/3
2	ATP	F	801	3	-	1/22/38/38	0/3/3/3
2	ATP	G	801	3	-	3/22/38/38	0/3/3/3
2	ATP	H	801	3	-	1/22/38/38	0/3/3/3
2	ATP	C	801	3	-	2/22/38/38	0/3/3/3
2	ATP	A	801	3	-	0/22/38/38	0/3/3/3
2	ATP	B	801	3	-	0/22/38/38	0/3/3/3
2	ATP	D	801	3	-	1/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	ATP	PB-O3B	6.21	1.66	1.59
2	F	801	ATP	PA-O3A	4.30	1.64	1.59
2	G	801	ATP	PB-O3B	4.22	1.64	1.59
2	A	801	ATP	PG-O1G	3.54	1.61	1.50
2	F	801	ATP	PG-O1G	3.51	1.61	1.50
2	B	801	ATP	C5-N7	-3.45	1.32	1.39
2	H	801	ATP	PG-O1G	3.44	1.61	1.50
2	H	801	ATP	C5-N7	-3.30	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	ATP	C5-N7	-3.29	1.33	1.39
2	D	801	ATP	PA-O1A	3.17	1.61	1.50
2	B	801	ATP	PB-O1B	3.16	1.61	1.50
2	G	801	ATP	C5-N7	-3.13	1.33	1.39
2	G	801	ATP	PB-O1B	3.10	1.61	1.50
2	B	801	ATP	PA-O1A	3.08	1.61	1.50
2	G	801	ATP	PA-O1A	3.07	1.61	1.50
2	F	801	ATP	C5-N7	-3.03	1.33	1.39
2	E	801	ATP	PB-O1B	3.00	1.61	1.50
2	D	801	ATP	C5-N7	-2.98	1.33	1.39
2	E	801	ATP	PA-O1A	2.91	1.60	1.50
2	H	801	ATP	PB-O3B	2.89	1.62	1.59
2	D	801	ATP	PB-O1B	2.84	1.60	1.50
2	C	801	ATP	C5-N7	-2.77	1.34	1.39
2	B	801	ATP	PA-O3A	2.70	1.62	1.59
2	D	801	ATP	PA-O3A	2.64	1.62	1.59
2	A	801	ATP	PG-O3G	2.46	1.63	1.54
2	H	801	ATP	C1'-N9	2.35	1.52	1.46
2	H	801	ATP	O4'-C1'	2.32	1.47	1.42
2	A	801	ATP	C5-N7	-2.25	1.35	1.39
2	G	801	ATP	PB-O3A	2.19	1.61	1.59
2	C	801	ATP	PG-O3G	2.18	1.62	1.54
4	B	804	PO4	P-O3	-2.18	1.48	1.54
2	D	801	ATP	PG-O2G	2.15	1.62	1.54
2	A	801	ATP	O4'-C1'	2.15	1.47	1.42
2	B	801	ATP	PG-O3G	2.14	1.62	1.54
2	B	801	ATP	C4-N9	-2.09	1.33	1.37
4	H	804	PO4	P-O4	-2.08	1.48	1.54
4	B	805	PO4	P-O2	-2.06	1.48	1.54
4	E	804	PO4	P-O2	-2.06	1.48	1.54
4	D	803	PO4	P-O4	-2.05	1.48	1.54
2	C	801	ATP	PA-O3A	2.05	1.61	1.59
4	D	803	PO4	P-O3	-2.03	1.48	1.54
4	E	804	PO4	P-O4	-2.01	1.48	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	ATP	N3-C2-N1	-5.42	120.38	128.58
2	D	801	ATP	C5-C4-N3	-5.30	119.42	126.72
2	F	801	ATP	N3-C2-N1	-5.26	120.61	128.58
2	H	801	ATP	N3-C2-N1	-5.19	120.72	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ATP	C5-C4-N3	-5.16	119.62	126.72
2	C	801	ATP	N3-C2-N1	-5.11	120.85	128.58
2	H	801	ATP	C5-C4-N3	-5.10	119.69	126.72
2	A	801	ATP	N3-C2-N1	-5.10	120.87	128.58
2	D	801	ATP	N3-C2-N1	-5.07	120.91	128.58
2	E	801	ATP	N3-C2-N1	-5.06	120.93	128.58
2	B	801	ATP	N3-C2-N1	-5.04	120.96	128.58
2	E	801	ATP	C5-C4-N3	-5.03	119.78	126.72
2	B	801	ATP	C5-C4-N3	-4.87	120.02	126.72
2	A	801	ATP	C5-C4-N3	-4.72	120.22	126.72
2	G	801	ATP	C5-C4-N3	-4.56	120.43	126.72
2	F	801	ATP	C5-C4-N3	-4.55	120.46	126.72
2	C	801	ATP	N3-C4-N9	4.04	134.03	127.17
2	D	801	ATP	N3-C4-N9	4.01	133.99	127.17
2	H	801	ATP	N3-C4-N9	3.85	133.72	127.17
2	E	801	ATP	C2-N3-C4	3.75	121.00	111.83
2	C	801	ATP	C2-N3-C4	3.74	120.98	111.83
2	D	801	ATP	C2-N3-C4	3.72	120.93	111.83
2	E	801	ATP	N3-C4-N9	3.72	133.49	127.17
2	H	801	ATP	C2-N3-C4	3.72	120.91	111.83
2	G	801	ATP	C2-N3-C4	3.66	120.76	111.83
2	B	801	ATP	C2-N3-C4	3.64	120.71	111.83
2	F	801	ATP	C2-N3-C4	3.62	120.67	111.83
2	B	801	ATP	N3-C4-N9	3.61	133.30	127.17
2	A	801	ATP	C2-N3-C4	3.56	120.53	111.83
2	G	801	ATP	N3-C4-N9	3.55	133.21	127.17
2	A	801	ATP	N3-C4-N9	3.43	133.00	127.17
2	B	801	ATP	C2'-C1'-N9	-3.35	104.98	113.30
2	F	801	ATP	N3-C4-N9	3.28	132.75	127.17
2	A	801	ATP	C2'-C1'-N9	-3.22	105.30	113.30
2	F	801	ATP	N9-C8-N7	-2.91	109.81	113.94
2	H	801	ATP	C5-N7-C8	2.81	107.86	103.45
2	F	801	ATP	C2'-C1'-N9	-2.76	106.44	113.30
2	A	801	ATP	N9-C8-N7	-2.75	110.03	113.94
2	C	801	ATP	C5-N7-C8	2.75	107.77	103.45
2	B	801	ATP	N9-C8-N7	-2.71	110.09	113.94
2	E	801	ATP	C5-N7-C8	2.68	107.67	103.45
2	A	801	ATP	O2G-PG-O3B	2.64	113.50	104.64
2	D	801	ATP	C5-N7-C8	2.64	107.60	103.45
2	A	801	ATP	C5-N7-C8	2.60	107.54	103.45
2	C	801	ATP	N9-C8-N7	-2.58	110.27	113.94
2	A	801	ATP	C4-C5-N7	-2.57	107.64	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	ATP	N9-C8-N7	-2.56	110.31	113.94
2	H	801	ATP	N9-C8-N7	-2.54	110.33	113.94
2	F	801	ATP	C5-N7-C8	2.54	107.44	103.45
2	B	801	ATP	C5-N7-C8	2.53	107.43	103.45
2	E	801	ATP	N9-C8-N7	-2.49	110.40	113.94
2	E	801	ATP	C4-C5-N7	-2.37	107.87	110.58
2	D	801	ATP	N9-C8-N7	-2.36	110.59	113.94
2	C	801	ATP	C4-C5-N7	-2.35	107.90	110.58
2	G	801	ATP	C5-N7-C8	2.33	107.11	103.45
2	F	801	ATP	O2G-PG-O3B	2.32	112.41	104.64
2	F	801	ATP	C4-C5-N7	-2.25	108.01	110.58
2	B	801	ATP	C4-C5-N7	-2.24	108.02	110.58
2	H	801	ATP	O3G-PG-O3B	2.23	112.11	104.64
2	A	801	ATP	O4'-C1'-N9	2.18	112.28	108.09
2	D	801	ATP	C4-C5-N7	-2.17	108.11	110.58
2	A	801	ATP	C4-N9-C8	2.15	108.00	105.74
2	G	801	ATP	C2'-C1'-N9	-2.15	107.96	113.30
2	H	801	ATP	C4-C5-N7	-2.15	108.13	110.58
2	D	801	ATP	C2'-C1'-N9	-2.14	107.99	113.30
2	B	801	ATP	O4'-C1'-N9	2.11	112.13	108.09
2	F	801	ATP	C4-N9-C8	2.10	107.95	105.74
2	A	801	ATP	C2'-C3'-C4'	-2.09	98.57	102.61
2	H	801	ATP	C2'-C3'-C4'	-2.04	98.67	102.61
2	A	801	ATP	C2-N1-C6	2.03	122.07	118.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

