



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:39 PM GMT

PDB ID : 1BMF  
Title : BOVINE MITOCHONDRIAL F1-ATPASE  
Authors : Abrahams, J.P.; Leslie, A.G.W.; Lutter, R.; Walker, J.E.  
Deposited on : 1996-03-13  
Resolution : 2.85 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

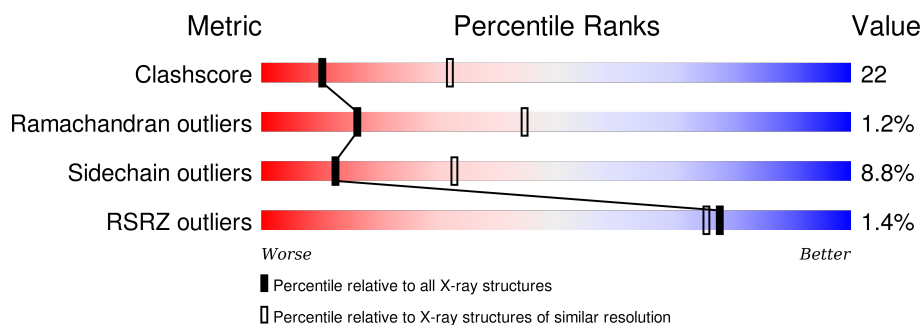
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	510	<div> <div></div> <div> <div></div> <div>50%</div> <div>37%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	510	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>36%</div> <div>6%</div> <div>5%</div> </div> </div>
1	C	510	<div> <div></div> <div> <div></div> <div>55%</div> <div>36%</div> <div>5%</div> <div></div> </div> </div>
2	D	482	<div> <div></div> <div> <div></div> <div>58%</div> <div>33%</div> <div>5%</div> <div></div> </div> </div>
2	E	482	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>43%</div> <div>6%</div> <div></div> </div> </div>
2	F	482	<div> <div></div> <div> <div></div> <div>60%</div> <div>33%</div> <div></div> <div></div> </div> </div>
3	G	272	<div> <div>2%</div> <div> <div></div> <div>24%</div> <div>17%</div> <div></div> <div>55%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	D	601	-	-	-	X
4	MG	F	601	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23481 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	487	Total	C	N	O	S	59	0	0
			3715	2341	656	706	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	ENGINEERED	UNP P19483
B	481	GLY	SER	ENGINEERED	UNP P19483
C	481	GLY	SER	ENGINEERED	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

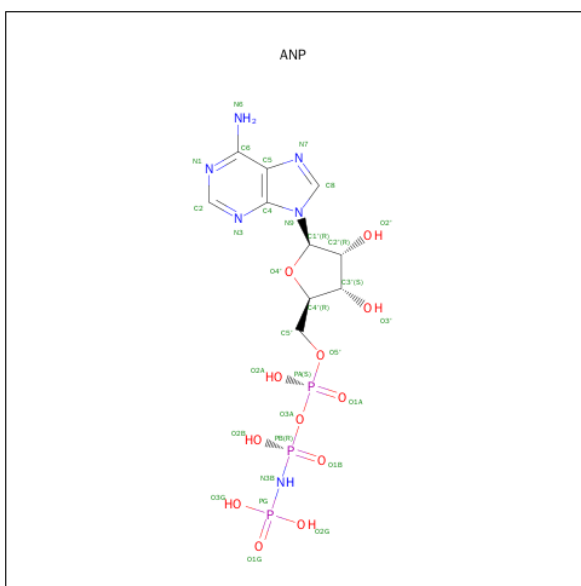
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	F	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

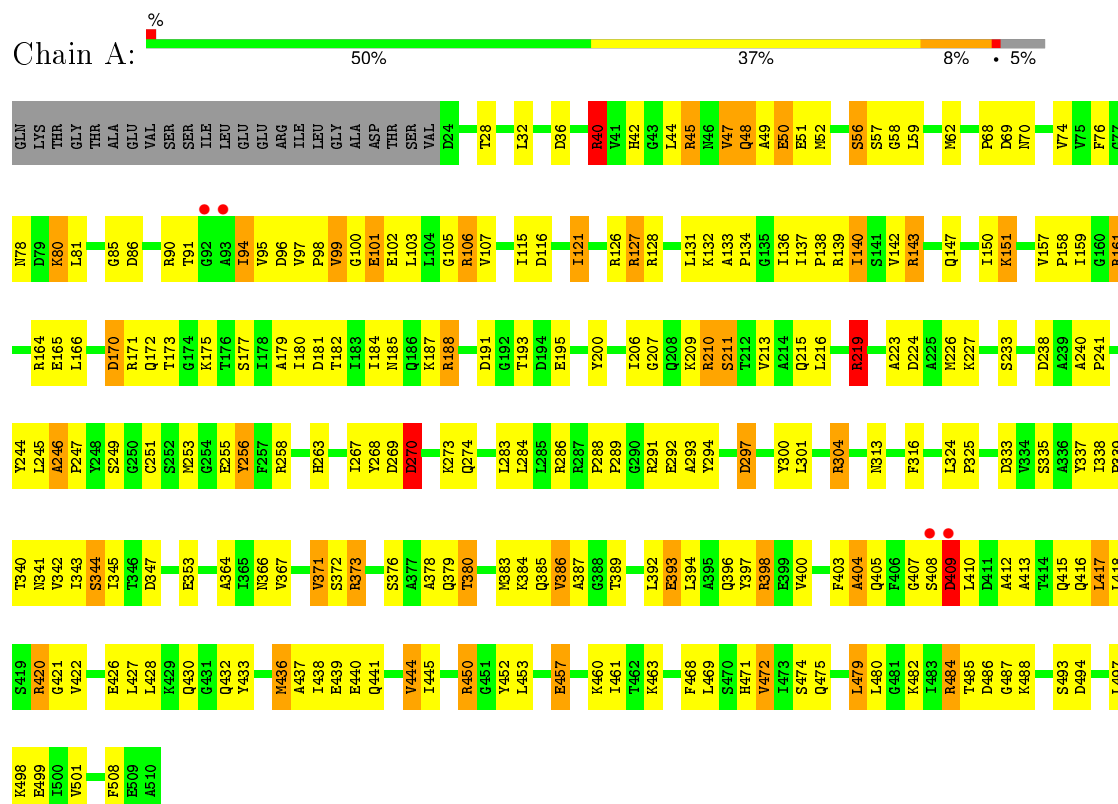
- Molecule 7 is water.

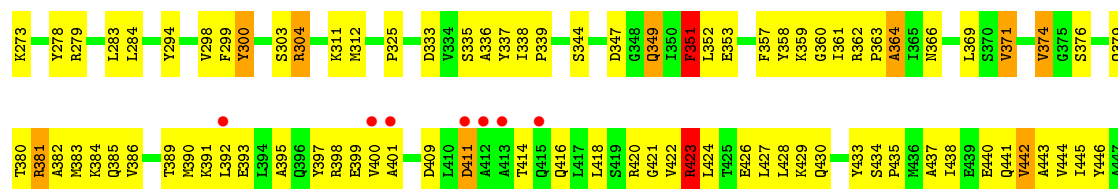
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	92	Total	O	0	0
			92	92		
7	B	96	Total	O	0	0
			96	96		
7	C	123	Total	O	0	0
			123	123		
7	D	105	Total	O	0	0
			105	105		
7	E	49	Total	O	0	0
			49	49		
7	F	104	Total	O	0	0
			104	104		
7	G	34	Total	O	0	0
			34	34		

### 3 Residue-property plots [i](#)

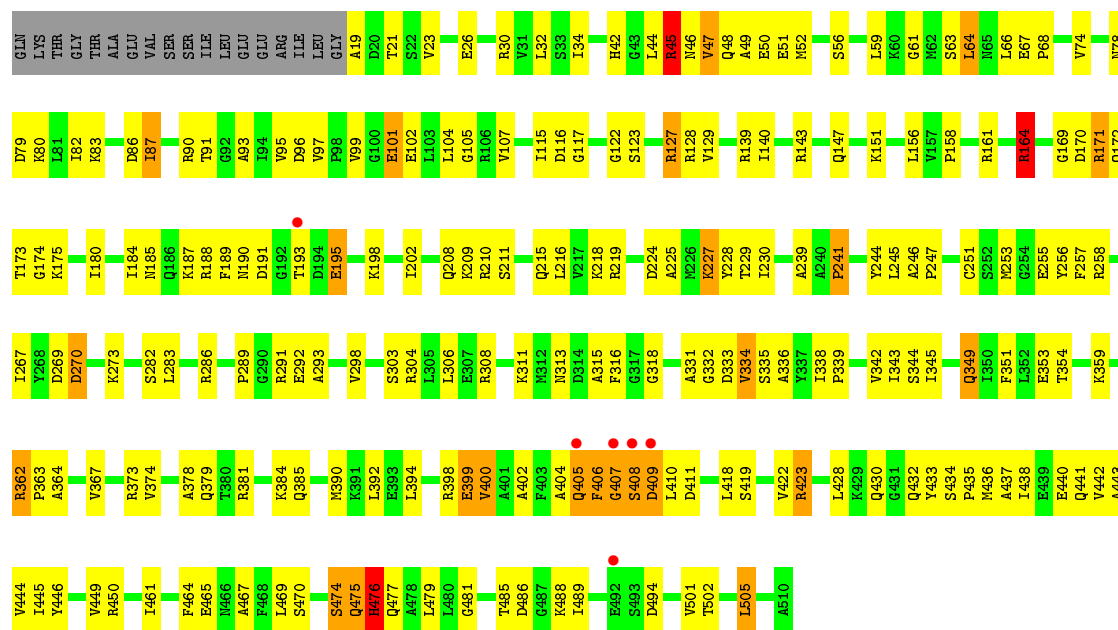
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: BOVINE MITOCHONDRIAL F1-ATPASE

