



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:07 PM GMT

PDB ID : 1E1R  
Title : BOVINE MITOCHONDRIAL F1-ATPASE INHIBITED BY MG2+ADP  
AND ALUMINIUM FLUORIDE  
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2000-05-10  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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.

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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

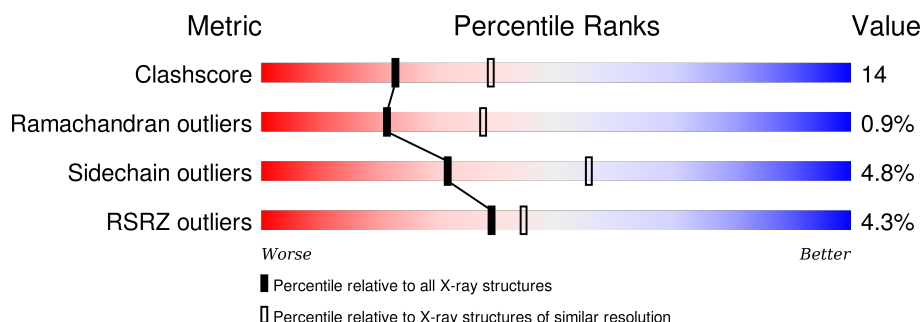
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>3%</div> <div>63% 30% 5%</div> </div>
1	B	510	<div> <div>5%</div> <div>59% 31% 6%</div> </div>
1	C	510	<div> <div>2%</div> <div>67% 26% . .</div> </div>
2	D	482	<div> <div>2%</div> <div>67% 26% . .</div> </div>
2	E	482	<div> <div>6%</div> <div>61% 33% . .</div> </div>
2	F	482	<div> <div>2%</div> <div>72% 22% . .</div> </div>
3	G	272	<div> <div>9%</div> <div>32% 12% . 55%</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
5	MG	D	601	-	-	-	X
5	MG	F	601	-	-	-	X
7	AF3	D	602	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23688 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	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	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	CONFLICT	UNP P19483
B	481	GLY	SER	CONFLICT	UNP P19483
C	481	GLY	SER	CONFLICT	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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

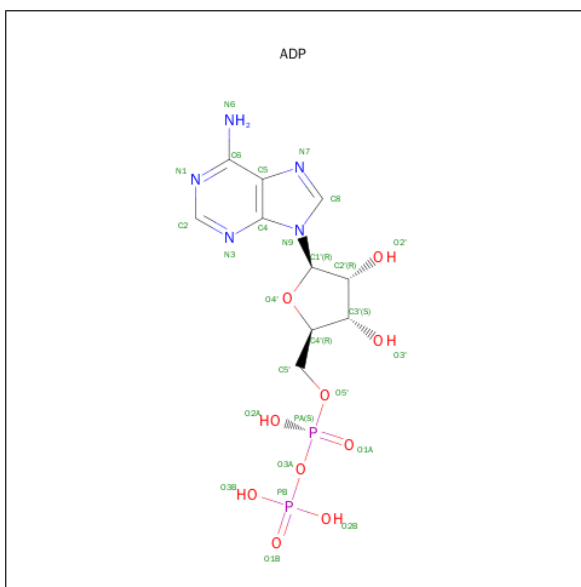


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	F	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

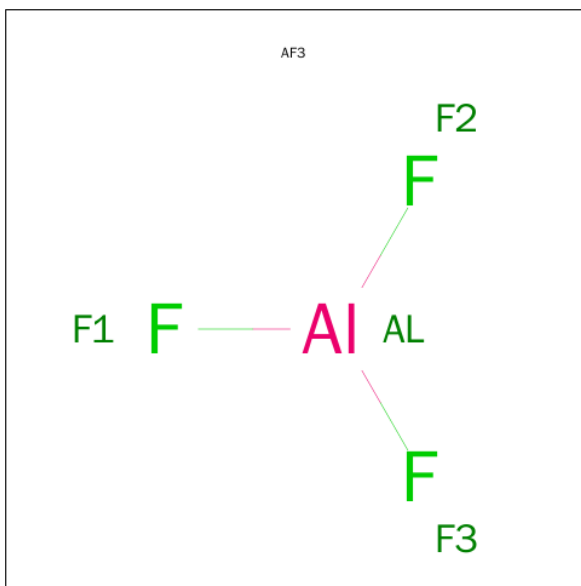
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

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



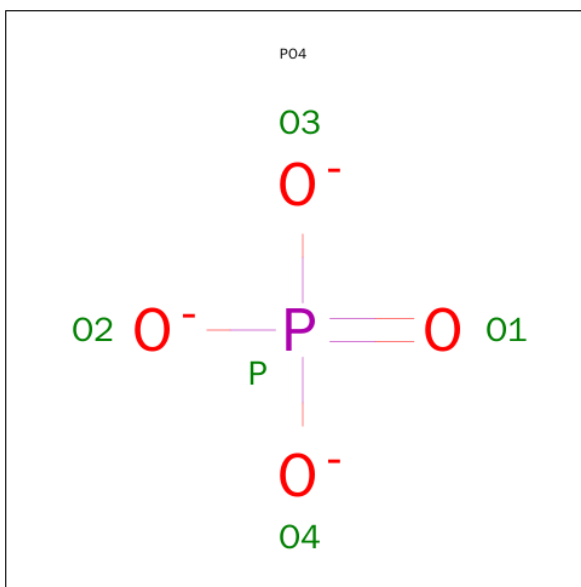
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $\text{AlF}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 4	Al 1	F 3	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		

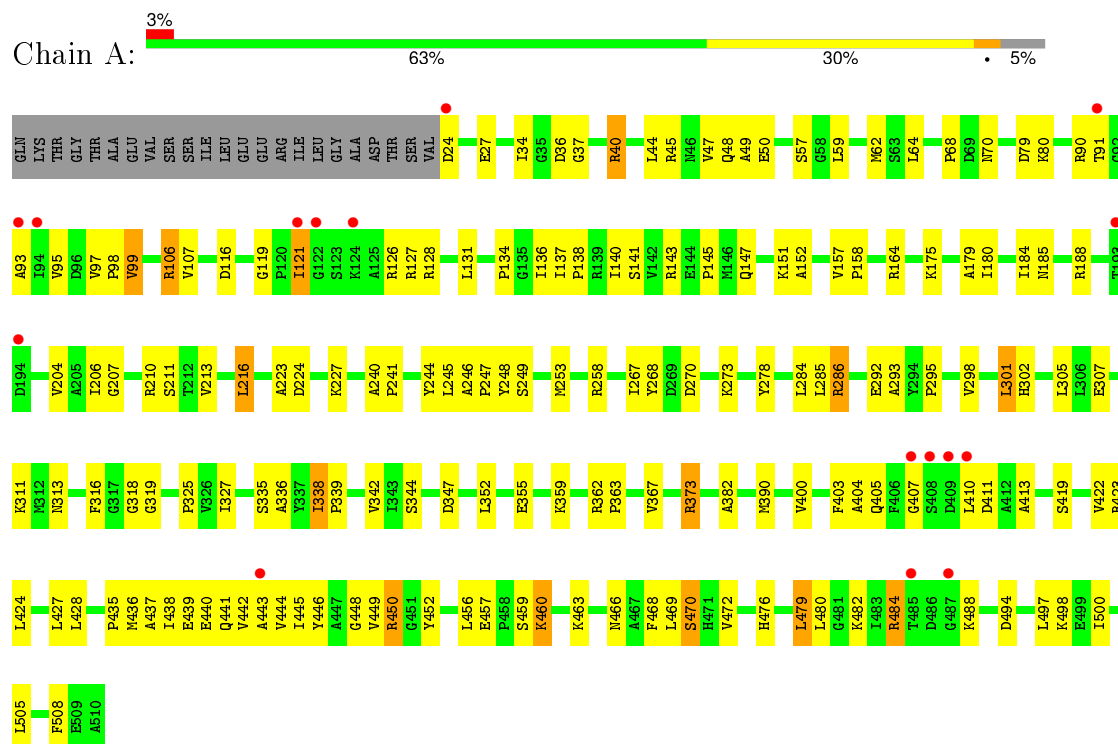
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	144	Total	O	0	0
			144	144		
9	B	126	Total	O	0	0
			126	126		
9	C	171	Total	O	0	0
			171	171		
9	D	145	Total	O	0	0
			145	145		
9	E	105	Total	O	0	0
			105	105		
9	F	148	Total	O	0	0
			148	148		
9	G	21	Total	O	0	0
			21	21		

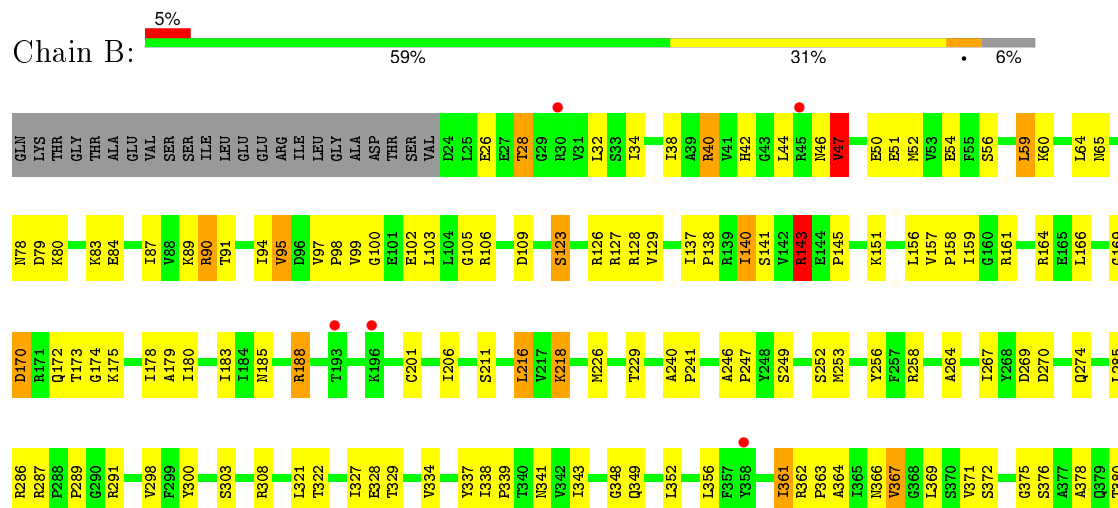
### 3 Residue-property plots

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.