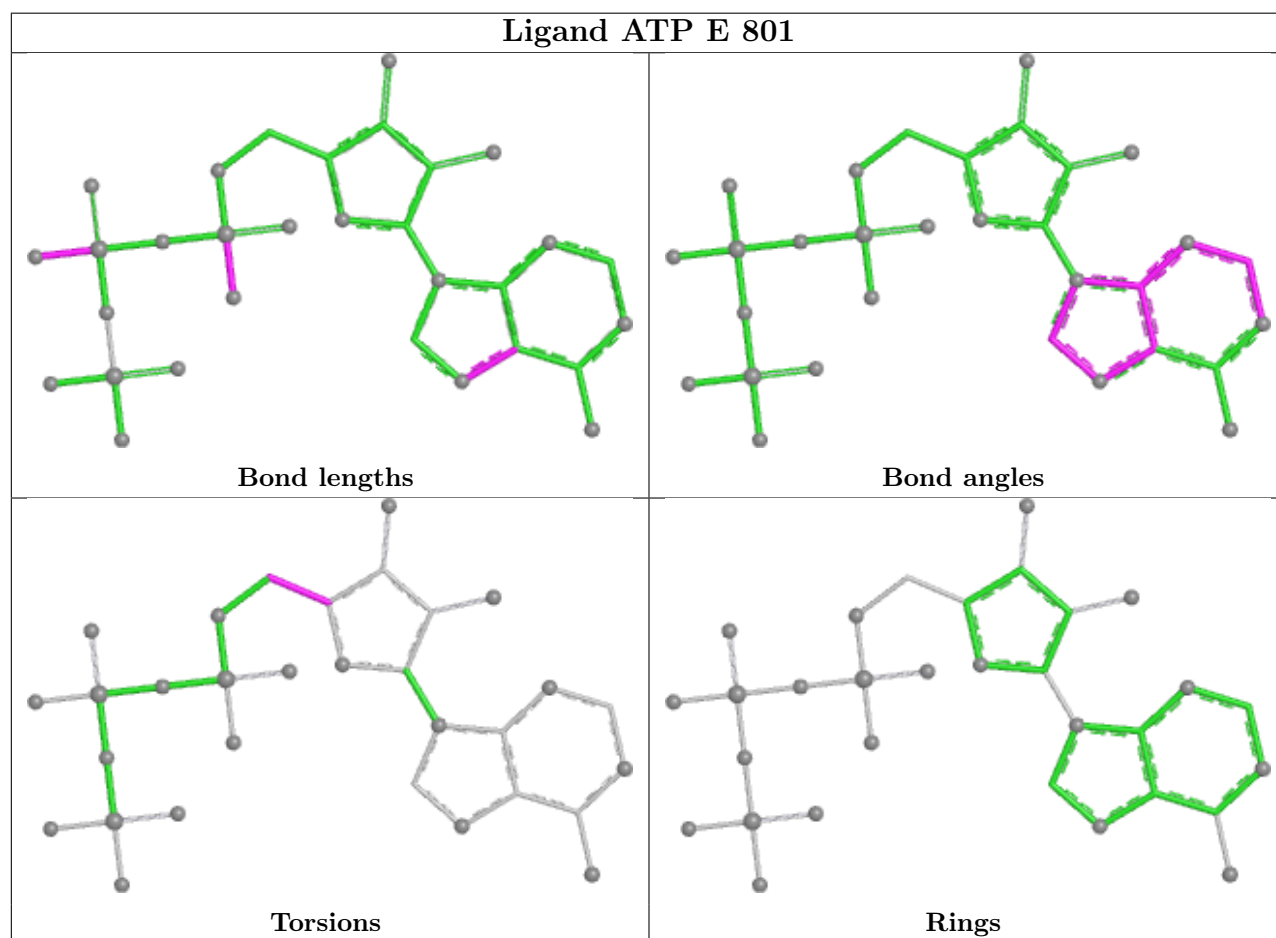
Mol	Chain	Res	Type	Atoms
2	G	801	ATP	O4'-C4'-C5'-O5'
2	G	801	ATP	C3'-C4'-C5'-O5'
2	C	801	ATP	O4'-C4'-C5'-O5'
2	C	801	ATP	C3'-C4'-C5'-O5'
2	D	801	ATP	O4'-C4'-C5'-O5'
2	E	801	ATP	O4'-C4'-C5'-O5'
2	G	801	ATP	C4'-C5'-O5'-PA
2	F	801	ATP	C5'-O5'-PA-O1A
2	H	801	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