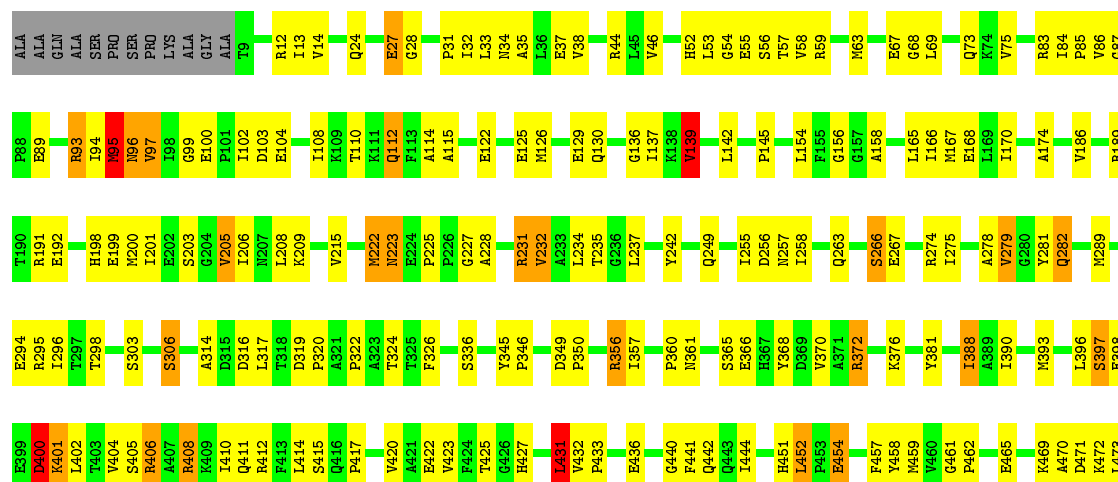




### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



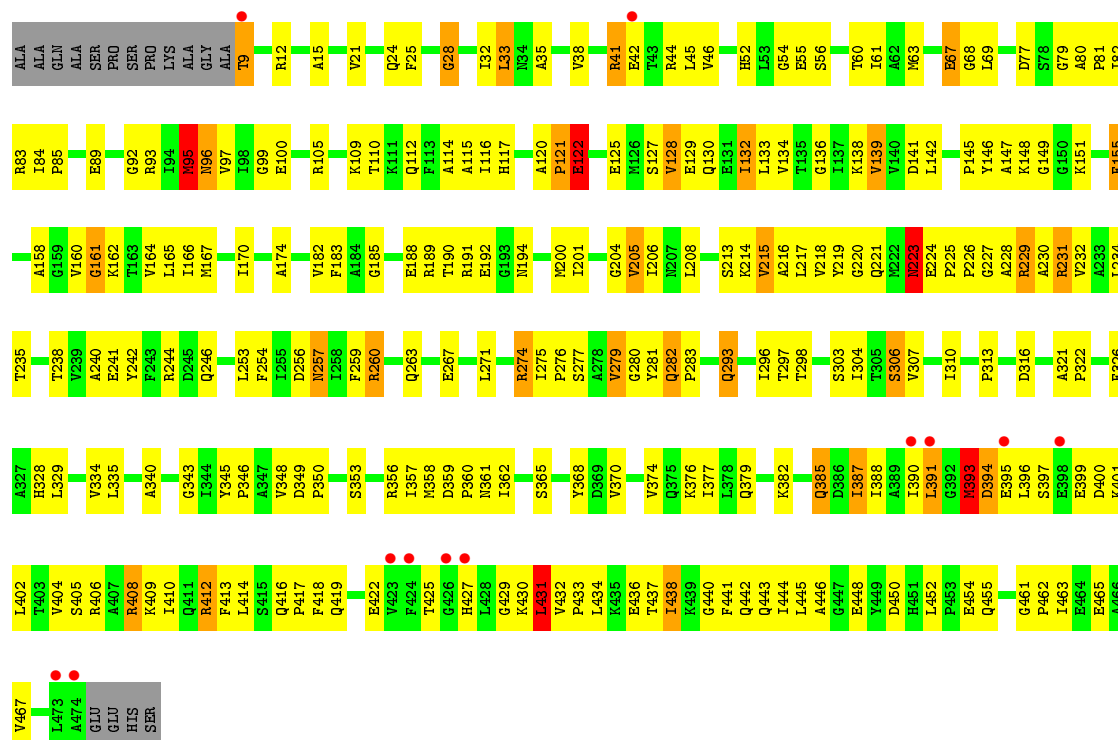
### • Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



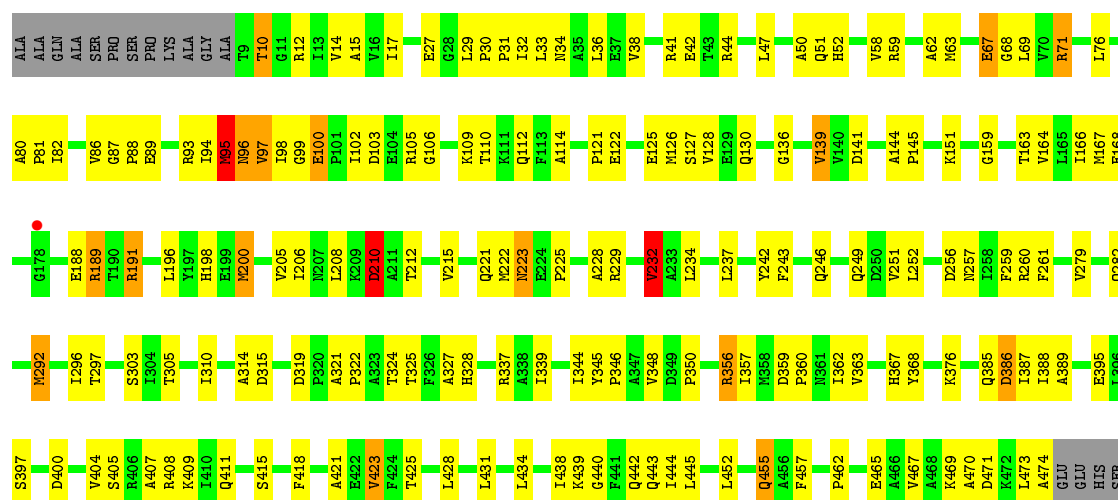




• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

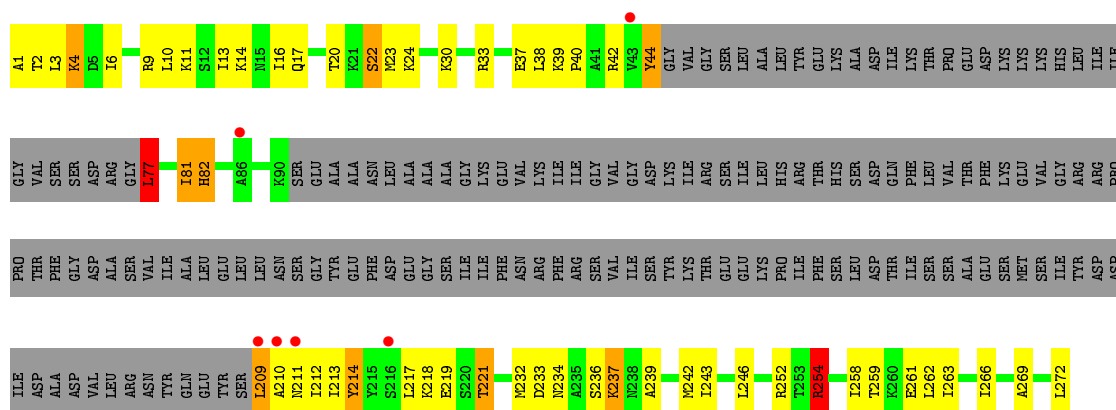


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	284.22Å 107.76Å 139.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.85 15.25 – 2.87	Depositor EDS
% Data completeness (in resolution range)	95.0 (6.00-2.85) 97.9 (15.25-2.87)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.86Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.163 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 88.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 96689 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.60	0/3766	1.31	27/5080 (0.5%)
1	B	0.63	2/3766 (0.1%)	1.37	35/5080 (0.7%)
1	C	0.62	0/3799	1.38	24/5126 (0.5%)
2	D	0.62	0/3596	1.36	23/4879 (0.5%)
2	E	0.60	0/3587	1.32	18/4867 (0.4%)
2	F	0.62	0/3587	1.36	27/4867 (0.6%)
3	G	0.52	0/949	1.15	5/1266 (0.4%)
All	All	0.61	2/23050 (0.0%)	1.34	159/31165 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	ALA	C-N	-7.54	1.16	1.34
1	B	409	ASP	C-N	-6.84	1.18	1.34