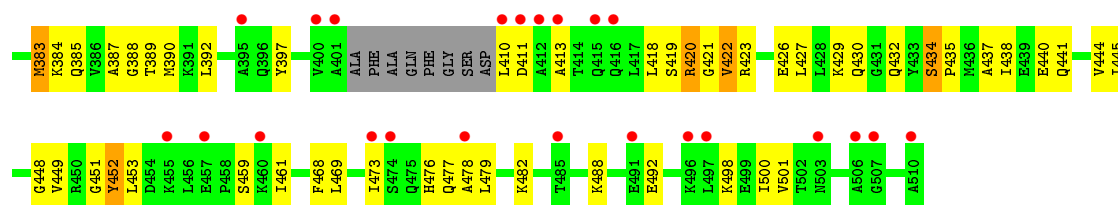
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



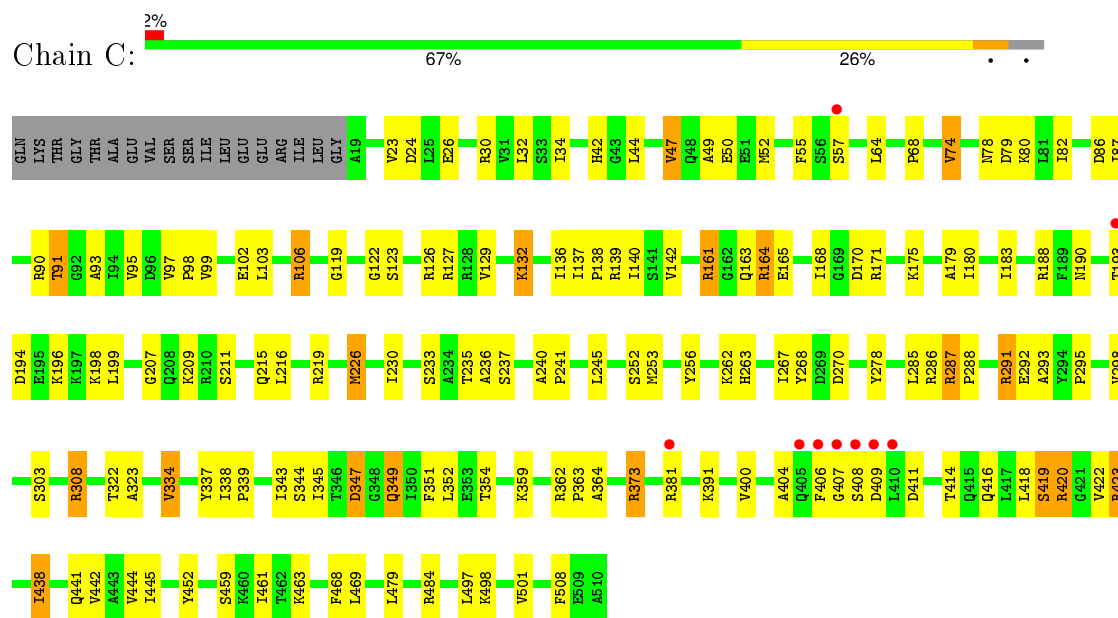
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



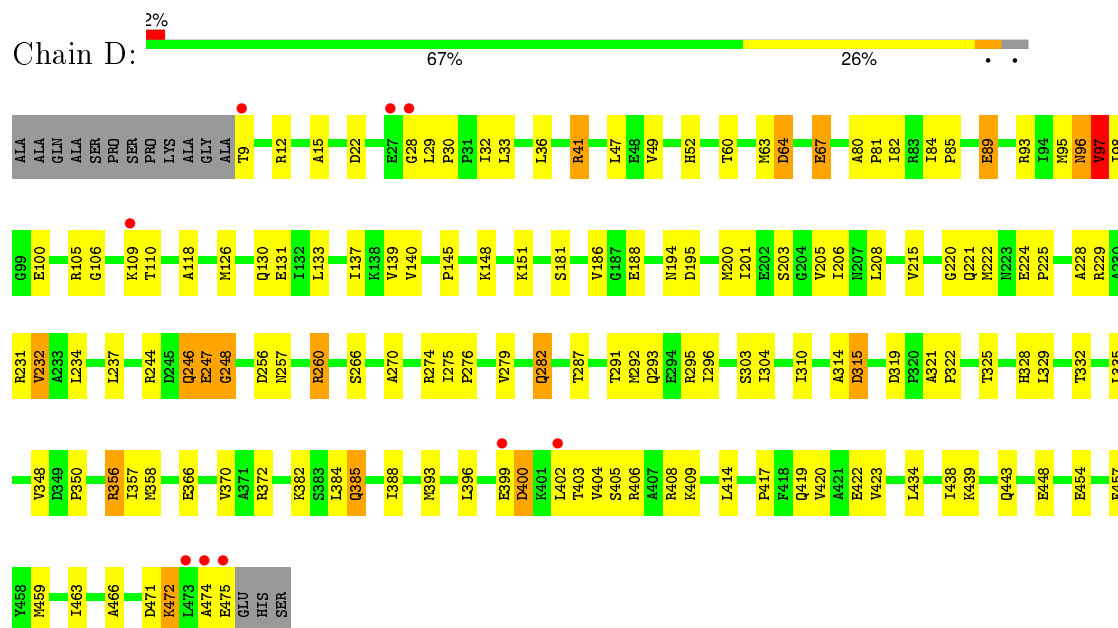




• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

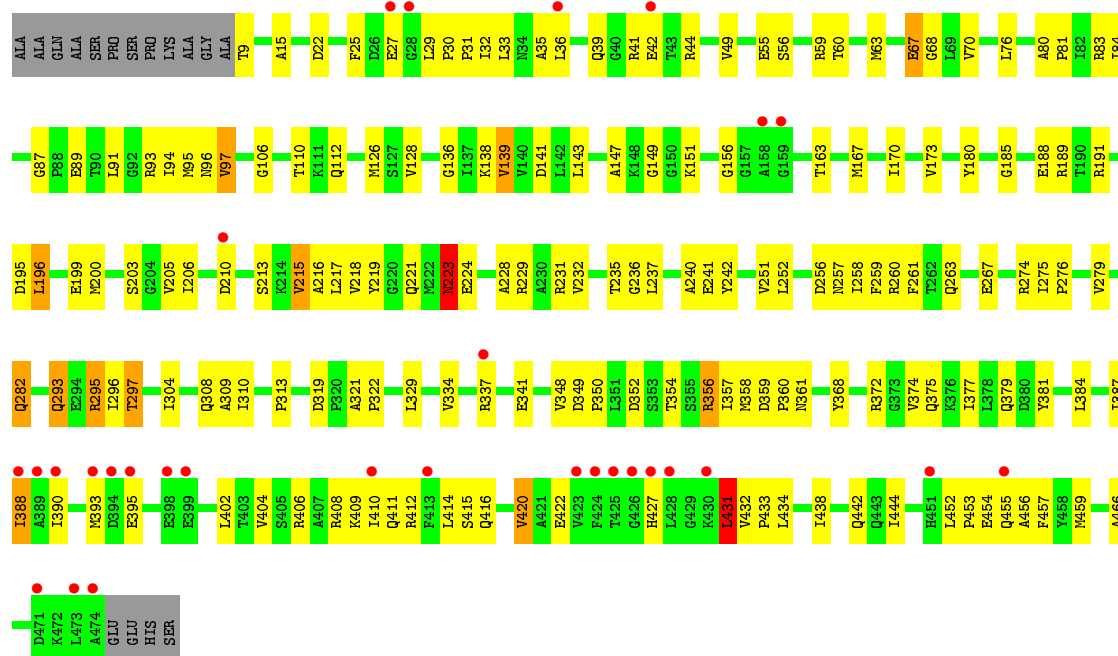


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

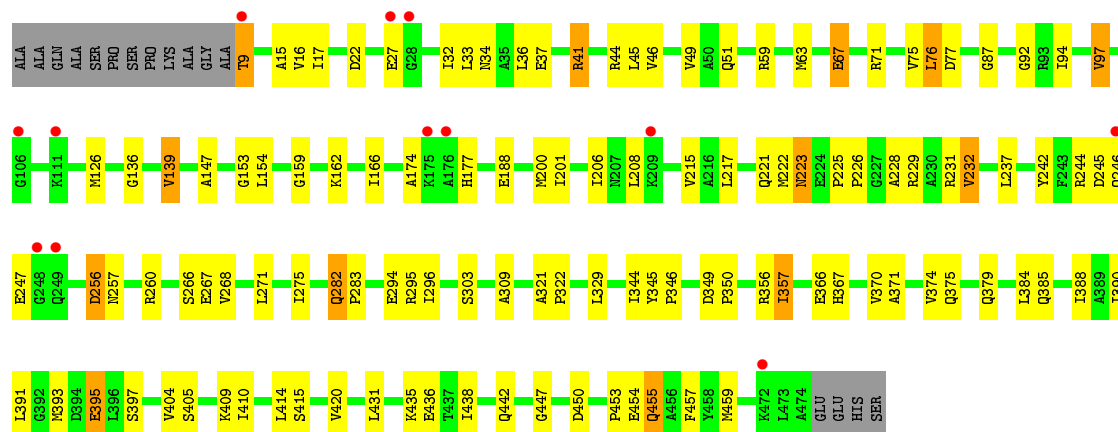


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

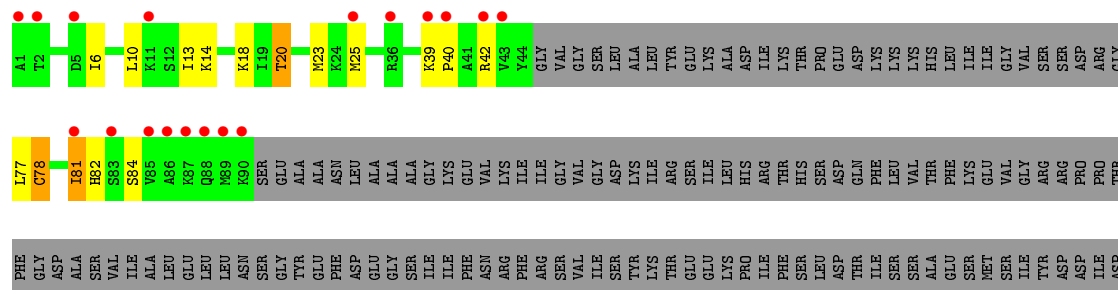
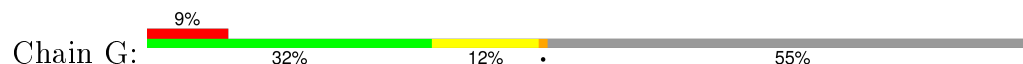




- Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



- 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, $\alpha$ , $\beta$ , $\gamma$	278.60 Å 106.70 Å 137.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.50) 95.4 (19.99-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.50 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.218 , 0.282 0.205 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 65.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 135815 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, PO4, ADP, AF3

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	0.51	0/3766	1.05	12/5080 (0.2%)
1	B	0.52	0/3704	1.09	19/4995 (0.4%)
1	C	0.56	0/3799	1.17	22/5126 (0.4%)
2	D	0.56	0/3596	1.13	17/4879 (0.3%)
2	E	0.51	0/3587	1.10	19/4867 (0.4%)
2	F	0.53	0/3587	1.09	13/4867 (0.3%)
3	G	0.46	0/949	1.01	3/1266 (0.2%)
All	All	0.53	0/22988	1.10	105/31080 (0.3%)