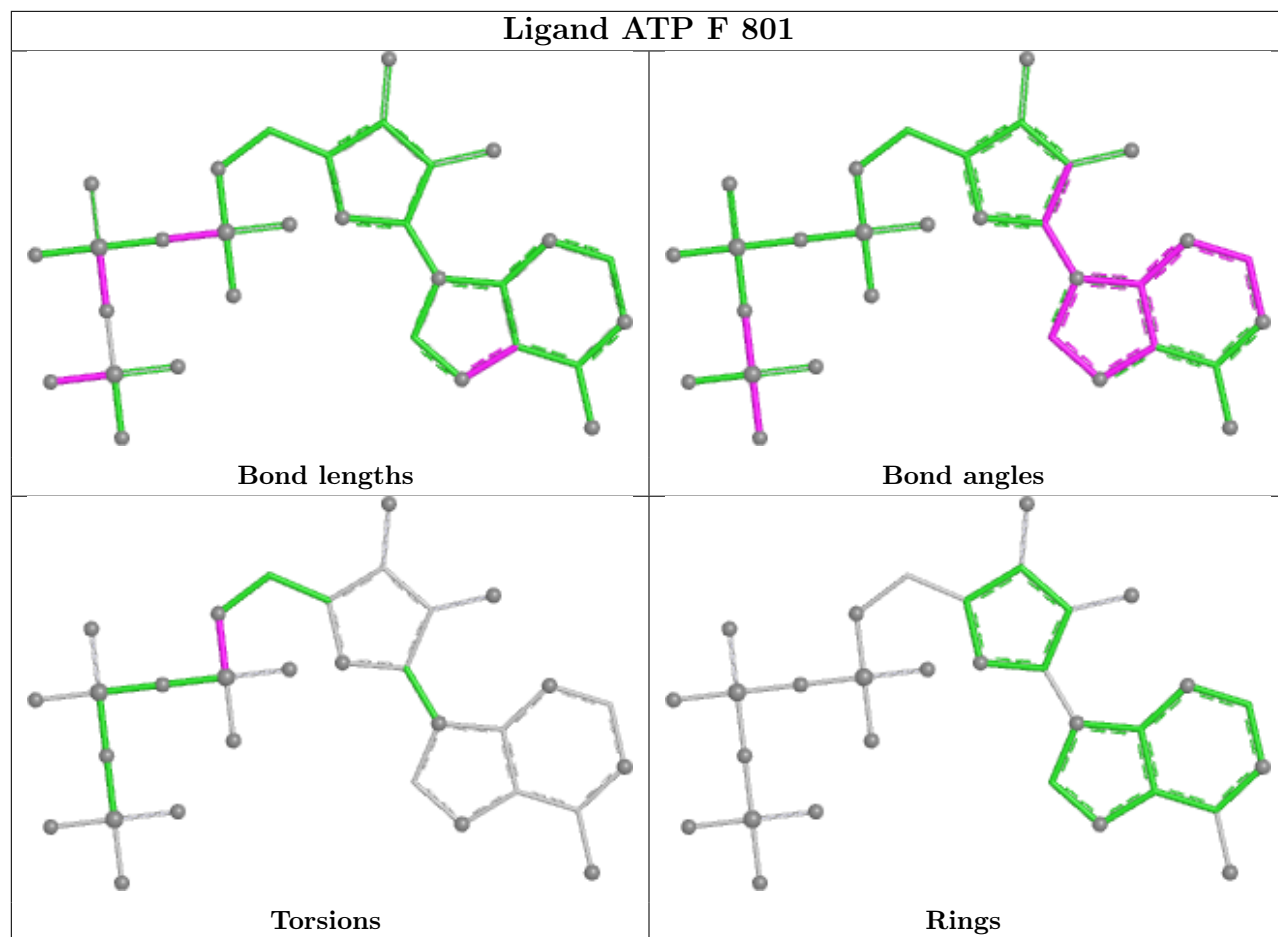
1 monomer is involved in 1 short contact:

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

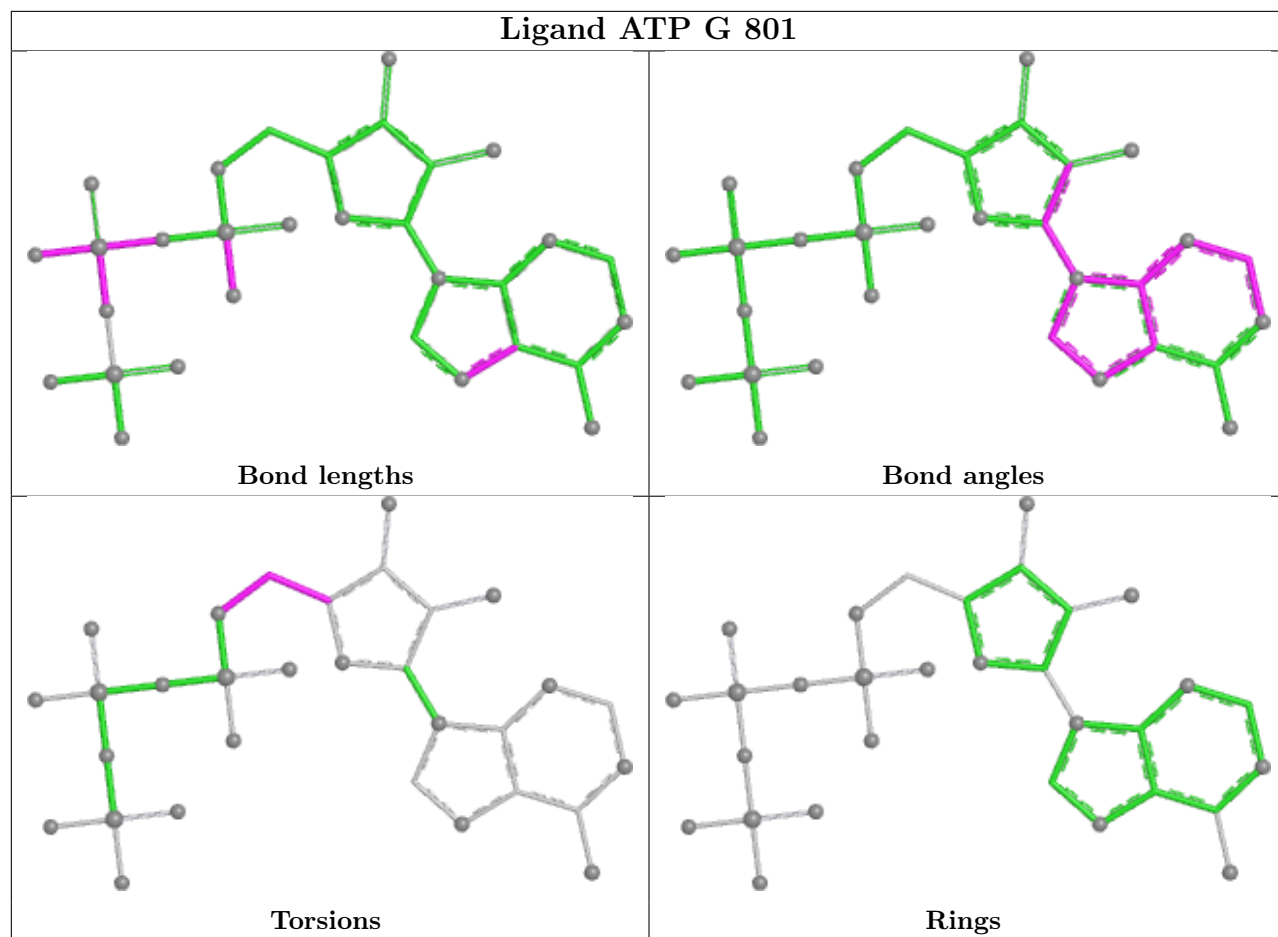
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