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	23.37	156.31	123.60
2	E	408	ARG	CD-NE-CZ	14.00	143.20	123.60
1	C	291	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	B	40	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	B	279	ARG	NE-CZ-NH1	12.88	126.74	120.30
2	F	356	ARG	NE-CZ-NH1	11.57	126.09	120.30
2	D	406	ARG	NE-CZ-NH1	-11.52	114.54	120.30
2	F	59	ARG	NE-CZ-NH1	-11.40	114.60	120.30
3	G	254	ARG	NE-CZ-NH2	-11.05	114.78	120.30
2	D	408	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	B	219	ARG	NE-CZ-NH2	10.35	125.47	120.30
2	F	282	GLN	CB-CG-CD	10.30	138.39	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	B	40	ARG	CD-NE-CZ	9.91	137.47	123.60
1	C	164	ARG	NE-CZ-NH1	-9.82	115.39	120.30
2	F	229	ARG	NE-CZ-NH1	-9.57	115.51	120.30
2	F	356	ARG	NE-CZ-NH2	-9.43	115.58	120.30
2	F	95	MET	CA-CB-CG	9.20	128.94	113.30
2	D	44	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	C	161	ARG	NE-CZ-NH1	9.11	124.85	120.30
2	F	59	ARG	NE-CZ-NH2	9.07	124.83	120.30
1	B	304	ARG	NE-CZ-NH1	-9.05	115.78	120.30
1	A	420	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	C	450	ARG	NE-CZ-NH2	-8.57	116.02	120.30
2	F	96	ASN	CB-CA-C	-8.55	93.29	110.40
2	E	95	MET	CA-CB-CG	8.52	127.79	113.30
2	E	83	ARG	NE-CZ-NH1	-8.50	116.05	120.30
2	E	260	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	A	373	ARG	NE-CZ-NH2	8.27	124.44	120.30
1	A	398	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	450	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	C	127	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	F	229	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	B	409	ASP	C-N-CA	7.98	141.66	121.70
2	E	229	ARG	NE-CZ-NH1	7.98	124.29	120.30
2	D	125	GLU	OE1-CD-OE2	-7.95	113.76	123.30
1	C	362	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	B	304	ARG	NE-CZ-NH2	7.87	124.24	120.30
1	B	219	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	B	279	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	C	450	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	C	304	ARG	NE-CZ-NH2	7.45	124.02	120.30
2	F	408	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	B	270	ASP	CB-CA-C	-7.38	95.63	110.40
2	D	93	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	C	161	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	450	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	E	41	ARG	CD-NE-CZ	7.13	133.58	123.60
1	A	270	ASP	CB-CA-C	-7.11	96.17	110.40
1	B	258	ARG	CD-NE-CZ	7.10	133.54	123.60
2	E	356	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	C	45	ARG	NE-CZ-NH2	-7.05	116.78	120.30
2	F	139	VAL	CB-CA-C	-7.04	98.02	111.40
2	E	356	ARG	NE-CZ-NH1	7.01	123.81	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	CD-NE-CZ	6.94	133.32	123.60
3	G	77	LEU	CA-CB-CG	6.92	131.22	115.30
2	F	95	MET	C-N-CA	6.75	138.58	121.70
2	D	95	MET	C-N-CA	6.66	138.35	121.70
2	D	96	ASN	CB-CA-C	-6.66	97.09	110.40
1	B	349	GLN	CA-CB-CG	6.63	127.99	113.40
1	C	308	ARG	NE-CZ-NH1	-6.55	117.03	120.30
2	D	231	ARG	NE-CZ-NH1	6.53	123.57	120.30
2	F	256	ASP	CB-CG-OD1	6.53	124.18	118.30
2	F	189	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	B	423	ARG	CD-NE-CZ	6.51	132.71	123.60
2	D	274	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	106	ARG	CD-NE-CZ	6.48	132.68	123.60
2	D	59	ARG	NE-CZ-NH1	-6.47	117.06	120.30
2	D	191	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	B	270	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	127	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	371	VAL	CB-CA-C	-6.42	99.20	111.40
2	E	44	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	372	SER	N-CA-CB	6.39	120.08	110.50
2	E	431	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	170	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	171	ARG	NE-CZ-NH2	6.33	123.46	120.30
2	F	12	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	C	308	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	D	372	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	210	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	398	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	C	381	ARG	CD-NE-CZ	6.22	132.31	123.60
1	C	291	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	127	ARG	CD-NE-CZ	6.17	132.24	123.60
1	C	476	HIS	N-CA-C	6.16	127.64	111.00
1	B	300	TYR	CB-CG-CD2	-6.14	117.31	121.00
1	B	128	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	F	97	VAL	CB-CA-C	-6.12	99.78	111.40
1	B	371	VAL	CB-CA-C	-6.11	99.79	111.40
2	E	274	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	C	423	ARG	CD-NE-CZ	6.04	132.05	123.60
1	C	164	ARG	CD-NE-CZ	-6.01	115.19	123.60
2	D	222	MET	CB-CA-C	-5.94	98.52	110.40
1	A	269	ASP	C-N-CA	5.87	136.38	121.70
1	B	401	ALA	O-C-N	-5.87	113.30	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH2	5.85	123.23	120.30
3	G	9	ARG	NE-CZ-NH1	5.77	123.19	120.30
2	F	103	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	219	ARG	CD-NE-CZ	5.70	131.57	123.60
1	A	297	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	398	ARG	NE-CZ-NH1	-5.68	117.46	120.30
2	F	41	ARG	CG-CD-NE	5.67	123.71	111.80
1	B	337	TYR	CB-CG-CD1	5.67	124.40	121.00
2	D	139	VAL	CB-CA-C	-5.66	100.64	111.40
1	B	139	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	D	474	ALA	C-N-CA	5.61	135.74	121.70
1	B	210	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	297	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	F	191	ARG	NE-CZ-NH2	-5.56	117.52	120.30
3	G	237	LYS	CB-CA-C	5.56	121.52	110.40
2	D	431	LEU	CA-CB-CG	5.56	128.08	115.30
2	D	454	GLU	CA-CB-CG	5.55	125.61	113.40
1	A	233	SER	N-CA-CB	-5.53	102.20	110.50
2	E	93	ARG	NE-CZ-NH1	-5.49	117.56	120.30
2	D	12	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	349	GLN	N-CA-CB	5.47	120.44	110.60
1	B	423	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	D	372	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	304	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	B	222	ASP	CB-CG-OD2	-5.41	113.43	118.30
2	F	191	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	335	SER	CB-CA-C	-5.39	99.86	110.10
1	C	349	GLN	CB-CA-C	-5.37	99.66	110.40
2	F	71	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	143	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	C	170	ASP	CB-CG-OD1	5.36	123.12	118.30
2	E	408	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	241	PRO	N-CA-CB	5.30	109.67	103.30
1	B	45	ARG	CB-CG-CD	-5.29	97.86	111.60
1	C	171	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	188	ARG	CG-CD-NE	5.25	122.83	111.80
2	E	260	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	B	40	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	F	100	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	B	278	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	C	336	ALA	N-CA-CB	-5.18	102.84	110.10
1	A	270	ASP	CB-CG-OD1	5.17	122.95	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PHE	N-CA-CB	5.17	119.90	110.60
2	E	231	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	258	ARG	CD-NE-CZ	5.14	130.80	123.60
2	F	423	VAL	CB-CA-C	-5.11	101.68	111.40
2	D	400	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	161	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	127	ARG	NH1-CZ-NH2	5.10	125.01	119.40
2	E	122	GLU	CA-CB-CG	5.10	124.62	113.40
2	D	356	ARG	CD-NE-CZ	-5.08	116.49	123.60
2	F	303	SER	N-CA-CB	-5.08	102.88	110.50
2	D	316	ASP	CB-CG-OD2	-5.07	113.73	118.30
2	F	337	ARG	CD-NE-CZ	5.07	130.69	123.60
2	E	96	ASN	N-CA-CB	-5.06	101.48	110.60
2	E	223	ASN	CB-CA-C	-5.06	100.29	110.40
3	G	44	TYR	CA-CB-CG	5.06	123.01	113.40
1	A	40	ARG	CG-CD-NE	5.05	122.42	111.80
2	F	232	VAL	CB-CA-C	-5.05	101.80	111.40
1	B	171	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	234	ALA	N-CA-C	-5.03	97.42	111.00
1	A	200	TYR	CA-CB-CG	-5.02	103.86	113.40
2	F	210	ASP	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3815	172	0
1	B	3715	0	3812	167	0
1	C	3748	0	3844	168	0
2	D	3539	0	3592	153	0
2	E	3530	0	3587	205	0
2	F	3530	0	3585	131	0
3	G	945	0	1019	55	0
4	A	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	31	0	13	2	0
5	B	31	0	13	5	0
5	C	31	0	13	4	0
5	F	31	0	13	4	0
6	D	27	0	12	2	0
7	A	92	0	0	9	0
7	B	96	0	0	14	0
7	C	123	0	0	11	0
7	D	105	0	0	6	0
7	E	49	0	0	6	0
7	F	104	0	0	3	0
7	G	34	0	0	1	0
All	All	23481	0	23318	994	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 22.