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
2	E	0	1

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	254	ARG	CD-NE-CZ	15.19	144.86	123.60
3	G	254	ARG	NE-CZ-NH1	10.28	125.44	120.30
2	D	231	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	C	127	ARG	NE-CZ-NH2	-9.83	115.39	120.30
2	D	229	ARG	NE-CZ-NH2	-9.80	115.40	120.30
2	E	260	ARG	CD-NE-CZ	9.70	137.18	123.60
1	C	291	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	B	40	ARG	CD-NE-CZ	9.19	136.46	123.60
1	A	450	ARG	NE-CZ-NH2	-9.11	115.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	260	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	40	ARG	NE-CZ-NH1	8.98	124.79	120.30
2	D	105	ARG	NE-CZ-NH1	-8.72	115.94	120.30
2	E	295	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	C	219	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	C	161	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	C	106	ARG	NE-CZ-NH2	-7.91	116.35	120.30
2	F	41	ARG	CG-CD-NE	7.84	128.27	111.80
1	B	128	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	C	423	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	E	231	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	E	44	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	D	12	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	373	ARG	NE-CZ-NH2	-7.45	116.58	120.30
2	F	229	ARG	CD-NE-CZ	7.33	133.87	123.60
1	C	423	ARG	CD-NE-CZ	7.28	133.79	123.60
2	E	231	ARG	NE-CZ-NH1	-7.22	116.69	120.30
2	E	59	ARG	NE-CZ-NH2	-7.12	116.74	120.30
3	G	254	ARG	NE-CZ-NH2	-7.11	116.75	120.30
2	D	356	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	C	423	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	D	41	ARG	CG-CD-NE	6.87	126.22	111.80
1	B	106	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	90	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	A	40	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	40	ARG	NE-CZ-NH2	6.64	123.62	120.30
2	D	95	MET	C-N-CA	6.64	138.29	121.70
1	C	484	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	373	ARG	NE-CZ-NH2	6.49	123.54	120.30
2	F	244	ARG	NE-CZ-NH2	-6.43	117.09	120.30
2	E	191	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	F	71	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	E	41	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	171	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	216	LEU	CA-CB-CG	6.28	129.74	115.30
2	E	44	ARG	CD-NE-CZ	6.22	132.31	123.60
2	E	41	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	450	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	E	295	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	143	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	D	319	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	127	ARG	NE-CZ-NH1	6.02	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	356	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	226	MET	CA-CB-CG	6.00	123.50	113.30
1	B	126	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	F	71	ARG	CD-NE-CZ	5.94	131.91	123.60
2	D	96	ASN	CB-CA-C	-5.91	98.59	110.40
1	A	164	ARG	NE-CZ-NH2	-5.89	117.35	120.30
2	D	315	ASP	CB-CG-OD1	5.89	123.60	118.30
2	D	222	MET	CB-CA-C	-5.83	98.74	110.40
1	B	308	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	C	90	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	106	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	E	431	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	90	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
2	D	260	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	E	44	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	E	274	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	C	287	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	C	308	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	B	420	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	126	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	47	VAL	CB-CA-C	-5.55	100.86	111.40
1	B	109	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	127	ARG	CD-NE-CZ	5.54	131.36	123.60
2	E	59	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	143	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	90	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	210	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	C	139	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	D	274	ARG	NE-CZ-NH1	-5.41	117.59	120.30
2	F	244	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	D	64	ASP	CB-CG-OD1	5.36	123.12	118.30
2	F	267	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	C	349	GLN	CB-CA-C	-5.33	99.74	110.40
1	C	219	ARG	NH1-CZ-NH2	5.32	125.26	119.40
2	F	256	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	170	ASP	CB-CG-OD1	5.31	123.08	118.30
2	F	77	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	127	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	347	ASP	CB-CG-OD1	5.21	122.98	118.30
1	C	420	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	E	189	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	E	95	MET	CA-CB-CG	5.16	122.07	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	260	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	84	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	B	287	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	F	295	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	F	44	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	D	97	VAL	CB-CA-C	-5.07	101.76	111.40
1	B	47	VAL	N-CA-CB	5.06	122.63	111.50
1	B	258	ARG	CD-NE-CZ	5.05	130.68	123.60
2	F	357	ILE	CA-CB-CG2	5.05	121.00	110.90
1	A	143	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	D	195	ASP	CB-CG-OD1	5.02	122.82	118.30
2	D	372	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	223	ASN	Mainchain

## 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	3814	124	0
1	B	3656	0	3765	117	0
1	C	3748	0	3844	96	0
2	D	3539	0	3592	92	0
2	E	3530	0	3587	121	0
2	F	3530	0	3586	89	0
3	G	945	0	1019	20	0
4	A	31	0	13	0	0
4	B	31	0	13	4	0
4	C	31	0	13	1	0
4	F	31	0	13	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	D	27	0	12	1	0
7	D	4	0	0	1	0
8	E	5	0	0	0	0
9	A	144	0	0	6	0
9	B	126	0	0	4	0
9	C	171	0	0	4	0
9	D	145	0	0	5	0
9	E	105	0	0	4	0
9	F	148	0	0	5	0
9	G	21	0	0	1	0
All	All	23688	0	23271	626	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 14.