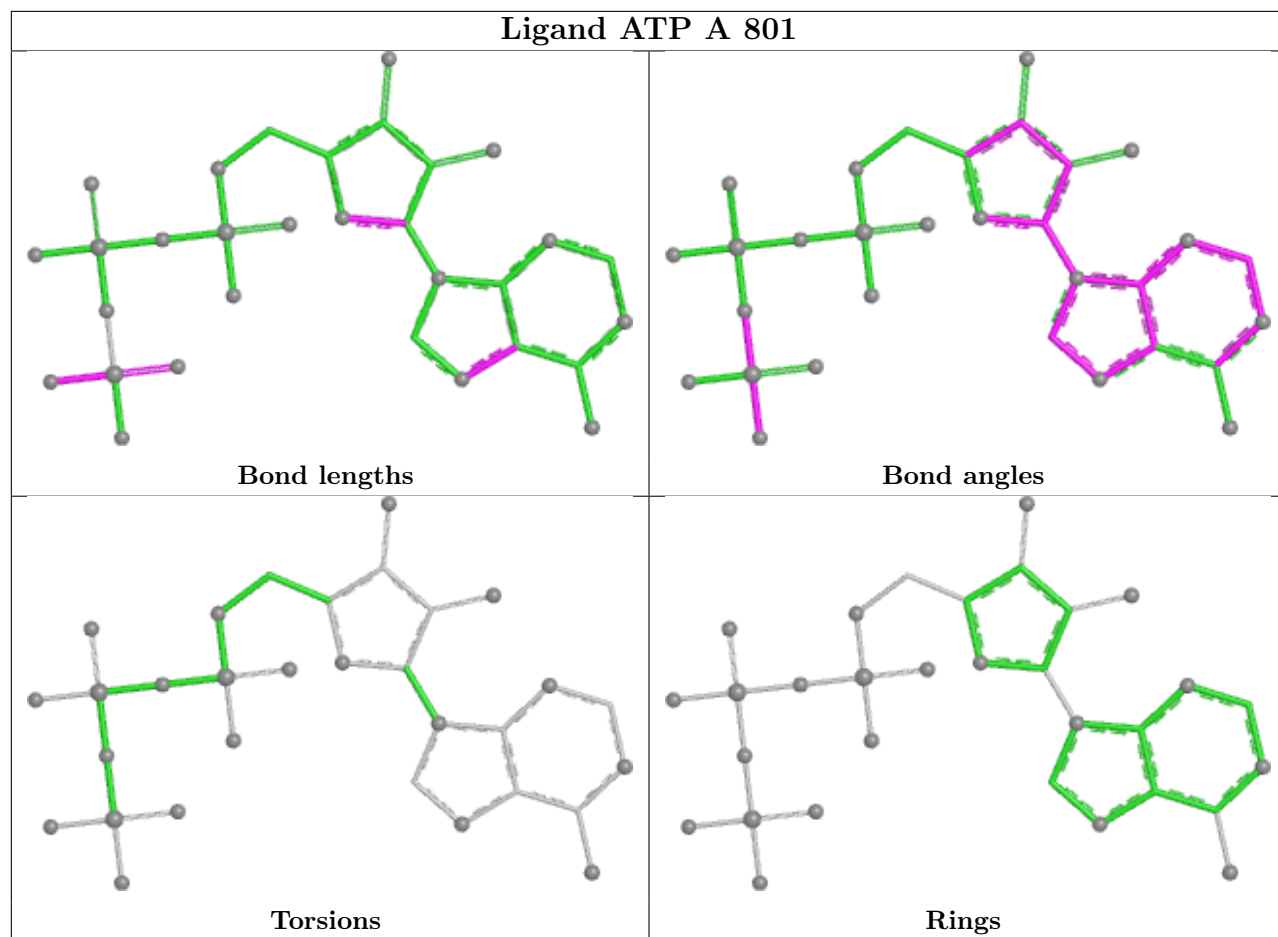
Ligand ATP F 801

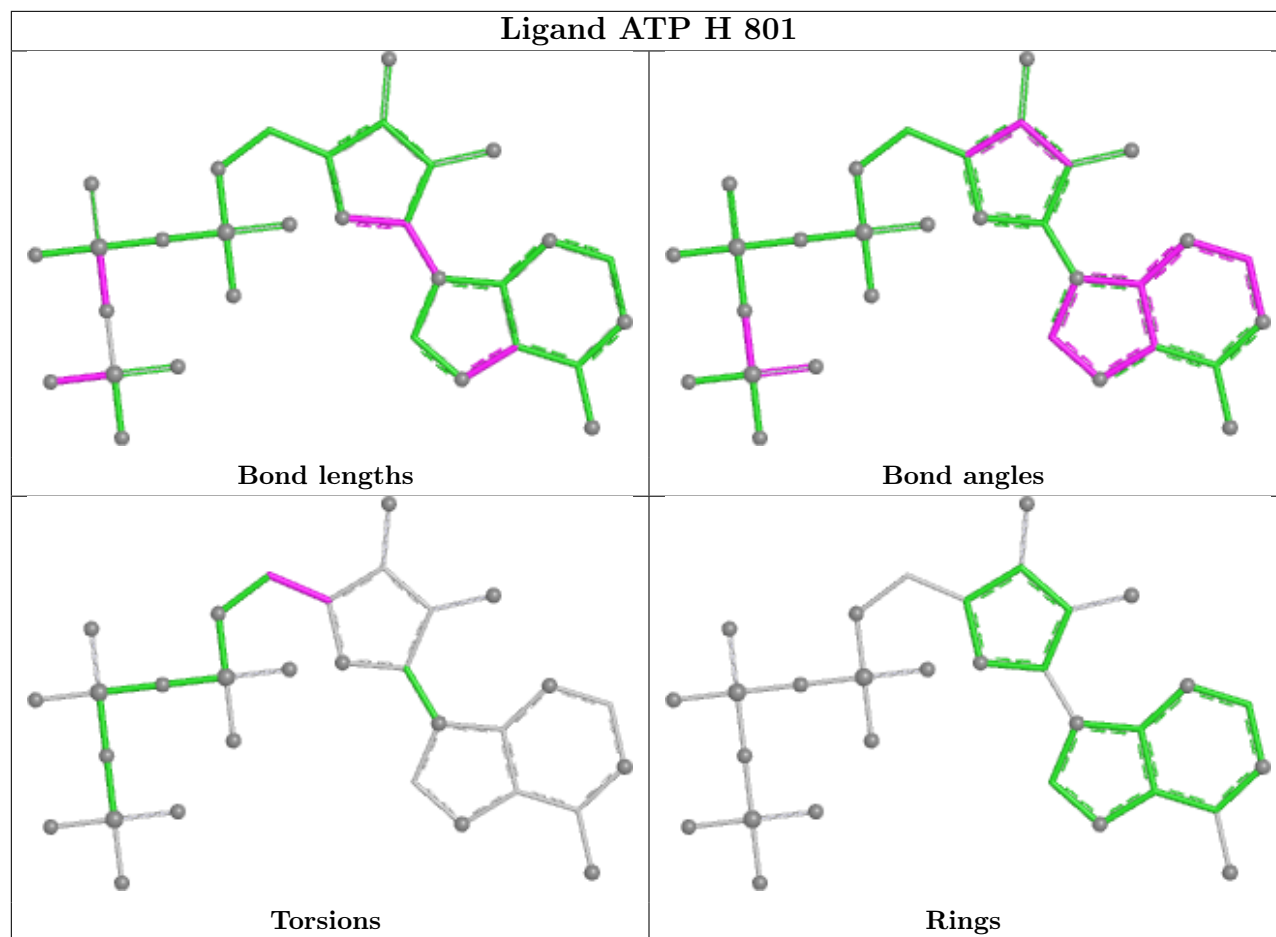


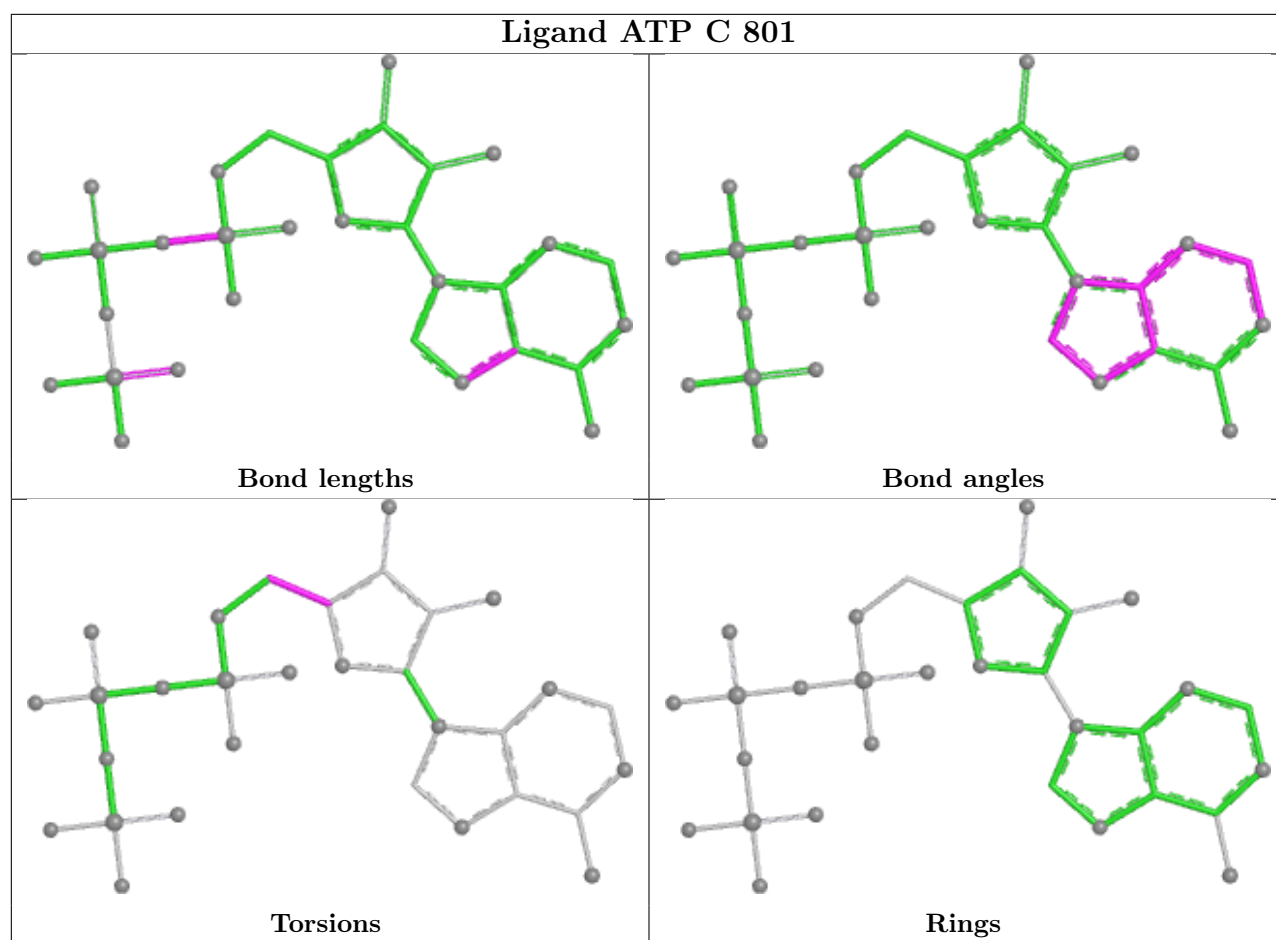
Ligand ATP G 801



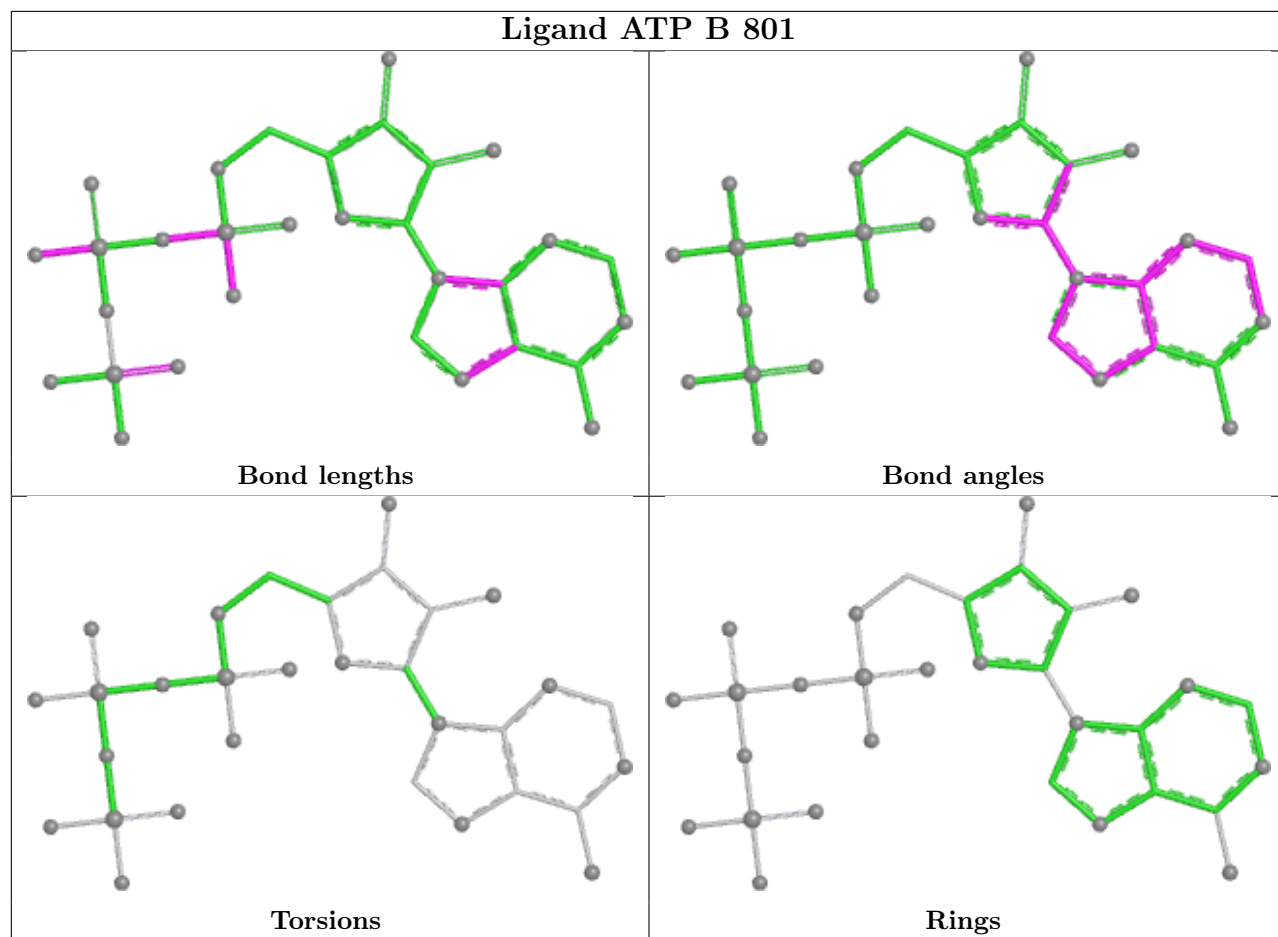
Ligand ATP A 801

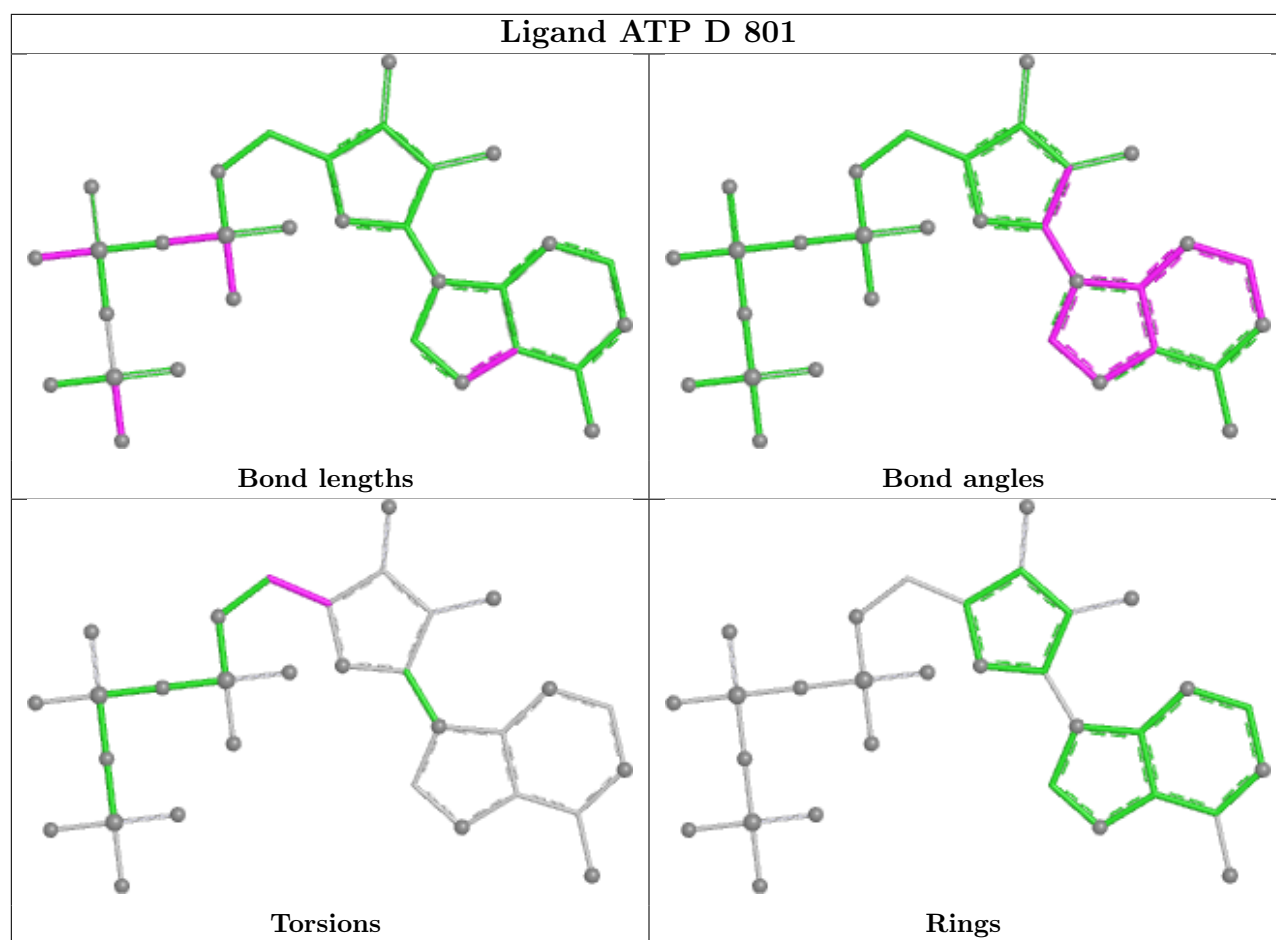






Ligand ATP B 801





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	768/812 (94%)	0.07	3 (0%) 88 76	25, 56, 83, 113	0
1	B	768/812 (94%)	0.19	10 (1%) 75 56	26, 55, 83, 114	0
1	C	760/812 (93%)	0.13	6 (0%) 82 65	36, 62, 93, 114	0
1	D	761/812 (93%)	-0.02	2 (0%) 90 80	36, 59, 86, 113	0