All (994) 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:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.15
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.12	1.12
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.35	1.09
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.73	1.02
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.40	1.02
2:F:223:ASN:HD22	2:F:223:ASN:H	1.08	1.02
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.30	0.95
1:C:404:ALA:C	1:C:406:PHE:H	1.64	0.93
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.93
2:E:223:ASN:H	2:E:223:ASN:HD22	1.00	0.92
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.91
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.91
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.89
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.89	0.88
1:C:398:ARG:HG2	7:C:627:HOH:O	1.72	0.88
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.55	0.87
1:B:456:LEU:HD12	1:B:457:GLU:H	1.42	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.60	0.84
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.79
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.79
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.79
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.79
1:B:211:SER:HB2	7:B:674:HOH:O	1.82	0.79
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.78
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.78
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.77
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.77
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.76
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.76
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.76
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.75
1:B:172:GLN:HA	5:B:600:ANP:HNB1	1.51	0.75
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.75
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.74
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
3:G:2:THR:HG22	3:G:4:LYS:H	1.51	0.74
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.68	0.74
2:F:159:GLY:HA2	5:F:600:ANP:HNB1	1.52	0.74
1:C:101:GLU:HB2	7:C:723:HOH:O	1.88	0.73
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.70	0.72
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.72
2:D:223:ASN:H	2:D:223:ASN:HD22	1.35	0.72
1:A:297:ASP:HA	7:A:628:HOH:O	1.89	0.72
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.72
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.72	0.72
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.72
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.71
2:D:156:GLY:HA2	7:D:659:HOH:O	1.90	0.71
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.71	0.71
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.72	0.71
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.71
1:A:291:ARG:HA	3:G:262:LEU:HD13	1.72	0.70
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.70
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.71	0.70
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.70
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.70
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.73	0.70
2:D:84:ILE:HB	2:D:95:MET:HE3	1.74	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.73	0.70
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.73	0.69
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.74	0.69
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.75	0.69
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.69
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.69
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.69
2:D:223:ASN:N	2:D:223:ASN:HD22	1.89	0.69
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	0.68
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.74	0.68
1:B:283:LEU:CD1	2:E:277:SER:HB3	2.22	0.68
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.67
2:E:425:THR:O	2:E:427:HIS:ND1	2.20	0.67
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.76	0.67
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.30	0.67
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.67
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.67
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.67
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.67
1:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.67
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.67
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.66
1:B:363:PRO:O	7:B:609:HOH:O	2.13	0.66
2:F:223:ASN:N	2:F:223:ASN:HD22	1.85	0.66
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.66
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.66
2:E:224:GLU:HG2	7:E:501:HOH:O	1.96	0.66
2:D:223:ASN:ND2	2:D:223:ASN:H	1.93	0.66
2:F:223:ASN:ND2	2:F:223:ASN:H	1.85	0.66
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.78	0.65
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.65
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	0.65
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.65
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.65
1:B:283:LEU:HD12	2:E:277:SER:HB3	1.78	0.65
3:G:24:LYS:HE3	3:G:233:ASP:HB2	1.78	0.65
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.96	0.65
2:E:223:ASN:HD22	2:E:223:ASN:N	1.84	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.65
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.65
1:A:403:PHE:CZ	3:G:22:SER:HB2	2.32	0.65
1:B:215:GLN:NE2	2:E:130:GLN:NE2	2.45	0.65
2:D:225:PRO:HB2	7:D:649:HOH:O	1.95	0.65
1:B:437:ALA:O	1:B:440:GLU:N	2.30	0.65
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.64
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.79	0.64
1:C:44:LEU:O	1:C:47:VAL:HG22	1.96	0.64
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.64
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.77	0.64
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.64
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.64
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.64
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.64
1:C:215:GLN:CG	2:F:356:ARG:HH22	2.02	0.63
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.63
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.63
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.63
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.63
1:C:52:MET:O	1:C:91:THR:HB	1.98	0.63
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.33	0.63
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.63
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.63	0.63
2:E:138:LYS:HE2	2:E:432:VAL:HG21	1.81	0.63
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.62
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
1:A:48:GLN:HB3	2:E:68:GLY:O	1.99	0.62
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.62
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.62
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	0.62
1:B:389:THR:HA	1:B:392:LEU:CD1	2.28	0.62
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.62
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.61
1:C:218:LYS:HD2	2:F:128:VAL:HG21	1.81	0.61
1:B:389:THR:HA	1:B:392:LEU:HD12	1.81	0.61
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.82	0.61
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.83	0.61
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.61
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.61
1:C:362:ARG:NH1	7:C:689:HOH:O	2.34	0.61
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.81	0.61
1:A:376:SER:C	1:A:378:ALA:H	2.03	0.61
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.61
1:A:121:ILE:H	1:A:121:ILE:HD13	1.66	0.61
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.61
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.82	0.61
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.61
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.61
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.15	0.61
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.60
2:D:93:ARG:HH11	2:D:93:ARG:HG3	1.66	0.60
1:A:52:MET:O	1:A:91:THR:HG23	2.01	0.60
2:E:92:GLY:N	2:E:215:VAL:O	2.30	0.60
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.60
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.60
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.60
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.60
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.02	0.60
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.60
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.60
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.34	0.60
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.60
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.60
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.60
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.60
1:B:362:ARG:HA	1:B:363:PRO:C	2.22	0.60
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.60
2:E:149:GLY:HA2	2:E:304:ILE:O	2.02	0.60
3:G:13:ILE:HG22	3:G:243:ILE:HG12	1.84	0.60
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.60
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.59
1:B:237:SER:HB3	7:B:687:HOH:O	2.02	0.59
1:C:175:LYS:HE3	5:C:600:ANP:O1B	2.02	0.59
2:E:263:GLN:HB3	7:E:490:HOH:O	2.00	0.59
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.59
2:E:316:ASP:OD2	3:G:254:ARG:NH1	2.35	0.59
1:A:132:LYS:HA	7:A:643:HOH:O	2.01	0.59
3:G:239:ALA:O	3:G:243:ILE:HG13	2.02	0.59
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.59
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.32	0.59
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.59
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.59
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.59
1:A:403:PHE:CE1	3:G:22:SER:HB2	2.38	0.59
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.66	0.59
1:B:215:GLN:HE22	2:E:130:GLN:NE2	1.99	0.59
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.59
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.59
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.18	0.59
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.59
1:B:499:GLU:O	1:B:502:THR:HB	2.03	0.59
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.59
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.59
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.03	0.59
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.58
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.58
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.85	0.58
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.58
2:E:408:ARG:O	2:E:412:ARG:HG3	2.02	0.58
7:B:617:HOH:O	2:F:67:GLU:HG3	2.02	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.58
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.58
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.58
2:E:246:GLN:NE2	2:E:246:GLN:HA	2.19	0.58
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.58
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	0.58
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.58
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.58
3:G:17:GLN:HB2	3:G:239:ALA:HB1	1.85	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.39	0.58
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.58
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.58
1:C:210:ARG:NH1	2:F:121:PRO:O	2.37	0.58
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.58
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.58
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.86	0.58
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.58
1:C:399:GLU:OE2	2:D:408:ARG:NH2	2.37	0.57
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
2:D:473:LEU:C	2:D:475:GLU:H	2.08	0.57
1:A:333:ASP:HB3	7:A:632:HOH:O	2.04	0.57
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.57
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.57
2:E:267:GLU:O	2:E:271:LEU:HG	2.05	0.57
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.57
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.57
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.57
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.57
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.57
2:E:138:LYS:O	2:E:142:LEU:HB3	2.03	0.57
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.57
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.57
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.56
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.56
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.56
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.56
1:A:286:ARG:HH22	3:G:272:LEU:HD13	1.68	0.56
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.40	0.56
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.56
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.56
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.56
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.56
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.56
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.56
3:G:20:THR:HG21	3:G:236:SER:N	2.21	0.56
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.56
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.36	0.56
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.56
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.56
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.56
1:B:218:LYS:NZ	2:E:129:GLU:OE2	2.39	0.56
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.56
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.56
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.87	0.56
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.56
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.55
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.55
2:F:63:MET:CE	2:F:97:VAL:HG11	2.37	0.55
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.72	0.55
1:B:70:ASN:OD1	7:B:632:HOH:O	2.18	0.55
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.55
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.55
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.55
2:D:278:ALA:HB1	3:G:261:GLU:OE2	2.06	0.55
1:B:175:LYS:HE3	5:B:600:ANP:O1B	2.06	0.55
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.55
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.55
2:D:425:THR:HG21	2:D:459:MET:HE1	1.87	0.55
2:F:32:ILE:O	2:F:33:LEU:HB2	2.05	0.55
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.55
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.55
2:E:84:ILE:HB	2:E:95:MET:HE1	1.88	0.55
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.55
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.55
1:B:482:LYS:O	1:B:486:ASP:N	2.37	0.55
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.55
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.55
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.55
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.54
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.42	0.54
1:B:172:GLN:HA	5:B:600:ANP:N3B	2.21	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.07	0.54
1:B:195:GLU:HB3	7:B:691:HOH:O	2.08	0.54
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.73	0.54
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.54
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.25	0.54
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.54
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.54
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.54
1:A:211:SER:N	2:D:126:MET:HE2	2.22	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.54
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.54
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.54
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.08	0.54
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.54
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.90	0.54
1:A:172:GLN:HA	5:A:600:ANP:N3B	2.23	0.54
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.54
2:F:395:GLU:OE2	3:G:77:LEU:HA	2.08	0.54
1:C:83:LYS:HB3	2:F:52:HIS:CE1	2.42	0.54
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.54
2:E:397:SER:C	2:E:399:GLU:N	2.57	0.54
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.54