All (626) 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:91:THR:HG22	1:C:93:ALA:H	1.27	1.00
2:F:282:GLN:H	2:F:282:GLN:HE21	0.99	0.98
2:F:166:ILE:HD11	2:F:309:ALA:HB2	1.41	0.98
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.50	0.94
2:D:282:GLN:H	2:D:282:GLN:HE21	1.11	0.93
1:A:382:ALA:HB2	1:A:488:LYS:HA	1.53	0.91
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.54	0.89
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.25	0.85
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.60	0.83
2:F:282:GLN:H	2:F:282:GLN:NE2	1.77	0.83
3:G:20:THR:HG22	3:G:236:SER:HB3	1.61	0.82
2:D:139:VAL:HG12	2:D:414:LEU:HD22	1.61	0.81
2:F:139:VAL:HG13	2:F:414:LEU:HD22	1.64	0.80
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.64	0.80
2:E:203:SER:HB2	2:E:420:VAL:HG22	1.64	0.78
1:C:419:SER:O	1:C:423:ARG:HG2	1.83	0.78
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.66	0.78
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.66	0.78
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.65	0.78
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.66	0.77
1:A:80:LYS:HE3	2:D:33:LEU:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.65	0.77
1:B:303:SER:HB2	2:F:222:MET:HB3	1.67	0.75
1:C:52:MET:O	1:C:91:THR:HB	1.86	0.74
1:A:99:VAL:HG23	1:A:253:MET:HA	1.70	0.74
1:C:175:LYS:HE3	4:C:600:ANP:O1B	1.88	0.74
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.68	0.74
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.03	0.74
2:F:282:GLN:HE21	2:F:282:GLN:N	1.82	0.72
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.71	0.72
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.71	0.72
1:A:390:MET:HE2	1:A:424:LEU:HB3	1.71	0.72
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.70	0.72
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.53	0.71
2:D:282:GLN:H	2:D:282:GLN:NE2	1.87	0.71
2:F:223:ASN:H	2:F:223:ASN:HD22	1.36	0.71
1:C:288:PRO:HG2	2:D:270:ALA:HB1	1.73	0.71
2:E:282:GLN:HE21	2:E:282:GLN:H	1.37	0.70
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.56	0.70
2:D:408:ARG:HD3	2:D:454:GLU:OE2	1.90	0.70
1:B:479:LEU:HA	1:B:482:LYS:HD2	1.73	0.70
2:F:405:SER:O	2:F:409:LYS:HG3	1.92	0.69
2:E:173:VAL:HG21	2:E:252:LEU:HD22	1.75	0.69
1:C:211:SER:HB3	2:F:126:MET:CE	2.23	0.69
1:C:344:SER:HA	7:D:602:AF3:F1	1.83	0.68
2:F:200:MET:HB3	2:F:206:ILE:HG12	1.76	0.68
2:D:188:GLU:O	2:D:221:GLN:HB3	1.95	0.68
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.74	0.68
2:D:393:MET:HE2	2:D:404:VAL:HG11	1.77	0.67
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.24	0.67
1:B:420:ARG:HH12	1:B:451:GLY:HA2	1.59	0.67
1:B:38:ILE:HG13	1:B:285:LEU:HD21	1.76	0.67
1:A:140:ILE:HG23	1:A:311:LYS:HG3	1.77	0.67
1:B:183:ILE:HD11	1:B:267:ILE:HD12	1.76	0.67
2:D:388:ILE:HD12	2:D:393:MET:HE3	1.77	0.66
1:C:285:LEU:O	1:C:286:ARG:HB2	1.94	0.66
2:F:188:GLU:O	2:F:222:MET:HG3	1.95	0.66
1:B:366:ASN:ND2	1:B:369:LEU:HD12	2.10	0.66
2:D:366:GLU:O	2:D:370:VAL:HG23	1.96	0.65
3:G:23:MET:SD	3:G:232:MET:HE2	2.36	0.65
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.79	0.65
1:A:286:ARG:HH11	1:A:286:ARG:HG2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.79	0.65
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.79	0.64
1:B:78:ASN:HD21	1:B:80:LYS:HD3	1.62	0.64
2:D:419:GLN:O	2:D:422:GLU:HG3	1.97	0.64
2:D:384:LEU:HD22	2:D:396:LEU:HD21	1.78	0.64
2:E:388:ILE:HG23	2:E:393:MET:SD	2.38	0.64
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.79	0.64
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.80	0.64
3:G:14:LYS:HA	3:G:243:ILE:HD11	1.80	0.64
1:C:211:SER:HB3	2:F:126:MET:HE1	1.78	0.64
1:C:91:THR:HG22	1:C:93:ALA:N	2.08	0.63
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.27	0.63
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.80	0.63
2:E:163:THR:HG21	2:E:199:GLU:OE1	1.98	0.63
2:F:223:ASN:H	2:F:223:ASN:ND2	1.96	0.63
1:C:52:MET:HE3	1:C:95:VAL:HG13	1.81	0.63
2:E:375:GLN:O	2:E:379:GLN:HG3	1.99	0.63
1:C:418:LEU:O	1:C:422:VAL:HG23	1.98	0.62
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.82	0.62
1:B:52:MET:HG2	1:B:95:VAL:HG22	1.81	0.62
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.81	0.62
2:E:223:ASN:H	2:E:223:ASN:HD22	1.47	0.62
1:C:400:VAL:HG23	1:C:418:LEU:HD21	1.82	0.61
1:C:237:SER:HB3	2:F:294:GLU:HG3	1.82	0.61
1:B:349:GLN:NE2	9:B:2113:HOH:O	2.33	0.61
2:F:9:THR:HG21	2:F:27:GLU:O	2.00	0.61
2:E:63:MET:CE	2:E:228:ALA:HA	2.30	0.61
1:A:204:VAL:HG12	1:A:206:ILE:HD11	1.83	0.61
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.81	0.61
1:C:463:LYS:HE2	1:C:508:PHE:CZ	2.35	0.61
1:B:419:SER:O	1:B:423:ARG:HG2	2.01	0.61
2:D:409:LYS:HD3	2:D:457:PHE:CE1	2.36	0.61
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.30	0.60
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.84	0.60
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.83	0.60
1:B:175:LYS:NZ	9:B:2122:HOH:O	2.33	0.60
1:B:175:LYS:HE3	4:B:600:ANP:O1B	2.02	0.60
2:D:139:VAL:HG11	9:D:2118:HOH:O	2.02	0.60
1:C:175:LYS:NZ	9:C:2061:HOH:O	2.34	0.60
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.32	0.60
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.37	0.59
2:F:223:ASN:N	2:F:223:ASN:HD22	1.96	0.59
2:D:205:VAL:HG12	2:D:215:VAL:HG23	1.84	0.59
2:E:89:GLU:HG3	2:E:110:THR:HA	1.85	0.59
1:A:211:SER:HB3	2:D:126:MET:HE3	1.83	0.59
1:A:151:LYS:HG2	1:A:441:GLN:HG2	1.83	0.59
2:F:275:ILE:O	2:F:283:PRO:HG3	2.02	0.59
2:E:149:GLY:HA2	2:E:304:ILE:O	2.02	0.59
1:A:403:PHE:HE1	3:G:18:LYS:HB3	1.65	0.59
1:C:183:ILE:HD11	1:C:267:ILE:HD13	1.84	0.59
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.83	0.59
2:E:282:GLN:H	2:E:282:GLN:NE2	2.00	0.59
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.85	0.59
1:C:404:ALA:C	1:C:406:PHE:H	2.05	0.59
1:C:359:LYS:HG3	2:F:379:GLN:HG2	1.84	0.59
2:E:195:ASP:O	2:E:199:GLU:HB2	2.03	0.58
1:C:23:VAL:O	1:C:23:VAL:HG12	2.03	0.58
1:A:440:GLU:O	1:A:444:VAL:HG13	2.03	0.58
2:D:89:GLU:HG3	2:D:110:THR:HA	1.86	0.58
1:C:168:ILE:HD11	1:C:339:PRO:HB3	1.84	0.58
1:B:26:GLU:HB3	1:B:46:ASN:ND2	2.18	0.58
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.86	0.58
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.58
2:E:126:MET:CE	2:E:297:THR:HG21	2.34	0.58
1:C:44:LEU:O	1:C:47:VAL:HG22	2.03	0.58
2:F:166:ILE:HD11	2:F:309:ALA:CB	2.28	0.57
3:G:6:ILE:HG21	3:G:250:PHE:HB2	1.86	0.57
2:D:382:LYS:HA	2:D:385:GLN:HE21	1.69	0.57
1:A:98:PRO:HD3	1:A:126:ARG:HH21	1.67	0.57
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.39	0.57
2:E:408:ARG:HH21	2:E:412:ARG:NH2	2.02	0.57
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.34	0.57
1:A:34:ILE:HD11	1:A:79:ASP:HB2	1.86	0.57
1:C:164:ARG:HG3	1:C:323:ALA:HB3	1.86	0.57
2:E:49:VAL:HA	2:E:60:THR:HG22	1.87	0.57
1:B:158:PRO:O	1:B:375:GLY:HA3	2.05	0.57
2:D:382:LYS:HA	2:D:385:GLN:NE2	2.19	0.57
2:D:314:ALA:O	2:D:315:ASP:HB2	2.03	0.57
1:A:91:THR:HA	9:A:2017:HOH:O	2.04	0.57
1:C:24:ASP:OD2	1:C:26:GLU:HB2	2.05	0.56
1:A:62:MET:CE	1:A:64:LEU:HD21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.70	0.56
2:E:334:VAL:HG21	2:E:352:ASP:HB3	1.87	0.56
2:E:223:ASN:ND2	2:E:223:ASN:H	2.02	0.56
1:B:141:SER:O	1:B:143:ARG:HD2	2.05	0.56
2:E:83:ARG:HD3	9:E:2018:HOH:O	2.05	0.56
1:A:419:SER:O	1:A:423:ARG:HD3	2.05	0.56
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.70	0.56
2:E:422:GLU:HG2	2:E:427:HIS:O	2.05	0.56
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.41	0.56
1:B:432:GLN:OE1	4:B:600:ANP:H2'	2.05	0.56
1:B:137:ILE:N	1:B:138:PRO:CD	2.69	0.56
2:E:402:LEU:HD23	2:E:406:ARG:HH21	1.70	0.56
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.88	0.56
2:E:404:VAL:O	2:E:408:ARG:HG3	2.05	0.56
2:D:246:GLN:O	2:D:247:GLU:HG3	2.06	0.56
2:F:384:LEU:O	2:F:388:ILE:HG12	2.06	0.56
1:C:30:ARG:HA	1:C:86:ASP:O	2.07	0.55
2:F:367:HIS:HA	2:F:438:ILE:HD12	1.88	0.55
1:C:411:ASP:OD1	1:C:414:THR:HG23	2.06	0.55
2:F:41:ARG:HD3	2:F:45:LEU:HD23	1.89	0.55
1:B:441:GLN:O	1:B:445:ILE:HG13	2.06	0.55
1:A:258:ARG:O	1:A:319:GLY:HA3	2.06	0.55
1:B:151:LYS:HE2	1:B:427:LEU:O	2.06	0.55
2:E:139:VAL:HG21	2:E:348:VAL:HB	1.89	0.55
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.71	0.55
2:D:404:VAL:O	2:D:408:ARG:HG3	2.07	0.55
1:A:241:PRO:O	1:A:244:TYR:HB3	2.07	0.55
2:D:93:ARG:NH2	2:D:106:GLY:O	2.40	0.55
2:D:474:ALA:O	2:D:475:GLU:HB2	2.07	0.55
2:F:228:ALA:O	2:F:232:VAL:HG22	2.07	0.54
1:C:68:PRO:HA	9:D:2001:HOH:O	2.06	0.54
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.89	0.54
2:E:63:MET:HE3	2:E:228:ALA:HA	1.88	0.54
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.43	0.54
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.54
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.89	0.54
1:A:184:ILE:HD12	1:A:223:ALA:HB3	1.89	0.54
1:B:78:ASN:ND2	1:B:80:LYS:HD3	2.22	0.54
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.89	0.54
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.22	0.54
1:A:411:ASP:OD2	1:A:413:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:O	1:B:188:ARG:HD2	2.08	0.54
1:A:286:ARG:HH12	3:G:272:LEU:HD13	1.72	0.54
1:B:216:LEU:O	1:B:216:LEU:HD22	2.08	0.54
2:D:266:SER:HB3	2:D:282:GLN:NE2	2.23	0.53
2:D:402:LEU:O	2:D:406:ARG:HG3	2.07	0.53
2:D:36:LEU:HB2	2:D:47:LEU:HB2	1.90	0.53
2:D:97:VAL:HG22	9:D:2062:HOH:O	2.07	0.53
2:F:188:GLU:H	2:F:221:GLN:NE2	2.06	0.53
2:F:154:LEU:HD12	2:F:166:ILE:HG12	1.91	0.53
2:F:126:MET:HE3	9:F:2039:HOH:O	2.09	0.53
2:F:438:ILE:O	2:F:442:GLN:HG3	2.08	0.53
1:B:352:LEU:HA	1:B:364:ALA:O	2.08	0.53
2:F:147:ALA:HB2	2:F:357:ILE:HG13	1.89	0.53
1:A:313:ASN:OD1	1:A:316:PHE:HD1	1.90	0.53
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.44	0.53
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.89	0.53
1:A:441:GLN:O	1:A:445:ILE:HG12	2.08	0.53
2:F:454:GLU:HG3	9:F:2139:HOH:O	2.08	0.53
1:B:388:GLY:O	1:B:392:LEU:HG	2.08	0.53
1:C:129:VAL:O	1:C:308:ARG:NH1	2.40	0.53
1:B:385:GLN:NE2	1:B:488:LYS:NZ	2.58	0.52
2:D:9:THR:HG21	2:D:28:GLY:HA3	1.91	0.52
2:F:34:ASN:O	2:F:49:VAL:HG23	2.09	0.52
1:B:348:GLY:HA2	1:B:371:VAL:HG13	1.91	0.52
1:C:99:VAL:HG13	1:C:253:MET:HA	1.90	0.52
2:F:201:ILE:HD13	2:F:208:LEU:HD11	1.91	0.52
1:B:151:LYS:HZ1	1:B:430:GLN:HB2	1.74	0.52
1:C:233:SER:OG	1:C:235:THR:HG23	2.10	0.52
1:B:172:GLN:NE2	2:E:356:ARG:NE	2.57	0.52
2:E:32:ILE:O	2:E:33:LEU:HB2	2.10	0.52
1:B:178:ILE:HD12	1:B:352:LEU:HD11	1.91	0.52
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.24	0.52
2:E:372:ARG:HD3	2:E:375:GLN:OE1	2.10	0.52
1:C:343:ILE:HG12	1:C:349:GLN:HG2	1.91	0.52
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.91	0.52
1:A:204:VAL:HG12	1:A:206:ILE:CD1	2.39	0.52
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.45	0.52
2:F:393:MET:SD	2:F:404:VAL:HG11	2.50	0.52
2:E:9:THR:HG21	2:E:27:GLU:O	2.09	0.52
2:D:220:GLY:CA	2:D:232:VAL:HG11	2.37	0.52
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:454:GLU:O	2:E:456:ALA:N	2.43	0.52
2:D:225:PRO:HB2	9:D:2013:HOH:O	2.09	0.51
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.92	0.51
1:A:48:GLN:HG2	2:E:70:VAL:CG2	2.40	0.51
1:B:44:LEU:O	1:B:47:VAL:HG22	2.11	0.51
1:B:102:GLU:HG3	1:B:123:SER:HA	1.92	0.51
2:D:203:SER:OG	2:D:205:VAL:HG23	2.11	0.51
1:C:211:SER:HB3	2:F:126:MET:HE2	1.92	0.51
2:E:126:MET:HE3	2:E:297:THR:HG21	1.92	0.51
2:E:456:ALA:HB1	2:E:466:ALA:O	2.11	0.51
2:E:374:VAL:O	2:E:377:ILE:HG22	2.11	0.51
1:C:137:ILE:HB	1:C:138:PRO:HD3	1.93	0.51
2:E:91:LEU:HD11	2:E:180:TYR:CD2	2.45	0.51
2:E:402:LEU:HD23	2:E:406:ARG:NH2	2.26	0.50
1:B:201:CYS:O	1:B:229:THR:HA	2.11	0.50
1:A:137:ILE:N	1:A:138:PRO:CD	2.74	0.50
1:B:83:LYS:HD3	2:E:31:PRO:HG3	1.91	0.50
1:A:460:LYS:HD2	1:A:460:LYS:N	2.27	0.50
1:C:103:LEU:HB2	1:C:230:ILE:HD13	1.93	0.50
2:E:293:GLN:HE22	2:E:308:GLN:NE2	2.02	0.50
2:E:170:ILE:HD13	2:E:215:VAL:HG22	1.92	0.50
1:C:240:ALA:N	1:C:241:PRO:CD	2.75	0.50
2:E:237:LEU:O	2:E:241:GLU:HG3	2.10	0.50
1:B:97:VAL:HG11	1:B:249:SER:HB3	1.92	0.50
1:A:99:VAL:CG2	1:A:253:MET:HA	2.38	0.50
1:A:106:ARG:NH2	1:A:119:GLY:O	2.39	0.50
2:D:151:LYS:HE2	2:D:328:HIS:O	2.12	0.50
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.41	0.50
2:D:348:VAL:O	2:D:350:PRO:HD3	2.12	0.50
1:B:426:GLU:OE1	1:B:429:LYS:HE3	2.12	0.50
1:A:134:PRO:HD3	9:A:2030:HOH:O	2.11	0.50
2:D:247:GLU:O	2:D:248:GLY:C	2.50	0.49
1:A:185:ASN:OD1	1:A:435:PRO:HB2	2.12	0.49
1:A:45:ARG:NH2	1:A:68:PRO:O	2.44	0.49
1:A:40:ARG:NH1	9:A:2004:HOH:O	2.44	0.49
2:F:206:ILE:HD11	2:F:215:VAL:HB	1.95	0.49
1:A:292:GLU:O	1:A:293:ALA:HB3	2.10	0.49
2:F:371:ALA:O	2:F:375:GLN:HG3	2.11	0.49
2:F:51:GLN:HG2	2:F:59:ARG:HB3	1.94	0.49
2:F:174:ALA:O	2:F:177:HIS:HB3	2.13	0.49
3:G:221:THR:O	3:G:225:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:293:GLN:NE2	2:E:308:GLN:HE22	2.02	0.49
2:F:63:MET:CE	2:F:231:ARG:HB2	2.41	0.49
1:C:400:VAL:HG23	1:C:418:LEU:CD2	2.41	0.49
2:E:310:ILE:HD11	2:E:329:LEU:HD11	1.94	0.49
2:E:147:ALA:HA	2:E:357:ILE:HD13	1.94	0.49
2:F:16:VAL:C	2:F:17:ILE:HD12	2.33	0.49
2:E:151:LYS:NZ	9:E:2042:HOH:O	2.38	0.49
2:D:399:GLU:O	2:D:403:THR:HG23	2.13	0.49
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.94	0.49
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.95	0.49
2:F:395:GLU:OE1	3:G:77:LEU:HD23	2.12	0.49
2:D:287:THR:O	2:D:291:THR:HG23	2.13	0.49
2:D:393:MET:CE	2:D:404:VAL:HG11	2.42	0.49
1:B:99:VAL:HG11	1:B:256:TYR:HB2	1.95	0.49
1:A:400:VAL:HG13	1:A:403:PHE:CD2	2.47	0.49
3:G:78:CYS:HG	3:G:82:HIS:CD2	2.30	0.49
1:A:466:ASN:O	1:A:470:SER:OG	2.30	0.49
2:F:97:VAL:HG13	2:F:232:VAL:HG13	1.95	0.49
2:D:133:LEU:HB2	2:D:148:LYS:HG2	1.95	0.49
1:C:354:THR:HG23	9:C:2128:HOH:O	2.12	0.49
1:A:307:GLU:HG3	2:E:223:ASN:ND2	2.27	0.49
1:A:91:THR:C	1:A:93:ALA:H	2.15	0.49
2:F:226:PRO:HB2	2:F:268:VAL:HG13	1.94	0.49
1:A:180:ILE:O	1:A:184:ILE:HG12	2.13	0.48
9:A:2007:HOH:O	2:E:67:GLU:HG3	2.12	0.48
1:C:292:GLU:O	1:C:293:ALA:HB3	2.12	0.48
1:C:170:ASP:O	1:C:175:LYS:HE2	2.13	0.48
2:D:400:ASP:O	2:D:404:VAL:HG23	2.12	0.48
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.95	0.48
1:B:103:LEU:N	1:B:103:LEU:HD12	2.28	0.48
1:C:400:VAL:HG13	9:C:2143:HOH:O	2.12	0.48
2:E:224:GLU:O	2:E:229:ARG:NH1	2.45	0.48
2:F:321:ALA:CB	2:F:322:PRO:CD	2.89	0.48
2:D:405:SER:O	2:D:409:LYS:HG3	2.14	0.48
1:A:136:ILE:HD13	2:E:94:ILE:HD13	1.95	0.48
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.44	0.48
1:C:55:PHE:CE1	1:C:82:ILE:HD13	2.49	0.48
1:C:102:GLU:HG2	1:C:122:GLY:O	2.13	0.48
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.95	0.48
1:A:27:GLU:O	1:A:90:ARG:HG3	2.13	0.48
2:E:390:ILE:HG13	3:G:25:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLN:HG3	1:C:347:ASP:HB2	1.95	0.48
1:B:383:MET:SD	1:B:387:ALA:HB2	2.53	0.48
1:B:397:TYR:HD1	1:B:418:LEU:HA	1.79	0.48
1:B:371:VAL:HG22	1:B:372:SER:N	2.28	0.48
1:B:105:GLY:HA2	1:B:226:MET:O	2.13	0.48