1	E	765/812 (94%)	0.01	3 (0%) 88 76	37, 59, 86, 114	0
1	F	761/812 (93%)	0.06	3 (0%) 88 76	36, 60, 86, 114	0
1	G	760/812 (93%)	0.04	6 (0%) 82 65	36, 62, 89, 113	0
1	H	739/812 (91%)	0.09	4 (0%) 87 73	38, 61, 87, 114	0
All	All	6082/6496 (93%)	0.07	37 (0%) 85 70	25, 60, 87, 114	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	704	ALA	3.5
1	B	673	GLN	3.4
1	E	20	LEU	3.3
1	C	673	GLN	3.3
1	F	672	MET	3.1
1	H	758	MET	2.9
1	C	672	MET	2.8
1	E	672	MET	2.7
1	F	673	GLN	2.7
1	G	780	GLN	2.7
1	G	672	MET	2.6
1	A	672	MET	2.6
1	B	781	PRO	2.5
1	B	385	ARG	2.5
1	E	326	GLY	2.4
1	G	779	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	629	THR	2.3
1	H	63	GLY	2.3
1	C	180	GLY	2.3
1	B	672	MET	2.3
1	G	674	GLN	2.2
1	A	207	SER	2.2
1	A	673	GLN	2.2
1	F	704	ALA	2.2
1	B	400	LYS	2.1
1	C	164	TYR	2.1
1	H	675	GLY	2.1
1	C	718	CYS	2.1
1	B	292	VAL	2.0
1	B	723	SER	2.0
1	B	331	ILE	2.0
1	G	111	ALA	2.0
1	G	673	GLN	2.0
1	D	671	HIS	2.0
1	C	158	ALA	2.0
1	B	674	GLN	2.0
1	B	357	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	H	802	1/1	0.65	0.12	47,47,47,47	0
4	PO4	F	804	5/5	0.70	0.22	104,105,105,105	0

Continued on next page...