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.54
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.90	0.54
1:B:33:SER:HB2	2:E:52:HIS:O	2.08	0.54
7:B:624:HOH:O	2:F:198:HIS:CE1	2.60	0.54
2:F:225:PRO:HB2	7:F:630:HOH:O	2.07	0.54
2:D:122:GLU:HA	2:D:122:GLU:OE1	2.07	0.54
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.89	0.53
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.53
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	0.53
2:D:412:ARG:HG3	2:D:412:ARG:HH11	1.73	0.53
2:F:96:ASN:HB2	2:F:100:GLU:H	1.74	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.08	0.53
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.91	0.53
3:G:17:GLN:HB2	3:G:239:ALA:CB	2.39	0.53
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.91	0.53
1:B:69:ASP:O	1:B:70:ASN:HB3	2.09	0.53
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.53
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:C:174:GLY:HA2	5:C:600:ANP:PA	2.49	0.53
1:B:171:ARG:HD2	7:E:496:HOH:O	2.08	0.53
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.53
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.89	0.53
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.38	0.53
1:C:335:SER:O	2:D:314:ALA:HA	2.09	0.53
3:G:14:LYS:HG2	3:G:243:ILE:HD13	1.91	0.53
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.53
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.53
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.53
1:B:358:TYR:C	1:B:360:GLY:H	2.12	0.53
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.53
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.52
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.52
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.52
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.52
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.91	0.52
2:E:279:VAL:O	2:E:279:VAL:HG12	2.10	0.52
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.52
2:D:356:ARG:HG2	2:D:356:ARG:O	2.09	0.52
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.52
1:C:172:GLN:HA	5:C:600:ANP:HNB1	1.75	0.52
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.52
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.52
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.52
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.52
1:B:284:LEU:CD2	2:E:274:ARG:HD3	2.39	0.52
2:E:216:ALA:HB1	7:E:487:HOH:O	2.09	0.52
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.52
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.52
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.52
1:B:333:ASP:HB2	3:G:252:ARG:HH21	1.74	0.52
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.52
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.52
1:C:436:MET:HE1	1:C:469:LEU:HD21	1.92	0.52
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.52
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.52
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.52
3:G:214:TYR:CZ	3:G:218:LYS:HG3	2.45	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.91	0.52
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.52
2:D:390:ILE:HD13	3:G:16:ILE:CD1	2.40	0.52
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.52
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.45	0.51
1:C:354:THR:HG23	7:C:664:HOH:O	2.10	0.51
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.51
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.51
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.51
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.51
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.51
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.51
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.46	0.51
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.51
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.92	0.51
1:B:303:SER:HB2	2:F:222:MET:HB3	1.92	0.51
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.91	0.51
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.93	0.51
3:G:37:GLU:OE1	3:G:218:LYS:HE3	2.10	0.51
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.10	0.51
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.92	0.51
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.93	0.51
3:G:6:ILE:HG23	3:G:246:LEU:HD22	1.93	0.51
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.51
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.92	0.51
3:G:38:LEU:HD11	3:G:42:ARG:NE	2.26	0.51
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.51
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.25	0.51
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	0.51
1:C:83:LYS:HB3	2:F:52:HIS:HE1	1.76	0.51
3:G:1:ALA:HB1	3:G:6:ILE:HD11	1.92	0.51
7:B:621:HOH:O	2:F:189:ARG:HG2	2.09	0.51
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.51
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.51
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.50
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.50
1:A:177:SER:OG	5:A:600:ANP:H8	2.11	0.50
1:B:157:VAL:N	1:B:158:PRO:HD3	2.25	0.50
1:C:344:SER:HA	7:D:664:HOH:O	2.10	0.50
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.93	0.50
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.50
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.93	0.50
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.50
1:A:137:ILE:N	1:A:138:PRO:CD	2.75	0.50
1:B:174:GLY:HA2	5:B:600:ANP:PA	2.52	0.50
2:E:221:GLN:N	2:E:224:GLU:OE1	2.44	0.50
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.50
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.50
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.24	0.50
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.27	0.50
1:A:175:LYS:NZ	7:A:625:HOH:O	2.35	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	0.50
2:F:234:LEU:O	2:F:237:LEU:HB3	2.10	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.12	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.50
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.46	0.50
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.50
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.50
3:G:39:LYS:CB	3:G:40:PRO:HD3	2.15	0.50
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.50
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.50
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.92	0.50
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.50
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.50
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.49
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.49
2:F:297:THR:HA	7:F:675:HOH:O	2.12	0.49
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.49
1:C:171:ARG:NH2	7:C:707:HOH:O	2.27	0.49
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.49
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.94	0.49
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.49
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.49
3:G:30:LYS:HA	3:G:33:ARG:HE	1.77	0.49
3:G:210:ALA:HA	3:G:213:ILE:HB	1.93	0.49
1:C:23:VAL:HG12	1:C:23:VAL:O	2.11	0.49
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.49
2:D:168:GLU:O	2:D:168:GLU:HG3	2.11	0.49
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.49
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.49
2:F:164:VAL:HG23	5:F:600:ANP:O1A	2.13	0.49
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.49
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.49
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.95	0.49
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:ARG:NH1	2:D:93:ARG:HG3	2.27	0.49
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.49
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.49
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.49
2:D:306:SER:HB2	7:D:629:HOH:O	2.12	0.49
3:G:82:HIS:CD2	3:G:82:HIS:H	2.29	0.49
1:C:343:ILE:HG22	2:D:158:ALA:HB1	1.94	0.49
2:D:376:LYS:HB2	7:D:631:HOH:O	2.11	0.49
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.94	0.49
1:B:49:ALA:O	1:B:50:GLU:HB2	2.12	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.13	0.49
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.49
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
1:B:24:ASP:O	1:B:28:THR:HB	2.12	0.49
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.49
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.78	0.49
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.49
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.49
3:G:20:THR:HG22	3:G:236:SER:HB3	1.94	0.49
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.43	0.49
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.48
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.48
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.48
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.48
1:B:423:ARG:HE	1:B:458:PRO:CD	2.25	0.48
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.48
1:B:96:ASP:HB2	1:B:127:ARG:O	2.12	0.48
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.48
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.48
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.48
1:C:286:ARG:NH1	7:C:639:HOH:O	2.46	0.48
1:A:373:ARG:NH1	1:A:373:ARG:HG3	2.28	0.48
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.48
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.48
2:D:63:MET:HE1	2:D:227:GLY:O	2.14	0.48
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.78	0.48
2:E:393:MET:O	2:E:393:MET:HE2	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.48
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.48
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.48
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.44	0.48
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.48
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.48
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.48
1:B:481:GLY:O	1:B:485:THR:HB	2.14	0.48
1:B:351:PHE:HE1	1:B:369:LEU:O	1.96	0.48
1:B:40:ARG:NH1	7:B:632:HOH:O	2.27	0.48
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.48
2:E:326:PHE:HB3	7:E:496:HOH:O	2.13	0.48
2:E:404:VAL:O	2:E:408:ARG:HG3	2.14	0.48
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.48
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.48
3:G:39:LYS:CB	3:G:40:PRO:CD	2.89	0.48
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.48
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.48
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.45	0.47
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.47
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.47
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.79	0.47
1:C:481:GLY:O	1:C:485:THR:HB	2.14	0.47
2:F:36:LEU:HD23	2:F:36:LEU:N	2.30	0.47
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.79	0.47
3:G:209:LEU:O	3:G:210:ALA:C	2.52	0.47
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.47
2:F:44:ARG:NH2	7:F:653:HOH:O	2.39	0.47
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.47
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.47
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.96	0.47
1:B:389:THR:HA	1:B:392:LEU:HG	1.97	0.47
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.15	0.47
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.80	0.47
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.47
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.47
2:D:129:GLU:OE1	2:D:129:GLU:HA	2.15	0.47
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.44	0.47
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.96	0.47
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.47
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.47
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.47
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.95	0.47
1:B:237:SER:CB	7:B:687:HOH:O	2.62	0.47
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.47
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.47
2:E:61:ILE:O	2:E:61:ILE:HG13	2.14	0.47
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.47
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.47
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.47
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.47
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.47
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.47
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.47
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.47
1:C:359:LYS:O	2:F:376:LYS:HE2	2.15	0.47
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.47
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.47
3:G:210:ALA:O	3:G:213:ILE:N	2.47	0.47
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.47
1:B:83:LYS:HG2	7:B:631:HOH:O	2.15	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
2:F:159:GLY:HA2	5:F:600:ANP:N3B	2.24	0.47
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.96	0.47
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.47
1:B:269:ASP:HA	1:B:270:ASP:HA	1.78	0.47
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.47
3:G:254:ARG:NH2	7:G:273:HOH:O	2.49	0.46
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.46
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.46
2:E:431:LEU:O	2:E:431:LEU:HD12	2.15	0.46
1:C:52:MET:HE3	1:C:95:VAL:HG13	1.96	0.46
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.46
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.46
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.46
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.46
2:F:200:MET:CG	2:F:206:ILE:HG12	2.45	0.46
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	0.46
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.46
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.46
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.44	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.46
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.96	0.46
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.16	0.46
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.46
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.98	0.46
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.46
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.46
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.46
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.46
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.46
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.46
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.46
2:E:63:MET:CE	2:E:228:ALA:HA	2.45	0.46
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.81	0.46
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.98	0.46
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.46
3:G:259:THR:O	3:G:263:ILE:HG13	2.16	0.46
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.46
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.46
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.46
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.46
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.31	0.46
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.45
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.45
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.45
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.45
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.45
1:C:476:HIS:N	1:C:476:HIS:ND1	2.64	0.45
2:E:85:PRO:HD2	2:E:95:MET:CE	2.46	0.45
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.45
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:432:VAL:HA	2:E:433:PRO:HD3	1.81	0.45
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.45
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.45
1:B:284:LEU:HD21	2:E:274:ARG:HD3	1.97	0.45
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.45
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.47	0.45
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
7:C:687:HOH:O	2:D:198:HIS:HE1	1.99	0.45
1:C:400:VAL:HG22	7:C:698:HOH:O	2.15	0.45
2:E:260:ARG:NH1	7:E:495:HOH:O	2.49	0.45
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.45
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.46	0.45
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.45
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.66	0.45