2:F:36:LEU:HB3	2:F:75:VAL:CG1	2.43	0.48
1:C:268:TYR:O	1:C:270:ASP:HA	2.13	0.48
2:E:163:THR:O	2:E:167:MET:HG3	2.14	0.48
2:F:32:ILE:O	2:F:33:LEU:HB2	2.13	0.48
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.95	0.48
1:A:456:LEU:HD12	1:A:457:GLU:H	1.78	0.48
1:A:36:ASP:O	1:A:284:LEU:HD13	2.14	0.48
1:B:289:PRO:HD2	9:G:2021:HOH:O	2.14	0.48
2:D:310:ILE:HD13	2:D:325:THR:HG21	1.96	0.47
1:C:438:ILE:O	1:C:442:VAL:HG23	2.13	0.47
9:C:2011:HOH:O	2:D:67:GLU:HG2	2.14	0.47
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.96	0.47
1:A:211:SER:N	2:D:126:MET:HE2	2.28	0.47
2:F:388:ILE:HD12	2:F:393:MET:HG2	1.95	0.47
1:B:411:ASP:OD2	1:B:413:ALA:HB3	2.14	0.47
2:F:345:TYR:HA	2:F:346:PRO:C	2.34	0.47
2:F:17:ILE:HG22	2:F:271:LEU:HD22	1.95	0.47
1:B:156:LEU:HD13	1:B:367:VAL:HG13	1.97	0.47
2:F:390:ILE:HG22	2:F:391:LEU:HD23	1.96	0.47
2:E:63:MET:HE1	2:E:228:ALA:HA	1.95	0.47
1:B:151:LYS:HG2	1:B:441:GLN:HG2	1.95	0.47
2:F:385:GLN:NE2	9:F:2124:HOH:O	2.47	0.47
1:B:300:TYR:HA	1:B:303:SER:OG	2.14	0.47
1:A:327:ILE:HD12	1:A:338:ILE:HG22	1.96	0.47
2:F:37:GLU:OE2	2:F:46:VAL:HG22	2.15	0.47
1:C:32:LEU:HD21	1:C:42:HIS:HB2	1.97	0.47
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.95	0.47
1:A:224:ASP:O	1:A:227:LYS:HE3	2.13	0.47
1:C:52:MET:CE	1:C:95:VAL:HG13	2.45	0.47
2:F:154:LEU:CD1	2:F:166:ILE:HG12	2.44	0.47
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.49	0.47
1:B:170:ASP:O	1:B:175:LYS:HE2	2.14	0.47
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.43	0.47
1:B:145:PRO:HG3	1:B:378:ALA:O	2.14	0.47
1:A:468:PHE:O	1:A:472:VAL:HG13	2.14	0.47
1:B:169:GLY:O	1:B:328:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.44	0.47
2:D:96:ASN:HB2	2:D:100:GLU:O	2.15	0.47
1:A:427:LEU:HD11	1:A:448:GLY:HA3	1.97	0.47
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.50	0.47
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.97	0.47
2:E:337:ARG:O	2:E:341:GLU:HG3	2.15	0.47
2:E:97:VAL:HG21	2:E:228:ALA:HB1	1.97	0.47
1:B:157:VAL:O	1:B:159:ILE:HD13	2.14	0.47
1:A:137:ILE:N	1:A:138:PRO:HD3	2.30	0.46
1:A:145:PRO:HB2	1:A:147:GLN:HE21	1.80	0.46
2:D:32:ILE:O	2:D:33:LEU:HB2	2.15	0.46
1:A:106:ARG:NH1	1:A:121:ILE:HG22	2.31	0.46
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.96	0.46
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.46
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.45	0.46
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.98	0.46
1:A:175:LYS:HE2	1:A:175:LYS:HB2	1.71	0.46
2:E:87:GLY:HA2	2:E:242:TYR:CE1	2.51	0.46
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.98	0.46
1:C:80:LYS:HA	2:F:32:ILE:HB	1.97	0.46
2:F:159:GLY:HA2	4:F:600:ANP:HNB1	1.80	0.46
2:F:266:SER:HB3	2:F:282:GLN:HE22	1.80	0.46
2:E:456:ALA:O	2:E:466:ALA:HA	2.16	0.46
1:B:102:GLU:CG	1:B:123:SER:HA	2.45	0.46
1:A:362:ARG:HA	1:A:363:PRO:C	2.35	0.46
1:C:362:ARG:HA	1:C:363:PRO:C	2.35	0.46
2:E:256:ASP:HA	2:E:257:ASN:HA	1.67	0.46
2:D:471:ASP:O	2:D:472:LYS:C	2.53	0.46
2:E:384:LEU:O	2:E:388:ILE:HG12	2.16	0.46
1:C:414:THR:O	1:C:418:LEU:HG	2.16	0.46
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.98	0.46
1:A:157:VAL:N	1:A:158:PRO:CD	2.79	0.46
2:D:200:MET:HE3	2:D:206:ILE:HD12	1.97	0.46
1:B:434:SER:N	1:B:435:PRO:HD3	2.30	0.46
1:B:476:HIS:CE1	1:B:500:ILE:HG12	2.51	0.46
2:D:63:MET:CE	2:D:228:ALA:HA	2.46	0.46
1:A:347:ASP:C	1:A:373:ARG:NH1	2.69	0.46
1:C:441:GLN:O	1:C:445:ILE:HG12	2.16	0.46
2:D:131:GLU:HB3	9:D:2037:HOH:O	2.15	0.46
1:B:32:LEU:HG	1:B:42:HIS:HB2	1.97	0.46
1:B:40:ARG:NH1	9:B:2003:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:N	1:A:339:PRO:CD	2.79	0.46
1:C:132:LYS:HE3	2:D:224:GLU:OE2	2.16	0.46
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.46
2:D:439:LYS:O	2:D:443:GLN:HG3	2.16	0.46
2:E:409:LYS:HG2	2:E:457:PHE:CE1	2.50	0.46
1:B:390:MET:HB2	1:B:449:VAL:HG21	1.98	0.45
1:B:240:ALA:N	1:B:241:PRO:CD	2.78	0.45
1:A:49:ALA:O	1:A:50:GLU:HB2	2.17	0.45
1:B:343:ILE:HG12	1:B:349:GLN:HG2	1.97	0.45
2:E:126:MET:HE1	2:E:297:THR:HG21	1.98	0.45
2:D:329:LEU:HD12	2:D:332:THR:HG22	1.97	0.45
2:E:138:LYS:HE3	2:E:416:GLN:HB2	1.98	0.45
1:A:443:ALA:O	1:A:446:TYR:HB3	2.16	0.45
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.82	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HG21	1.98	0.45
1:A:278:TYR:CD2	1:A:301:LEU:HD13	2.52	0.45
2:D:49:VAL:HA	2:D:60:THR:HG22	1.99	0.45
1:A:268:TYR:CZ	1:A:305:LEU:HD11	2.52	0.45
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.52	0.45
1:A:136:ILE:HG22	9:E:2049:HOH:O	2.17	0.45
2:E:409:LYS:HG2	2:E:457:PHE:CD1	2.52	0.45
2:F:447:GLY:HA2	2:F:450:ASP:OD1	2.17	0.45
1:B:432:GLN:HG3	4:B:600:ANP:C5	2.47	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HG2	1.82	0.45
3:G:10:LEU:O	3:G:14:LYS:HG3	2.16	0.45
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.99	0.45
1:A:476:HIS:CD2	1:A:500:ILE:HD11	2.51	0.45
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.17	0.45
2:E:258:ILE:O	2:E:261:PHE:HB3	2.17	0.45
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.31	0.45
1:B:100:GLY:O	1:B:103:LEU:HD13	2.17	0.45
2:E:96:ASN:OD1	2:E:97:VAL:HG23	2.16	0.45
1:C:132:LYS:NZ	2:D:64:ASP:OD1	2.50	0.45
1:B:362:ARG:HA	1:B:363:PRO:C	2.36	0.45
2:E:411:GLN:HG3	9:E:2101:HOH:O	2.16	0.45
1:C:420:ARG:HH11	1:C:420:ARG:HG2	1.82	0.45
2:D:63:MET:HE3	2:D:228:ALA:HA	1.99	0.45
2:E:55:GLU:O	2:E:56:SER:HB2	2.16	0.45
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.98	0.45
1:A:338:ILE:N	1:A:339:PRO:HD2	2.32	0.44
1:C:338:ILE:N	1:C:339:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HG23	1:A:423:ARG:HD2	1.99	0.44
1:A:422:VAL:HG23	1:A:423:ARG:N	2.33	0.44
1:A:450:ARG:NH2	1:A:494:ASP:OD1	2.50	0.44
1:C:352:LEU:HA	1:C:364:ALA:O	2.17	0.44
2:F:87:GLY:HA2	2:F:242:TYR:CE1	2.51	0.44
2:F:225:PRO:CB	2:F:226:PRO:HD2	2.47	0.44
2:E:258:ILE:HD12	2:E:258:ILE:HA	1.86	0.44
2:E:387:ILE:HD12	2:E:387:ILE:N	2.32	0.44
2:E:39:GLN:NE2	2:E:76:LEU:HG	2.33	0.44
2:F:162:LYS:O	2:F:166:ILE:HG13	2.17	0.44
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.74	0.44
2:E:141:ASP:HB3	2:E:434:LEU:HD13	2.00	0.44
2:E:251:VAL:HG12	2:E:252:LEU:N	2.32	0.44
1:A:213:VAL:O	1:A:216:LEU:HB3	2.18	0.44
2:E:200:MET:HB3	2:E:206:ILE:HG13	1.98	0.44
1:B:28:THR:HG23	1:B:89:LYS:HG2	1.99	0.44
1:B:356:LEU:HB3	1:B:361:ILE:HB	2.00	0.44
2:E:349:ASP:HA	2:E:350:PRO:HD2	1.79	0.44
1:B:140:ILE:HG13	1:B:141:SER:N	2.33	0.44
1:A:347:ASP:C	1:A:373:ARG:HH11	2.21	0.44
2:D:63:MET:CE	2:D:97:VAL:HG11	2.48	0.44
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.99	0.44
2:E:91:LEU:HD23	2:E:216:ALA:HB2	2.00	0.44
2:E:218:VAL:HG21	2:E:236:GLY:HA2	1.97	0.44
2:F:94:ILE:HG12	2:F:217:LEU:HD12	1.99	0.44
2:D:463:ILE:HD12	2:D:466:ALA:HB3	2.00	0.44
2:F:256:ASP:HA	2:F:257:ASN:HA	1.76	0.44
2:E:188:GLU:O	2:E:221:GLN:HA	2.18	0.44
2:E:263:GLN:HA	2:E:263:GLN:NE2	2.33	0.44
1:B:385:GLN:NE2	1:B:488:LYS:HZ3	2.16	0.44
1:B:54:GLU:HG2	1:B:60:LYS:HZ3	1.82	0.44
1:B:420:ARG:NH1	1:B:448:GLY:O	2.51	0.44
1:A:95:VAL:HG11	1:A:245:LEU:HD13	1.99	0.44
1:B:52:MET:O	1:B:91:THR:HG23	2.18	0.44
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.99	0.44
2:E:432:VAL:HA	2:E:433:PRO:HD3	1.80	0.44
1:A:441:GLN:O	1:A:444:VAL:HG22	2.18	0.43
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.99	0.43
1:C:303:SER:HA	1:C:345:ILE:HD13	1.99	0.43
1:B:329:THR:HG21	1:B:334:VAL:HG12	1.99	0.43
1:C:199:LEU:HD12	1:C:263:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.53	0.43
2:E:360:PRO:HD3	2:E:368:TYR:CE1	2.53	0.43
1:B:94:ILE:O	1:B:95:VAL:C	2.57	0.43
1:A:37:GLY:HA2	9:A:2012:HOH:O	2.17	0.43
2:D:82:ILE:HD13	2:D:98:ILE:HG22	2.00	0.43
1:B:50:GLU:O	1:B:95:VAL:HG23	2.19	0.43
1:B:269:ASP:HA	1:B:270:ASP:HA	1.41	0.43
1:C:207:GLY:O	1:C:236:ALA:HB2	2.18	0.43
2:F:453:PRO:O	2:F:454:GLU:C	2.57	0.43
1:B:249:SER:O	1:B:253:MET:HG3	2.18	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.18	0.43
2:D:256:ASP:HA	2:D:257:ASN:HA	1.81	0.43
1:A:204:VAL:CG1	1:A:206:ILE:HD11	2.46	0.43
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.99	0.43
1:C:452:TYR:OH	1:C:498:LYS:HG3	2.18	0.43
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.53	0.43
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.90	0.43
1:B:38:ILE:HG13	1:B:285:LEU:CD2	2.47	0.43
1:A:311:LYS:NZ	1:A:318:GLY:O	2.49	0.43
1:A:240:ALA:N	1:A:241:PRO:CD	2.82	0.43
1:C:137:ILE:N	1:C:138:PRO:CD	2.81	0.43
2:D:151:LYS:NZ	2:D:293:GLN:O	2.52	0.43
1:A:355:GLU:O	1:A:359:LYS:HB2	2.19	0.43
1:B:161:ARG:HA	1:B:322:THR:OG1	2.19	0.43
1:B:473:ILE:O	1:B:477:GLN:HG2	2.18	0.43
2:D:275:ILE:HG23	2:D:276:PRO:HD2	2.00	0.43
2:F:9:THR:O	2:F:76:LEU:HD12	2.18	0.43
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.52	0.43
1:B:410:LEU:O	1:B:411:ASP:HB3	2.18	0.43
2:D:200:MET:HB2	2:D:200:MET:HE3	1.87	0.43
1:C:444:VAL:HG23	1:C:445:ILE:HD13	2.01	0.43
1:B:206:ILE:HG21	1:B:274:GLN:HB2	2.00	0.43
1:C:168:ILE:HD13	1:C:334:VAL:HG12	2.01	0.43
2:E:381:TYR:CE1	2:E:404:VAL:HG13	2.53	0.43
1:C:129:VAL:HA	1:C:252:SER:OG	2.19	0.43
1:B:422:VAL:O	1:B:426:GLU:HG2	2.19	0.43
2:D:97:VAL:HG13	2:D:232:VAL:HG13	2.01	0.43
1:B:338:ILE:O	1:B:341:ASN:HB2	2.17	0.43
1:B:444:VAL:CG1	1:B:469:LEU:HD13	2.48	0.43
2:E:196:LEU:HD23	2:E:219:TYR:OH	2.18	0.43
1:C:163:GLN:O	1:C:322:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:CG1	1:C:241:PRO:HB3	2.48	0.42
3:G:42:ARG:HA	3:G:215:TYR:HE1	1.83	0.42
1:A:121:ILE:HD13	1:A:121:ILE:H	1.83	0.42
2:F:459:MET:HG3	9:F:2141:HOH:O	2.19	0.42
1:A:446:TYR:CD2	1:A:497:LEU:HD13	2.54	0.42
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.02	0.42
1:B:28:THR:CG2	1:B:87:ILE:HG23	2.50	0.42
1:B:291:ARG:HB3	1:B:337:TYR:CD2	2.54	0.42
1:C:106:ARG:NH2	1:C:119:GLY:O	2.44	0.42
2:F:409:LYS:NZ	2:F:450:ASP:HA	2.34	0.42
2:F:275:ILE:HD13	3:G:271:ALA:HB1	2.01	0.42
2:E:257:ASN:HB2	2:E:309:ALA:O	2.20	0.42
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.99	0.42
9:B:2010:HOH:O	2:F:67:GLU:HG2	2.18	0.42
2:D:244:ARG:HD3	2:D:304:ILE:HG13	2.01	0.42
2:F:17:ILE:CG2	2:F:271:LEU:HD22	2.49	0.42
2:D:234:LEU:HD23	2:D:292:MET:HG3	2.00	0.42
2:E:352:ASP:O	2:E:354:THR:HG23	2.20	0.42
1:B:453:LEU:HD13	1:B:461:ILE:HD12	2.01	0.42
2:E:408:ARG:NH2	2:E:412:ARG:NH2	2.66	0.42
1:A:44:LEU:O	1:A:47:VAL:HG22	2.20	0.42
1:C:194:ASP:OD1	1:C:196:LYS:HB2	2.19	0.42
2:D:29:LEU:HA	2:D:30:PRO:HD2	1.87	0.42
1:B:338:ILE:N	1:B:339:PRO:CD	2.82	0.42
2:E:93:ARG:NH2	2:E:106:GLY:O	2.39	0.42
1:A:128:ARG:HB3	1:A:131:LEU:HD21	2.01	0.42
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.20	0.42
1:A:151:LYS:CE	1:A:427:LEU:O	2.67	0.42
2:D:139:VAL:HG23	2:D:140:VAL:N	2.34	0.42
1:A:390:MET:CE	1:A:424:LEU:HD22	2.50	0.42
1:B:180:ILE:HD12	1:B:216:LEU:HD21	2.02	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.42
1:A:40:ARG:HD2	1:A:70:ASN:OD1	2.19	0.42
3:G:78:CYS:SG	3:G:228:ARG:NH2	2.92	0.42
1:B:54:GLU:HG2	1:B:60:LYS:NZ	2.35	0.42
1:A:407:GLY:HA3	1:A:410:LEU:CD1	2.50	0.42
1:B:51:GLU:HA	1:B:94:ILE:HA	2.01	0.42
2:E:374:VAL:HG13	2:E:410:ILE:HG21	2.02	0.42
2:E:30:PRO:HA	2:E:31:PRO:HD3	1.85	0.42
2:E:200:MET:HG2	2:E:205:VAL:CG2	2.49	0.42
1:A:336:ALA:HB3	1:A:339:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:PRO:HG3	3:G:268:GLY:HA3	2.01	0.42
2:F:349:ASP:HA	2:F:350:PRO:HD2	1.89	0.42
2:D:80:ALA:HB1	2:D:81:PRO:HD2	2.02	0.42
1:B:218:LYS:HG2	2:E:128:VAL:HB	2.02	0.42
1:C:91:THR:CG2	1:C:93:ALA:HB3	2.49	0.41
1:A:390:MET:HG3	1:A:424:LEU:HD13	2.02	0.41
2:E:143:LEU:HD22	2:E:375:GLN:HG3	2.02	0.41
2:E:319:ASP:HB3	2:E:322:PRO:HD2	2.02	0.41
1:A:245:LEU:O	1:A:246:ALA:C	2.59	0.41
1:B:174:GLY:HA2	4:B:600:ANP:PA	2.60	0.41
2:E:452:LEU:HB3	2:E:453:PRO:HD2	2.01	0.41
2:F:201:ILE:CD1	2:F:208:LEU:HD11	2.50	0.41
1:A:24:ASP:OD2	1:A:27:GLU:HB2	2.19	0.41
2:E:411:GLN:HA	2:E:414:LEU:HD12	2.03	0.41
1:A:34:ILE:HD11	1:A:79:ASP:CB	2.51	0.41
1:B:157:VAL:N	1:B:158:PRO:CD	2.84	0.41
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.34	0.41
1:A:34:ILE:CG2	2:D:52:HIS:HB2	2.51	0.41
1:A:175:LYS:CG	1:A:352:LEU:HD12	2.51	0.41
1:C:142:VAL:HG13	1:C:161:ARG:O	2.20	0.41
2:D:434:LEU:O	2:D:438:ILE:HG13	2.20	0.41
2:E:359:ASP:OD2	2:E:361:ASN:HB2	2.21	0.41
2:D:118:ALA:O	2:D:295:ARG:HD2	2.20	0.41
1:B:390:MET:CE	1:B:445:ILE:HG23	2.51	0.41
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.55	0.41
1:A:285:LEU:O	1:A:286:ARG:HB2	2.21	0.41
1:C:68:PRO:HD3	2:D:15:ALA:HB2	2.03	0.41
2:F:393:MET:HE2	9:F:2125:HOH:O	2.19	0.41
1:B:28:THR:HG22	1:B:87:ILE:HG23	2.01	0.41
1:A:439:GLU:H	1:A:439:GLU:CD	2.24	0.41
1:A:248:TYR:CE1	1:A:305:LEU:HB2	2.55	0.41
1:A:335:SER:HB2	9:A:2103:HOH:O	2.19	0.41
3:G:81:ILE:HG13	3:G:224:GLU:HA	2.03	0.41
2:F:435:LYS:HG3	2:F:436:GLU:N	2.35	0.41
1:A:140:ILE:CG2	1:A:311:LYS:HG3	2.49	0.41
2:E:321:ALA:N	2:E:322:PRO:HD2	2.36	0.41
1:A:446:TYR:CE2	1:A:497:LEU:HB3	2.56	0.41
1:B:166:LEU:HD11	1:B:327:ILE:HB	2.03	0.41
3:G:13:ILE:HD13	3:G:242:MET:SD	2.61	0.41
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.84	0.41
2:D:139:VAL:HG12	2:D:414:LEU:CD2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:240:ALA:O	2:E:251:VAL:HG21	2.20	0.41
1:C:497:LEU:O	1:C:501:VAL:HG13	2.21	0.41
1:A:40:ARG:HD3	1:A:40:ARG:HA	1.89	0.41
1:A:152:ALA:HA	1:A:428:LEU:HD22	2.03	0.41
2:F:245:ASP:C	2:F:247:GLU:H	2.24	0.41
2:E:35:ALA:O	2:E:36:LEU:HD23	2.21	0.40
1:B:173:THR:O	1:B:352:LEU:HD13	2.22	0.40
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.84	0.40
2:D:279:VAL:O	2:D:279:VAL:HG12	2.20	0.40
1:C:287:ARG:HA	1:C:288:PRO:HD3	1.88	0.40
1:B:478:ALA:O	1:B:482:LYS:HG3	2.22	0.40
2:E:251:VAL:HG12	2:E:252:LEU:H	1.86	0.40
1:C:406:PHE:O	1:C:408:SER:N	2.55	0.40
1:A:301:LEU:HD23	1:A:302:HIS:CD2	2.56	0.40
1:C:136:ILE:HG23	2:D:194:ASN:HA	2.04	0.40
2:D:84:ILE:HB	2:D:85:PRO:HD2	2.03	0.40
2:E:415:SER:HB2	2:E:459:MET:SD	2.61	0.40
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.51	0.40
2:E:147:ALA:HB2	2:E:357:ILE:CG2	2.51	0.40
1:B:383:MET:HG2	1:B:438:ILE:HD11	2.02	0.40
1:A:438:ILE:O	1:A:442:VAL:HG13	2.22	0.40
2:F:366:GLU:O	2:F:370:VAL:HG23	2.21	0.40
1:B:129:VAL:HA	1:B:252:SER:OG	2.22	0.40
1:B:264:ALA:HB3	1:B:321:LEU:HD13	2.03	0.40
1:C:404:ALA:C	1:C:406:PHE:N	2.74	0.40
1:B:47:VAL:HG13	1:B:90:ARG:HG2	2.03	0.40
1:C:444:VAL:CG1	1:C:469:LEU:HD13	2.52	0.40
1:A:268:TYR:O	1:A:270:ASP:HA	2.21	0.40
1:A:295:PRO:HD2	1:A:298:VAL:HB	2.02	0.40
2:D:186:VAL:HG12	2:D:260:ARG:HB2	2.02	0.40
2:F:344:ILE:HG23	2:F:415:SER:HB3	2.03	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%)	449 (93%)	33 (7%)	3 (1%)	30	50
1	B	475/510 (93%)	447 (94%)	25 (5%)	3 (1%)	30	50
1	C	490/510 (96%)	462 (94%)	26 (5%)	2 (0%)	39	61
2	D	465/482 (96%)	432 (93%)	26 (6%)	7 (2%)	13	22
2	E	464/482 (96%)	423 (91%)	35 (8%)	6 (1%)	15	26
2	F	464/482 (96%)	430 (93%)	31 (7%)	3 (1%)	30	50
3	G	116/272 (43%)	110 (95%)	4 (3%)	2 (2%)	11	19
All	All	2959/3248 (91%)	2753 (93%)	180 (6%)	26 (1%)	21	37