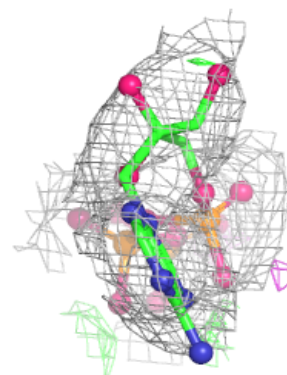
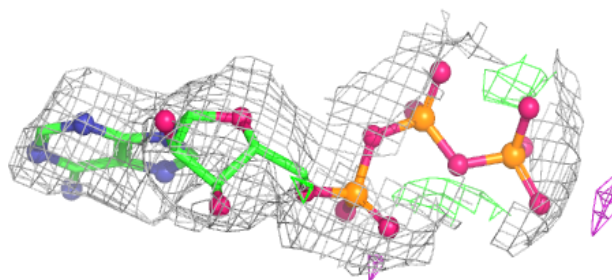
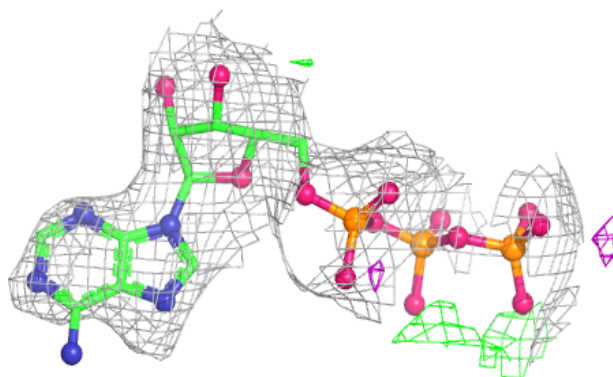
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	C	804	5/5	0.76	0.11	113,113,114,114	0
3	MG	H	803	1/1	0.77	0.11	67,67,67,67	0
4	PO4	B	805	5/5	0.79	0.17	120,120,121,121	0
4	PO4	G	804	5/5	0.79	0.11	90,91,91,92	0
3	MG	C	802	1/1	0.81	0.11	60,60,60,60	0
3	MG	D	802	1/1	0.81	0.12	37,37,37,37	0
3	MG	G	803	1/1	0.82	0.08	40,40,40,40	0
4	PO4	A	805	5/5	0.82	0.13	103,103,103,104	0
3	MG	A	802	1/1	0.82	0.10	43,43,43,43	0
4	PO4	G	805	5/5	0.84	0.11	113,113,114,114	0
3	MG	E	803	1/1	0.85	0.07	40,40,40,40	0
4	PO4	F	805	5/5	0.85	0.09	90,91,91,91	0
3	MG	F	802	1/1	0.85	0.13	54,54,54,54	0
3	MG	G	802	1/1	0.85	0.08	36,36,36,36	0
3	MG	E	802	1/1	0.87	0.11	39,39,39,39	0
2	ATP	E	801	31/31	0.89	0.11	79,88,95,95	0
2	ATP	C	801	31/31	0.90	0.10	78,86,92,93	0
4	PO4	D	803	5/5	0.90	0.10	83,83,84,84	0
4	PO4	A	804	5/5	0.90	0.10	65,66,67,67	0
2	ATP	G	801	31/31	0.91	0.08	72,75,78,78	0
4	PO4	E	804	5/5	0.91	0.10	77,78,78,78	0
3	MG	B	802	1/1	0.92	0.12	13,13,13,13	0
2	ATP	H	801	31/31	0.92	0.08	74,83,85,86	0
3	MG	C	803	1/1	0.92	0.09	34,34,34,34	0
4	PO4	H	804	5/5	0.92	0.07	75,75,76,76	0
4	PO4	B	804	5/5	0.93	0.10	66,67,67,69	0
2	ATP	F	801	31/31	0.95	0.09	45,54,62,62	0
2	ATP	D	801	31/31	0.95	0.08	55,69,82,83	0
2	ATP	A	801	31/31	0.95	0.07	46,50,53,54	0
3	MG	F	803	1/1	0.96	0.06	32,32,32,32	0
2	ATP	B	801	31/31	0.97	0.07	36,45,53,53	0
3	MG	A	803	1/1	0.97	0.04	18,18,18,18	0
5	CO	F	806	1/1	0.97	0.05	71,71,71,71	1
5	CO	B	806	1/1	0.99	0.04	48,48,48,48	0
3	MG	B	803	1/1	0.99	0.10	13,13,13,13	0

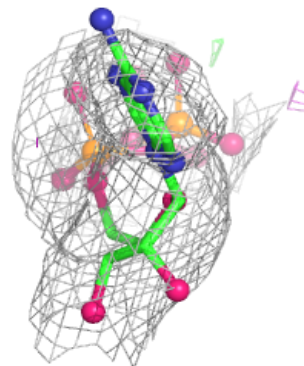
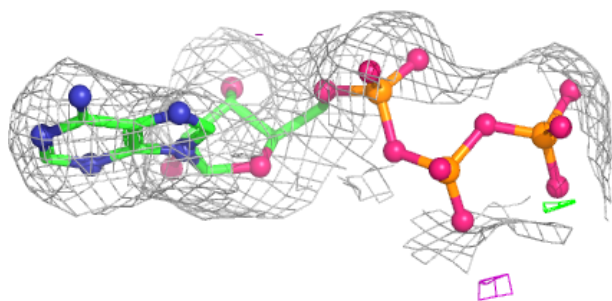
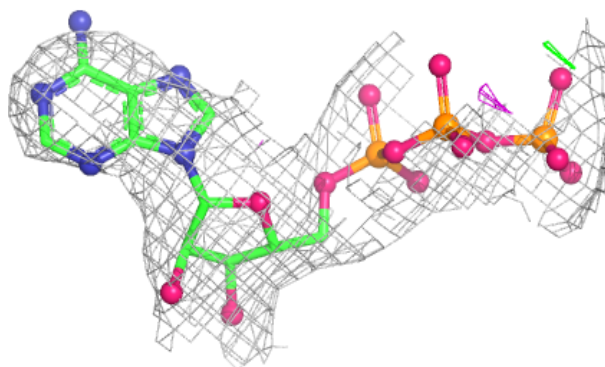
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

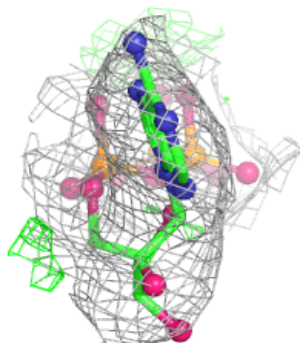
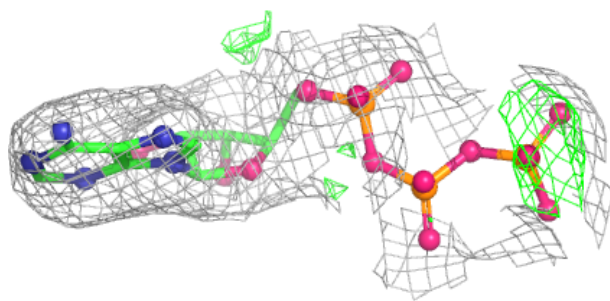
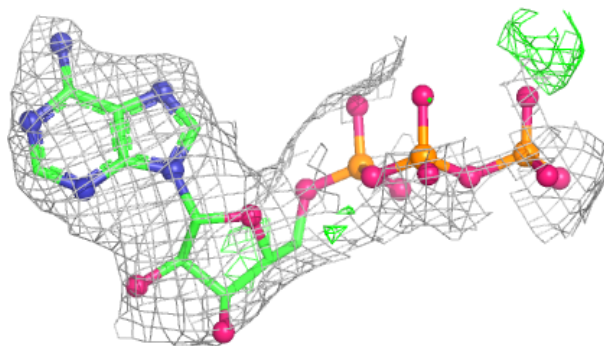
**Electron density around ATP C 801:**

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

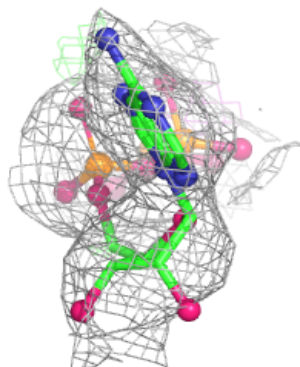
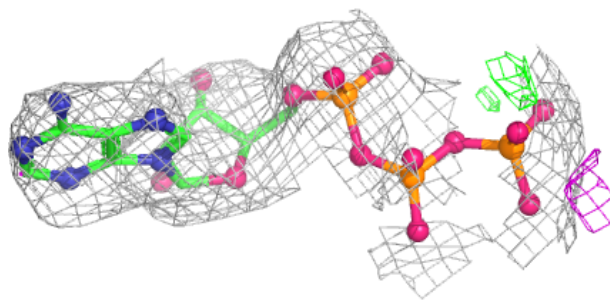
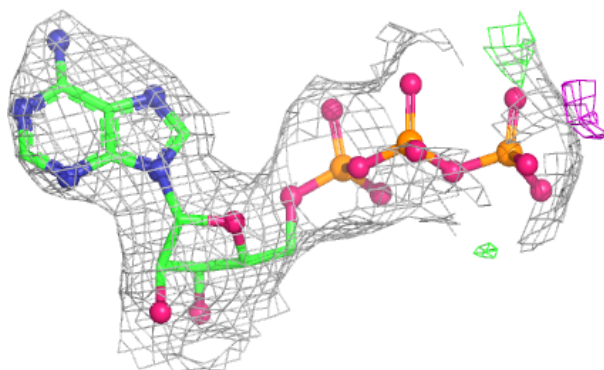