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.45
1:A:101:GLU:OE2	7:A:641:HOH:O	2.20	0.45
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.45
2:F:252:LEU:HA	2:F:252:LEU:HD23	1.81	0.45
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.45
1:B:420:ARG:O	1:B:423:ARG:N	2.50	0.45
3:G:234:ASN:HA	3:G:237:LYS:HB2	1.98	0.45
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.45
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.45
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.45
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.98	0.45
1:C:211:SER:HB3	2:F:126:MET:HE3	1.99	0.45
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.45
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.45
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.74	0.45
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.45
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.45
1:B:48:GLN:HB3	2:F:68:GLY:HA2	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.98	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.81	0.45
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.45
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.98	0.45
1:A:270:ASP:OD2	7:A:625:HOH:O	2.20	0.45
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.45
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.45
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.98	0.45
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.17	0.45
1:B:212:THR:O	1:B:216:LEU:HB2	2.18	0.45
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.45
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.45
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.45
1:B:423:ARG:HE	1:B:458:PRO:CG	2.31	0.44
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.44
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.81	0.44
1:B:465:GLU:O	1:B:469:LEU:HB2	2.17	0.44
1:A:62:MET:HE2	1:A:76:PHE:HZ	1.82	0.44
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.44
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.44
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.33	0.44
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.98	0.44
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.44
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.44
1:C:390:MET:HE2	1:C:428:LEU:HD11	1.99	0.44
2:D:470:ALA:O	2:D:474:ALA:N	2.51	0.44
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.17	0.44
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.99	0.44
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.44
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.44
2:E:402:LEU:O	2:E:406:ARG:HG3	2.16	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.44
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.44
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.44
3:G:82:HIS:CD2	3:G:82:HIS:N	2.85	0.44
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.44
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.44
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.47	0.44
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.44
1:A:151:LYS:H	1:A:151:LYS:HG2	1.67	0.44
2:D:209:LYS:HA	2:D:209:LYS:HD3	1.83	0.44
1:B:45:ARG:HD3	1:B:45:ARG:HH11	1.53	0.44
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.44
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.44
7:B:624:HOH:O	2:F:198:HIS:HE1	1.99	0.44
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.44
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.44
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.44
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.44
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.99	0.44
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.44
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.44
2:F:50:ALA:O	2:F:51:GLN:HB3	2.17	0.44
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.44
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.44
2:D:108:ILE:HG22	2:D:110:THR:HG23	2.00	0.44
1:C:172:GLN:HA	5:C:600:ANP:N3B	2.32	0.44
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.29	0.44
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.44
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.43
1:A:460:LYS:HD2	1:A:460:LYS:N	2.32	0.43
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.43
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.00	0.43
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	0.43
1:C:353:GLU:O	1:C:364:ALA:HB1	2.19	0.43
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.48	0.43
2:D:189:ARG:O	2:D:192:GLU:HB2	2.18	0.43
2:D:103:ASP:O	2:D:104:GLU:HB2	2.18	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.43
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.43
2:E:67:GLU:H	2:E:67:GLU:HG3	1.16	0.43
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.79	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.43
1:C:311:LYS:HE3	1:C:318:GLY:O	2.17	0.43
1:A:136:ILE:HG22	7:A:608:HOH:O	2.19	0.43
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.43
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.48	0.43
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.43
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.43
1:C:303:SER:HB2	2:D:222:MET:HB3	1.99	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.00	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.43
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.43
1:B:438:ILE:HD12	1:B:438:ILE:HA	1.87	0.43
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.43
1:A:224:ASP:HA	7:A:616:HOH:O	2.19	0.43
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.43
1:C:128:ARG:NH1	7:C:694:HOH:O	2.50	0.43
2:E:21:VAL:O	2:E:60:THR:OG1	2.35	0.43
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.43
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.43
1:A:48:GLN:HA	2:E:69:LEU:O	2.18	0.43
1:B:389:THR:HA	1:B:392:LEU:CG	2.48	0.43
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.43
1:C:211:SER:HB3	2:F:126:MET:CE	2.49	0.43
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.19	0.43
1:C:90:ARG:HB3	1:C:90:ARG:HE	1.61	0.43
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.43
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.43
1:A:99:VAL:HG23	1:A:253:MET:HA	2.01	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.41	0.43
3:G:209:LEU:O	3:G:212:ILE:N	2.51	0.43
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.00	0.43
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.42
2:E:89:GLU:HG2	2:E:110:THR:CG2	2.39	0.42
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.42
2:E:63:MET:HE3	2:E:228:ALA:HA	1.99	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.42
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.42
1:A:62:MET:HE2	1:A:76:PHE:CZ	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.42
1:B:65:ASN:HD22	2:F:17:ILE:CG1	2.33	0.42
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.02	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.42
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.42
2:D:345:TYR:HB3	6:D:600:ADP:C6	2.54	0.42
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	0.42
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.42
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.42
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.42
3:G:254:ARG:O	3:G:258:ILE:HG13	2.20	0.42
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.42
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.52	0.42
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.02	0.42
3:G:213:ILE:HA	3:G:213:ILE:HD13	1.89	0.42
3:G:23:MET:HB2	3:G:232:MET:HE2	2.00	0.42
2:F:400:ASP:O	2:F:404:VAL:HG23	2.20	0.42
2:E:425:THR:C	2:E:427:HIS:N	2.72	0.42
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.42
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.34	0.42
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.64	0.42
2:E:280:GLY:HA2	3:G:262:LEU:HD21	2.01	0.42
1:B:218:LYS:HB2	2:E:128:VAL:CG1	2.44	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.50	0.42
2:D:412:ARG:NH1	7:D:696:HOH:O	2.40	0.42
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.42
1:B:175:LYS:NZ	7:B:655:HOH:O	2.21	0.42
1:B:357:PHE:HZ	5:B:600:ANP:O4'	2.02	0.42
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.42
2:D:200:MET:CE	2:D:215:VAL:HG21	2.50	0.42
2:D:406:ARG:HH11	2:D:406:ARG:HD2	1.60	0.42
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
1:C:105:GLY:N	1:C:229:THR:O	2.41	0.42
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.42
3:G:2:THR:O	3:G:3:LEU:C	2.57	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.42
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.42
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.42
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.42
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.42
2:D:63:MET:CE	2:D:228:ALA:HA	2.50	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.42
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.42
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.42
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.02	0.42
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.42
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.00	0.42
2:D:401:LYS:H	2:D:401:LYS:HG2	1.72	0.42
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.42
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.35	0.42
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.42
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.42
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
2:F:438:ILE:H	2:F:438:ILE:HG12	1.73	0.42
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.42
1:A:139:ARG:C	1:A:140:ILE:HG22	2.40	0.42
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.88	0.42
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.42
1:B:273:LYS:HB3	7:B:676:HOH:O	2.19	0.42
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.42
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.42
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.42
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.42
1:C:392:LEU:HB3	2:D:458:TYR:OH	2.20	0.42
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.41
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.41
2:D:84:ILE:HD12	2:D:95:MET:CE	2.50	0.41
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.41
3:G:10:LEU:O	3:G:14:LYS:HG3	2.20	0.41
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	0.41
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.41
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.41
3:G:217:LEU:O	3:G:221:THR:HG23	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.41
2:E:349:ASP:HA	2:E:350:PRO:HD2	1.86	0.41
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.41
1:A:210:ARG:HG3	2:D:294:GLU:OE2	2.20	0.41
3:G:13:ILE:HD13	3:G:242:MET:HG2	2.02	0.41
1:A:180:ILE:O	1:A:181:ASP:C	2.56	0.41
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.41
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
1:A:238:ASP:HA	7:A:677:HOH:O	2.19	0.41
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.41
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.41
2:E:434:LEU:O	2:E:437:THR:HB	2.21	0.41
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.41
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.03	0.41
1:B:36:ASP:OD1	2:E:274:ARG:NE	2.53	0.41
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.41
3:G:209:LEU:HB3	3:G:210:ALA:H	1.60	0.41
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.41
2:F:442:GLN:O	2:F:445:LEU:HB2	2.21	0.41
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.49	0.41
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.41
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.41
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.45	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.19	0.41
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.41
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.41
1:A:103:LEU:O	1:A:106:ARG:HB2	2.20	0.41
2:F:423:VAL:HG12	2:F:423:VAL:O	2.20	0.41
1:A:206:ILE:O	1:A:273:LYS:HD2	2.20	0.41
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.41
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.41
2:D:281:TYR:CD2	2:D:320:PRO:HG2	2.56	0.41
2:E:387:ILE:HG22	2:E:388:ILE:N	2.36	0.41
1:A:407:GLY:CA	1:A:410:LEU:HD21	2.48	0.41
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	0.41
2:E:359:ASP:O	2:E:362:ILE:N	2.45	0.41
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.86	0.41
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.41
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.41
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.41
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.41
1:A:136:ILE:HD11	2:E:219:TYR:HE2	1.86	0.41
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
1:A:403:PHE:O	1:A:404:ALA:C	2.59	0.41
1:B:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.41
1:C:143:ARG:HD2	7:C:641:HOH:O	2.19	0.41
2:D:402:LEU:O	2:D:406:ARG:HG3	2.21	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
3:G:42:ARG:HG2	3:G:219:GLU:OE2	2.20	0.41
3:G:210:ALA:O	3:G:211:ASN:C	2.59	0.41
1:A:294:TYR:CE2	1:A:338:ILE:HD13	2.56	0.41
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.41
1:C:104:LEU:HD21	1:C:257:PHE:CZ	2.56	0.41
1:C:465:GLU:HG2	1:C:465:GLU:O	2.21	0.41
1:B:209:LYS:HE3	2:E:151:LYS:HZ3	1.86	0.41
1:B:201:CYS:O	1:B:229:THR:HA	2.21	0.41
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.41
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.02	0.41
2:E:105:ARG:NH1	2:E:208:LEU:HD23	2.36	0.41
1:C:289:PRO:HB2	7:C:618:HOH:O	2.21	0.41
1:A:441:GLN:O	1:A:445:ILE:HG12	2.21	0.41
1:B:353:GLU:OE2	1:B:366:ASN:ND2	2.50	0.41
1:A:422:VAL:O	1:A:426:GLU:HG2	2.21	0.41
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.41
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.41
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.40
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.03	0.40
2:F:63:MET:HE3	2:F:97:VAL:HG11	2.02	0.40
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.40
2:D:97:VAL:HG11	2:D:231:ARG:HB2	2.03	0.40
1:A:147:GLN:OE1	1:A:438:ILE:HD13	2.21	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.23	0.40
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.40
1:B:450:ARG:HA	1:B:450:ARG:HD3	1.87	0.40
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.40
1:B:344:SER:HA	5:F:600:ANP:O3G	2.21	0.40
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.40
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.56	0.40
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.40
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.40
1:B:187:LYS:HE3	1:B:227:LYS:HZ1	1.86	0.40
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.40
2:D:349:ASP:HA	2:D:350:PRO:HD2	1.85	0.40
2:E:282:GLN:NE2	2:E:282:GLN:H	2.19	0.40
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.53	0.40
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.40
2:D:84:ILE:HB	2:D:85:PRO:HD2	2.04	0.40
1:A:444:VAL:HG12	1:A:469:LEU:HD13	2.03	0.40
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.52	0.40
1:B:239:ALA:HB1	1:B:241:PRO:HD2	2.03	0.40
1:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.40
2:E:413:PHE:HE2	2:E:440:GLY:HA3	1.87	0.40
1:C:384:LYS:HE3	1:C:384:LYS:HB2	1.94	0.40
2:E:416:GLN:NE2	2:E:430:LYS:O	2.55	0.40
1:B:382:ALA:O	1:B:385:GLN:HB2	2.22	0.40
2:E:35:ALA:HB1	2:E:46:VAL:CG1	2.52	0.40
2:D:63:MET:HE3	2:D:228:ALA:HA	2.03	0.40
1:C:116:ASP:O	1:C:117:GLY:C	2.60	0.40
2:D:256:ASP:HA	2:D:257:ASN:HA	1.87	0.40
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.40
2:D:27:GLU:H	2:D:27:GLU:HG3	1.77	0.40
2:F:357:ILE:O	2:F:359:ASP:N	2.48	0.40
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.03	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
1:A:408:SER:O	1:A:409:ASP:HB2	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	485/510 (95%)	442 (91%)	36 (7%)	7 (1%)	14	40
1	B	485/510 (95%)	435 (90%)	43 (9%)	7 (1%)	14	40
1	C	490/510 (96%)	444 (91%)	38 (8%)	8 (2%)	12	36
2	D	465/482 (96%)	419 (90%)	43 (9%)	3 (1%)	30	63
2	E	464/482 (96%)	408 (88%)	47 (10%)	9 (2%)	10	32
2	F	464/482 (96%)	432 (93%)	30 (6%)	2 (0%)	39	71
3	G	116/272 (43%)	97 (84%)	18 (16%)	1 (1%)	21	52
All	All	2969/3248 (91%)	2677 (90%)	255 (9%)	37 (1%)	16	44