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	388	ILE
1	B	95	VAL
1	B	367	VAL
1	C	409	ASP
2	D	247	GLU
2	D	248	GLY
2	E	210	ASP
2	E	455	GLN
1	A	404	ALA
1	A	405	GLN
2	D	109	LYS
2	D	385	GLN
3	G	211	ASN
2	D	472	LYS
2	E	42	GLU
2	F	246	GLN
1	A	484	ARG
1	B	452	TYR
2	D	246	GLN
2	D	448	GLU
2	F	455	GLN
2	E	156	GLY
3	G	81	ILE
2	F	420	VAL
2	E	279	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	375 (95%)	18 (5%)	33	57
1	B	388/412 (94%)	365 (94%)	23 (6%)	24	44
1	C	397/412 (96%)	372 (94%)	25 (6%)	22	40
2	D	377/386 (98%)	364 (97%)	13 (3%)	44	72
2	E	376/386 (97%)	359 (96%)	17 (4%)	34	59
2	F	376/386 (97%)	364 (97%)	12 (3%)	46	74
3	G	102/230 (44%)	94 (92%)	8 (8%)	16	29
All	All	2409/2624 (92%)	2293 (95%)	116 (5%)	31	55

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	59	LEU
1	A	99	VAL
1	A	121	ILE
1	A	141	SER
1	A	249	SER
1	A	286	ARG
1	A	301	LEU
1	A	338	ILE
1	A	344	SER
1	A	367	VAL
1	A	436	MET
1	A	449	VAL
1	A	459	SER
1	A	460	LYS
1	A	470	SER
1	A	479	LEU
1	A	505	LEU
1	B	28	THR
1	B	47	VAL