Electron density around ATP G 801:

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

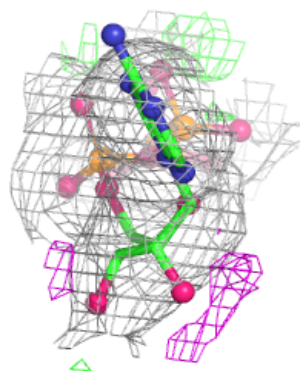
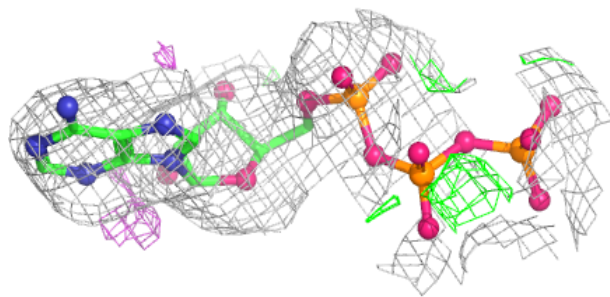
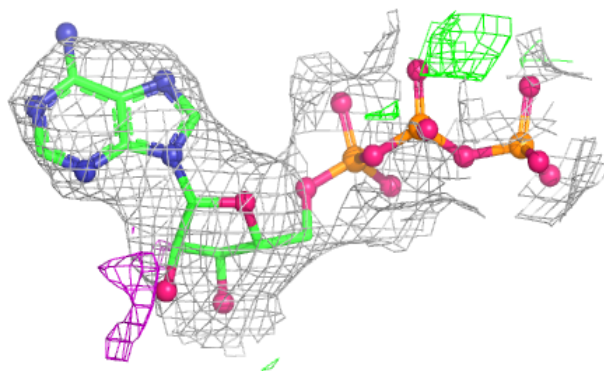
**Electron density around ATP H 801:**

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

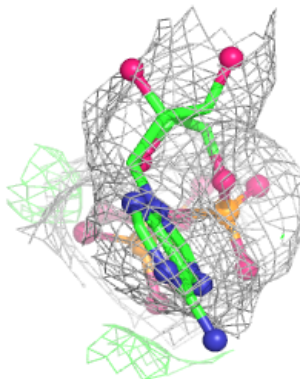
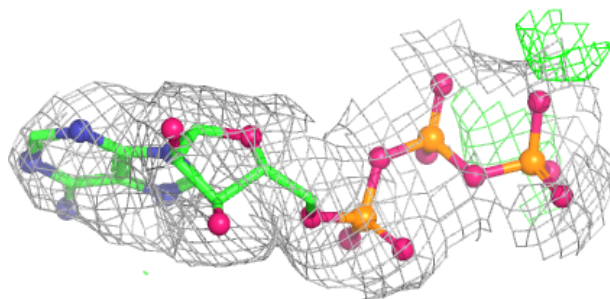
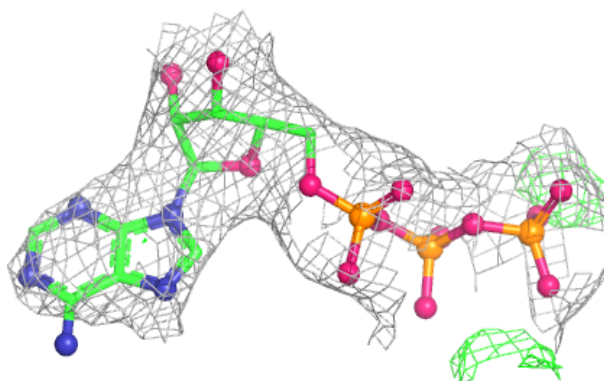


Electron density around ATP F 801:

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

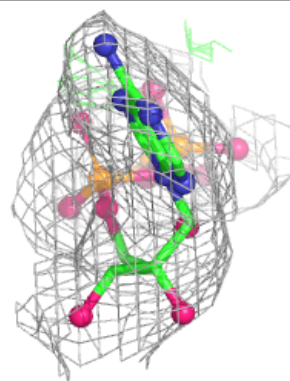
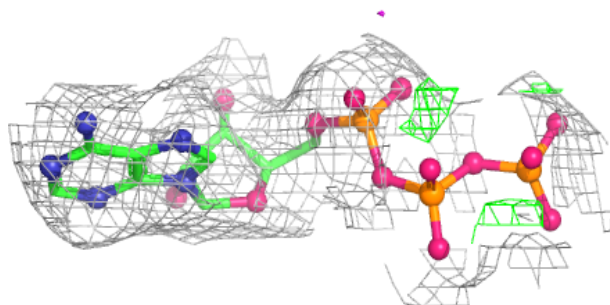
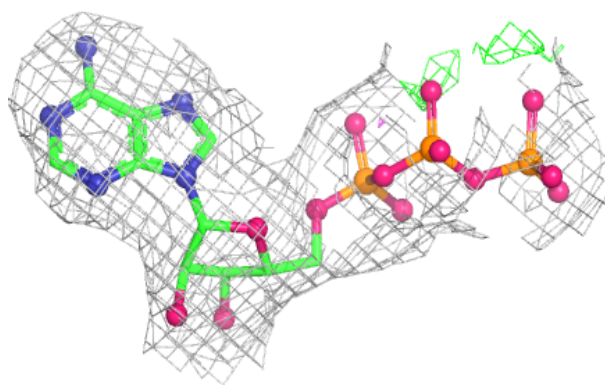
**Electron density around ATP D 801:**

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

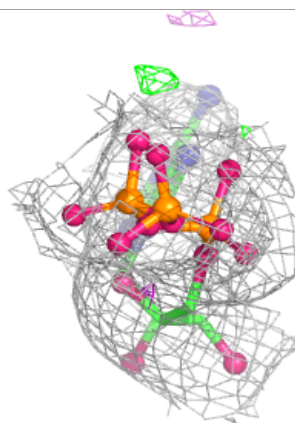
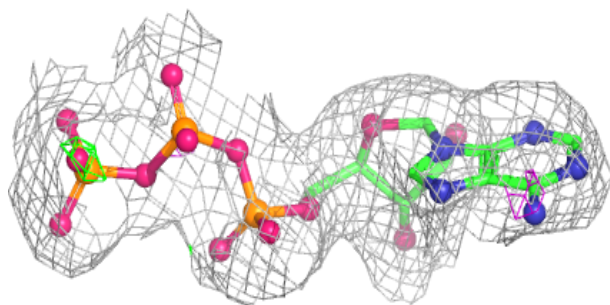
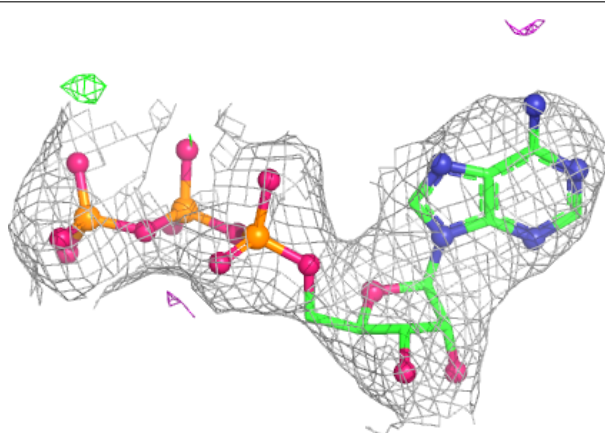


Electron density around ATP A 801:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.