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	409	ASP
1	B	364	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP
1	C	476	HIS
2	D	28	GLY
2	E	161	GLY
2	E	205	VAL
3	G	81	ILE
1	A	364	ALA
1	A	404	ALA
1	B	236	ALA
1	B	452	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	121	PRO
2	E	455	GLN
1	B	411	ASP
1	C	405	GLN
1	C	475	GLN
2	D	474	ALA
2	E	122	GLU
2	F	327	ALA
1	A	484	ARG
1	B	359	LYS
1	C	409	ASP
2	E	33	LEU
1	B	458	PRO
2	E	28	GLY
2	E	279	VAL
1	B	68	PRO
2	F	279	VAL
2	D	279	VAL
1	A	246	ALA

### 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	393/412 (95%)	351 (89%)	42 (11%)	8	22
1	B	393/412 (95%)	346 (88%)	47 (12%)	6	16
1	C	397/412 (96%)	369 (93%)	28 (7%)	18	44
2	D	377/386 (98%)	346 (92%)	31 (8%)	14	36
2	E	376/386 (97%)	343 (91%)	33 (9%)	12	33
2	F	376/386 (97%)	354 (94%)	22 (6%)	24	54
3	G	102/230 (44%)	92 (90%)	10 (10%)	10	27
All	All	2414/2624 (92%)	2201 (91%)	213 (9%)	12	33