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Mol	Chain	Res	Type
1	B	56	SER
1	B	59	LEU
1	B	123	SER
1	B	140	ILE
1	B	143	ARG
1	B	164	ARG
1	B	188	ARG
1	B	211	SER
1	B	216	LEU
1	B	218	LYS
1	B	298	VAL
1	B	361	ILE
1	B	376	SER
1	B	380	THR
1	B	383	MET
1	B	384	LYS
1	B	389	THR
1	B	422	VAL
1	B	434	SER
1	B	459	SER
1	B	492	GLU
1	C	47	VAL
1	C	57	SER
1	C	64	LEU
1	C	74	VAL
1	C	87	ILE
1	C	91	THR
1	C	123	SER
1	C	132	LYS
1	C	140	ILE
1	C	164	ARG
1	C	165	GLU
1	C	188	ARG
1	C	193	THR
1	C	209	LYS
1	C	226	MET
1	C	262	LYS
1	C	298	VAL
1	C	334	VAL
1	C	381	ARG
1	C	391	LYS
1	C	416	GLN

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Mol	Chain	Res	Type
1	C	419	SER
1	C	438	ILE
1	C	459	SER
1	C	479	LEU
2	D	41	ARG
2	D	67	GLU
2	D	89	GLU
2	D	97	VAL
2	D	137	ILE
2	D	232	VAL
2	D	282	GLN
2	D	303	SER
2	D	335	LEU
2	D	358	MET
2	D	400	ASP
2	D	420	VAL
2	D	423	VAL
2	E	67	GLU
2	E	97	VAL
2	E	112	GLN
2	E	139	VAL
2	E	196	LEU
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	232	VAL
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	358	MET
2	E	395	GLU
2	E	420	VAL
2	E	431	LEU
2	E	444	ILE
2	F	9	THR
2	F	67	GLU
2	F	76	LEU
2	F	97	VAL
2	F	139	VAL
2	F	223	ASN
2	F	232	VAL
2	F	282	GLN