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	40	ARG
1	A	45	ARG
1	A	47	VAL
1	A	48	GLN
1	A	50	GLU
1	A	56	SER
1	A	80	LYS
1	A	94	ILE
1	A	99	VAL
1	A	101	GLU
1	A	102	GLU
1	A	121	ILE
1	A	140	ILE
1	A	143	ARG
1	A	151	LYS
1	A	164	ARG
1	A	173	THR
1	A	188	ARG
1	A	193	THR
1	A	195	GLU
1	A	211	SER
1	A	219	ARG
1	A	256	TYR
1	A	270	ASP
1	A	344	SER
1	A	367	VAL
1	A	371	VAL
1	A	380	THR
1	A	386	VAL
1	A	393	GLU
1	A	409	ASP
1	A	417	LEU
1	A	420	ARG
1	A	436	MET
1	A	444	VAL
1	A	457	GLU
1	A	472	VAL
1	A	474	SER
1	A	479	LEU
1	A	497	LEU
1	A	499	GLU
1	B	38	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	47	VAL
1	B	52	MET
1	B	79	ASP
1	B	80	LYS
1	B	123	SER
1	B	141	SER
1	B	143	ARG
1	B	145	PRO
1	B	164	ARG
1	B	173	THR
1	B	186	GLN
1	B	188	ARG
1	B	189	PHE
1	B	193	THR
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	221	THR
1	B	227	LYS
1	B	233	SER
1	B	256	TYR
1	B	270	ASP
1	B	298	VAL
1	B	299	PHE
1	B	335	SER
1	B	349	GLN
1	B	351	PHE
1	B	371	VAL
1	B	374	VAL
1	B	376	SER
1	B	380	THR
1	B	381	ARG
1	B	399	GLU
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
1	B	454	ASP
1	B	474	SER
1	B	479	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	482	LYS
1	B	484	ARG
1	B	490	SER
1	B	505	LEU
1	C	45	ARG
1	C	47	VAL
1	C	56	SER
1	C	63	SER
1	C	64	LEU
1	C	87	ILE
1	C	101	GLU
1	C	164	ARG
1	C	189	PHE
1	C	195	GLU
1	C	208	GLN
1	C	227	LYS
1	C	270	ASP
1	C	282	SER
1	C	298	VAL
1	C	334	VAL
1	C	349	GLN
1	C	399	GLU
1	C	400	VAL
1	C	406	PHE
1	C	440	GLU
1	C	444	VAL
1	C	474	SER
1	C	477	GLN
1	C	479	LEU
1	C	501	VAL
1	C	502	THR
1	C	505	LEU
2	D	27	GLU
2	D	37	GLU
2	D	56	SER
2	D	67	GLU
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	137	ILE
2	D	139	VAL
2	D	166	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	199	GLU
2	D	205	VAL
2	D	223	ASN
2	D	232	VAL
2	D	249	GLN
2	D	266	SER
2	D	282	GLN
2	D	306	SER
2	D	322	PRO
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	397	SER
2	D	400	ASP
2	D	401	LYS
2	D	405	SER
2	D	423	VAL
2	D	431	LEU
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	67	GLU
2	E	95	MET
2	E	127	SER
2	E	128	VAL
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	148	LYS
2	E	155	PHE
2	E	164	VAL
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	225	PRO
2	E	257	ASN
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	306	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	358	MET
2	E	365	SER
2	E	385	GLN
2	E	387	ILE
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	412	ARG
2	E	431	LEU
2	E	438	ILE
2	E	452	LEU
2	F	10	THR
2	F	27	GLU
2	F	42	GLU
2	F	67	GLU
2	F	95	MET
2	F	112	GLN
2	F	127	SER
2	F	139	VAL
2	F	166	ILE
2	F	191	ARG
2	F	200	MET
2	F	210	ASP
2	F	223	ASN
2	F	232	VAL
2	F	261	PHE
2	F	292	MET
2	F	386	ASP
2	F	387	ILE
2	F	397	SER
2	F	405	SER
2	F	428	LEU
2	F	455	GLN
3	G	4	LYS
3	G	11	LYS
3	G	22	SER
3	G	44	TYR
3	G	77	LEU
3	G	82	HIS
3	G	209	LEU
3	G	214	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	G	221	THR
3	G	254	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	349	GLN
1	A	396	GLN
1	B	48	GLN
1	B	65	ASN
1	B	70	ASN
1	B	349	GLN
1	C	260	ASN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	442	GLN
2	E	39	GLN
2	E	51	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	246	GLN
2	E	367	HIS
2	F	39	GLN
2	F	96	ASN
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	443	GLN
3	G	82	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z  > 2$
5	ANP	A	600	4	27,33,33	1.26	4 (14%)	30,52,52	1.22	3 (10%)
5	ANP	B	600	4	27,33,33	1.32	4 (14%)	30,52,52	1.53	6 (20%)
5	ANP	C	600	4	27,33,33	1.54	4 (14%)	30,52,52	1.71	10 (33%)
6	ADP	D	600	4	22,29,29	0.96	1 (4%)	27,45,45	1.29	3 (11%)
5	ANP	F	600	4	27,33,33	1.26	3 (11%)	30,52,52	1.46	5 (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
5	ANP	A	600	4	-	0/12/38/38	0/3/3/3
5	ANP	B	600	4	-	2/12/38/38	0/3/3/3
5	ANP	C	600	4	-	0/12/38/38	0/3/3/3
6	ADP	D	600	4	-	0/12/32/32	0/3/3/3
5	ANP	F	600	4	-	0/12/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	600	ANP	PG-O3G	-4.29	1.44	1.56
5	B	600	ANP	PG-O2G	-3.45	1.47	1.56
5	A	600	ANP	PG-O3G	-3.30	1.47	1.56
5	C	600	ANP	PB-O2B	-3.29	1.47	1.56
5	F	600	ANP	PG-O3G	-3.00	1.48	1.56
5	A	600	ANP	PB-O2B	-2.61	1.49	1.56
5	B	600	ANP	PG-O3G	-2.21	1.50	1.56
5	B	600	ANP	PB-O2B	-2.15	1.50	1.56
5	F	600	ANP	PG-O2G	-2.01	1.51	1.56
6	D	600	ADP	O4'-C1'	2.12	1.43	1.41
5	A	600	ANP	PB-O1B	2.17	1.48	1.46
5	C	600	ANP	PG-O1G	2.17	1.48	1.46
5	A	600	ANP	C2-N1	2.29	1.38	1.33
5	B	600	ANP	PG-O1G	2.32	1.48	1.46
5	F	600	ANP	PG-O1G	3.34	1.49	1.46
5	C	600	ANP	PB-O3A	3.59	1.63	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	ANP	C2'-C1'-N9	-4.70	107.11	114.29
5	B	600	ANP	O4'-C1'-N9	-3.99	99.75	108.10
5	F	600	ANP	O1G-PG-N3B	-3.89	105.94	111.90
5	C	600	ANP	PA-O3A-PB	-3.69	120.30	132.67
5	C	600	ANP	O2G-PG-O1G	-3.19	105.00	113.49
5	C	600	ANP	O3A-PB-N3B	-3.08	97.97	106.44
5	C	600	ANP	O3'-C3'-C2'	-2.76	102.85	111.83
5	C	600	ANP	O2'-C2'-C3'	-2.49	103.73	111.83
5	B	600	ANP	O3A-PA-O5'	-2.43	96.48	102.94
5	F	600	ANP	C2'-C1'-N9	-2.23	110.89	114.29
5	B	600	ANP	O1G-PG-N3B	-2.16	108.58	111.90
5	C	600	ANP	C1'-N9-C4	-2.14	123.72	126.94
5	C	600	ANP	O1G-PG-N3B	-2.12	108.65	111.90
6	D	600	ADP	O3'-C3'-C2'	-2.10	105.00	111.83
5	B	600	ANP	C1'-N9-C4	-2.08	123.80	126.94
5	F	600	ANP	O5'-C5'-C4'	-2.04	101.60	109.12
5	A	600	ANP	O2'-C2'-C3'	2.14	118.78	111.83
5	A	600	ANP	C4-C5-N7	2.16	111.47	109.48
5	B	600	ANP	O3G-PG-O2G	2.20	114.11	107.58
6	D	600	ADP	N6-C6-N1	2.30	124.14	119.20
5	C	600	ANP	O3A-PA-O5'	2.41	109.32	102.94
5	B	600	ANP	O2A-PA-O3A	2.50	116.44	105.09
5	F	600	ANP	O1B-PB-N3B	2.60	115.88	111.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	600	ANP	O3G-PG-O1G	2.71	120.69	113.49
5	C	600	ANP	O1B-PB-N3B	2.78	116.16	111.90
5	F	600	ANP	C4-C5-N7	2.82	112.08	109.48
6	D	600	ADP	C4-C5-N7	3.02	112.26	109.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	600	ANP	O1G-PG-N3B-PB
5	B	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ANP	2	0
5	B	600	ANP	5	0
5	C	600	ANP	4	0
6	D	600	ADP	2	0
5	F	600	ANP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	487/510 (95%)	-0.66	4 (0%) 87 86	16, 38, 67, 97	0
1	B	479/510 (93%)	-0.59	13 (2%) 58 52	15, 37, 75, 98	0
1	C	492/510 (96%)	-0.79	6 (1%) 81 78	13, 33, 63, 95	0
2	D	467/482 (96%)	-0.88	0 100 100	13, 34, 62, 83	0
2	E	466/482 (96%)	-0.44	12 (2%) 59 54	18, 45, 79, 98	0
2	F	466/482 (96%)	-0.83	1 (0%) 95 95	13, 34, 63, 87	0
3	G	122/272 (44%)	0.00	6 (4%) 33 27	13, 60, 100, 100	0
All	All	2979/3248 (91%)	-0.67	42 (1%) 78 75	13, 37, 74, 100	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	473	LEU	4.4
1	C	407	GLY	4.3
1	C	408	SER	4.1
1	A	408	SER	3.8
2	E	395	GLU	3.6
1	B	400	VAL	3.6
1	B	193	THR	3.5
3	G	211	ASN	3.5
3	G	43	VAL	3.5
2	E	390	ILE	3.3
3	G	216	SER	3.3
1	B	412	ALA	3.2
3	G	210	ALA	3.1
1	B	492	GLU	3.0
1	B	474	SER	3.0
2	E	398	GLU	2.9
1	C	409	ASP	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	423	VAL	2.8
1	A	92	GLY	2.8
1	B	415	GLN	2.8
1	B	510	ALA	2.8
1	A	93	ALA	2.7
1	B	392	LEU	2.6
2	E	474	ALA	2.6
2	F	178	GLY	2.6
1	B	506	ALA	2.5
1	C	193	THR	2.4
2	E	424	PHE	2.4
2	E	426	GLY	2.4
1	A	409	ASP	2.4
1	B	413	ALA	2.4
2	E	9	THR	2.4
3	G	86	ALA	2.3
1	B	401	ALA	2.2
1	C	492	GLU	2.2
2	E	42	GLU	2.2
1	B	503	ASN	2.2
1	C	405	GLN	2.2
2	E	427	HIS	2.1
1	B	411	ASP	2.1
3	G	209	LEU	2.1
2	E	391	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	F	601	1/1	0.94	0.29	16.38	24,24,24,24	0
4	MG	D	601	1/1	0.93	0.36	11.22	22,22,22,22	0
5	ANP	B	600	31/31	0.97	0.12	-0.42	30,34,37,38	0
5	ANP	A	600	31/31	0.97	0.11	-0.51	25,27,32,32	0
5	ANP	F	600	31/31	0.98	0.10	-0.63	26,28,29,31	0
6	ADP	D	600	27/27	0.99	0.09	-0.68	20,23,24,25	0
5	ANP	C	600	31/31	0.98	0.09	-1.09	19,24,26,29	0
4	MG	B	601	1/1	0.94	0.22	-	36,36,36,36	0
4	MG	A	601	1/1	0.93	0.16	-	26,26,26,26	0
4	MG	C	601	1/1	0.96	0.23	-	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.