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Mol	Chain	Res	Type
2	F	303	SER
2	F	395	GLU
2	F	397	SER
2	F	455	GLN
3	G	20	THR
3	G	78	CYS
3	G	84	SER
3	G	226	SER
3	G	240	SER
3	G	254	ARG
3	G	260	LYS
3	G	262	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	432	GLN
1	A	471	HIS
1	B	46	ASN
1	B	48	GLN
1	B	65	ASN
1	B	172	GLN
1	B	215	GLN
1	B	260	ASN
1	B	432	GLN
1	B	476	HIS
1	B	503	ASN
1	C	260	ASN
1	C	263	HIS
1	C	432	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	282	GLN
2	D	385	GLN
2	D	411	GLN
2	E	39	GLN
2	E	130	GLN
2	E	221	GLN
2	E	223	ASN
2	E	263	GLN

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Mol	Chain	Res	Type
2	E	282	GLN
2	E	293	GLN
2	E	379	GLN
2	E	385	GLN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	361	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ANP	A	600	5	27,33,33	1.37	4 (14%)	30,52,52	1.14	1 (3%)
4	ANP	B	600	5	27,33,33	1.46	4 (14%)	30,52,52	1.32	2 (6%)
4	ANP	C	600	5	27,33,33	1.36	4 (14%)	30,52,52	1.26	3 (10%)
6	ADP	D	600	5,7	22,29,29	1.15	2 (9%)	27,45,45	1.02	0
7	AF3	D	602	9,1,5,6	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PO4	E	602	-	4,4,4	0.22	0	6,6,6	0.27	0
4	ANP	F	600	5	27,33,33	1.36	3 (11%)	30,52,52	1.22	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	600	5	-	1/12/38/38	0/3/3/3
4	ANP	B	600	5	-	1/12/38/38	0/3/3/3
4	ANP	C	600	5	-	1/12/38/38	0/3/3/3
6	ADP	D	600	5,7	-	0/12/32/32	0/3/3/3
7	AF3	D	602	9,1,5,6	-	0/0/0/0	0/0/0/0
8	PO4	E	602	-	-	0/0/0/0	0/0/0/0
4	ANP	F	600	5	-	2/12/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	600	ANP	PG-O2G	-4.41	1.44	1.56
4	A	600	ANP	PG-O2G	-3.88	1.45	1.56
4	C	600	ANP	PG-O3G	-3.39	1.47	1.56
4	B	600	ANP	PG-O2G	-3.21	1.47	1.56
4	F	600	ANP	PB-O2B	-3.10	1.48	1.56
4	C	600	ANP	PG-O2G	-3.09	1.48	1.56
4	B	600	ANP	PB-O2B	-3.08	1.48	1.56
4	A	600	ANP	PG-O3G	-3.04	1.48	1.56
4	C	600	ANP	PB-O2B	-2.97	1.48	1.56
4	A	600	ANP	PB-O2B	-2.95	1.48	1.56
4	B	600	ANP	PG-O3G	-2.75	1.49	1.56
6	D	600	ADP	PB-O2B	-2.55	1.45	1.54
6	D	600	ADP	PB-O3B	-2.52	1.45	1.54
4	C	600	ANP	PA-O2A	-2.13	1.45	1.54
4	A	600	ANP	PG-O1G	2.53	1.49	1.46
4	B	600	ANP	PB-O3A	2.81	1.62	1.59
4	F	600	ANP	PB-O1B	2.94	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ANP	O1G-PG-N3B	-3.52	106.51	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	ANP	O1G-PG-N3B	-3.16	107.05	111.90
4	F	600	ANP	C1'-N9-C4	-2.92	122.54	126.94
4	F	600	ANP	O1G-PG-N3B	-2.74	107.69	111.90
4	F	600	ANP	C2'-C1'-N9	-2.51	110.46	114.29
4	B	600	ANP	C2'-C1'-N9	-2.32	110.75	114.29
4	C	600	ANP	C2'-C3'-C4'	2.06	106.86	102.61
4	C	600	ANP	C4-C5-N7	2.11	111.42	109.48
4	B	600	ANP	O1B-PB-N3B	4.57	118.91	111.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	ANP	O1G-PG-N3B-PB
4	B	600	ANP	O1B-PB-N3B-PG
4	A	600	ANP	O1G-PG-N3B-PB
4	F	600	ANP	O1G-PG-N3B-PB
4	F	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	ANP	4	0
4	C	600	ANP	1	0
6	D	600	ADP	1	0
7	D	602	AF3	1	0
4	F	600	ANP	1	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%)	-0.19	16 (3%)	50	55	26, 46, 76, 110	0
1	B	479/510 (93%)	-0.05	28 (5%)	26	30	25, 43, 97, 110	0
1	C	492/510 (96%)	-0.35	9 (1%)	71	75	24, 38, 65, 106	0
2	D	467/482 (96%)	-0.33	9 (1%)	70	73	24, 40, 73, 103	0
2	E	466/482 (96%)	0.17	30 (6%)	23	25	26, 51, 102, 119	0
2	F	466/482 (96%)	-0.28	12 (2%)	59	63	24, 41, 72, 90	0
3	G	122/272 (44%)	0.75	24 (19%)	1	1	29, 68, 108, 111	0
All	All	2979/3248 (91%)	-0.14	128 (4%)	39	44	24, 44, 88, 119	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	389	ALA	9.4
2	E	390	ILE	8.5
1	C	408	SER	6.5
2	E	28	GLY	6.3
3	G	209	LEU	5.9
1	A	408	SER	5.8
2	E	424	PHE	5.8
3	G	1	ALA	5.5
1	C	409	ASP	5.5
3	G	89	MET	5.5
2	E	394	ASP	5.3
2	E	474	ALA	5.2
1	B	416	GLN	5.2
1	B	510	ALA	5.2
1	C	407	GLY	5.0
3	G	90	LYS	4.9
2	E	398	GLU	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	475	GLU	4.8
3	G	210	ALA	4.8
2	E	388	ILE	4.7
2	E	395	GLU	4.7
3	G	86	ALA	4.5
3	G	87	LYS	4.4
3	G	88	GLN	4.3
3	G	43	VAL	4.3
1	B	358	TYR	4.2
2	E	393	MET	4.1
1	B	400	VAL	4.0
1	B	410	LEU	4.0
3	G	85	VAL	4.0
2	E	27	GLU	3.9
3	G	36	ARG	3.9
2	F	246	GLN	3.9
2	E	471	ASP	3.9
1	A	485	THR	3.8
1	B	497	LEU	3.8
1	B	485	THR	3.8
1	A	409	ASP	3.7
1	C	410	LEU	3.7
2	D	9	THR	3.7
2	F	248	GLY	3.6
1	B	496	LYS	3.5
1	A	93	ALA	3.5
1	C	193	THR	3.5
1	A	24	ASP	3.5
1	C	405	GLN	3.4
2	E	473	LEU	3.4
1	B	455	LYS	3.2
2	E	159	GLY	3.2
1	B	473	ILE	3.1
1	B	413	ALA	3.1
2	E	423	VAL	3.1
2	D	27	GLU	3.1
1	A	94	ILE	3.1
2	D	474	ALA	3.0
2	F	9	THR	3.0
1	B	196	LYS	3.0
2	E	427	HIS	3.0
2	E	428	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	214	TYR	2.9
2	E	337	ARG	2.9
1	B	412	ALA	2.8
3	G	40	PRO	2.8
1	B	507	GLY	2.8
3	G	83	SER	2.8
1	B	30	ARG	2.7
1	A	487	GLY	2.7
2	E	158	ALA	2.7
2	E	426	GLY	2.7
2	E	455	GLN	2.7
1	C	381	ARG	2.6
1	A	407	GLY	2.6
1	B	506	ALA	2.6
2	D	473	LEU	2.6
1	B	503	ASN	2.5
3	G	212	ILE	2.5
1	B	411	ASP	2.5
1	B	415	GLN	2.5
2	F	472	LYS	2.4
1	B	460	LYS	2.4
1	A	193	THR	2.4
1	A	443	ALA	2.4
2	F	176	ALA	2.4
3	G	39	LYS	2.4
2	D	28	GLY	2.4
1	B	45	ARG	2.4
1	C	57	SER	2.3
2	F	106	GLY	2.3
2	E	451	HIS	2.3
3	G	42	ARG	2.3
1	A	122	GLY	2.3
1	B	457	GLU	2.3
3	G	215	TYR	2.3
1	B	401	ALA	2.3
1	A	91	THR	2.2
2	E	399	GLU	2.2
2	E	430	LYS	2.2
2	F	28	GLY	2.2
3	G	211	ASN	2.2
2	D	109	LYS	2.2
3	G	5	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	474	SER	2.1
3	G	81	ILE	2.1
1	A	410	LEU	2.1
2	E	413	PHE	2.1
2	E	425	THR	2.1
3	G	2	THR	2.1
1	B	395	ALA	2.1
3	G	25	MET	2.1
2	E	210	ASP	2.1
2	E	36	LEU	2.1
1	B	478	ALA	2.1
2	F	249	GLN	2.1
1	B	491	GLU	2.1
2	F	209	LYS	2.1
3	G	11	LYS	2.1
1	A	121	ILE	2.1
1	C	406	PHE	2.1
2	D	402	LEU	2.1
2	F	111	LYS	2.1
1	A	194	ASP	2.1
2	F	27	GLU	2.0
2	F	175	LYS	2.0
2	D	399	GLU	2.0
2	E	410	ILE	2.0
1	B	193	THR	2.0
2	E	42	GLU	2.0
1	A	124	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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(Å <sup>2</sup> )	Q<0.9
5	MG	F	601	1/1	0.93	0.17	3.57	32,32,32,32	0
5	MG	D	601	1/1	0.98	0.15	2.95	33,33,33,33	0
7	AF3	D	602	4/4	0.93	0.17	2.33	41,41,43,45	0
8	PO4	E	602	5/5	0.79	0.24	0.65	86,87,87,87	0
4	ANP	B	600	31/31	0.98	0.10	-0.75	32,47,51,54	0
4	ANP	C	600	31/31	0.98	0.10	-0.88	29,37,41,45	0
6	ADP	D	600	27/27	0.99	0.09	-0.97	28,33,35,36	0
4	ANP	F	600	31/31	0.98	0.10	-1.37	34,38,45,45	0
4	ANP	A	600	31/31	0.98	0.08	-1.59	29,36,40,42	0
5	MG	A	601	1/1	0.84	0.12	-	41,41,41,41	0
5	MG	C	601	1/1	0.98	0.06	-	28,28,28,28	0
5	MG	B	601	1/1	0.83	0.07	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.