



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:52 PM GMT

PDB ID : 1COW
Title : BOVINE MITOCHONDRIAL F1-ATPASE COMPLEXED WITH AU-ROVERTIN B
Authors : Van Raaij, M.; Abrahams, J.P.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 1996-05-08
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

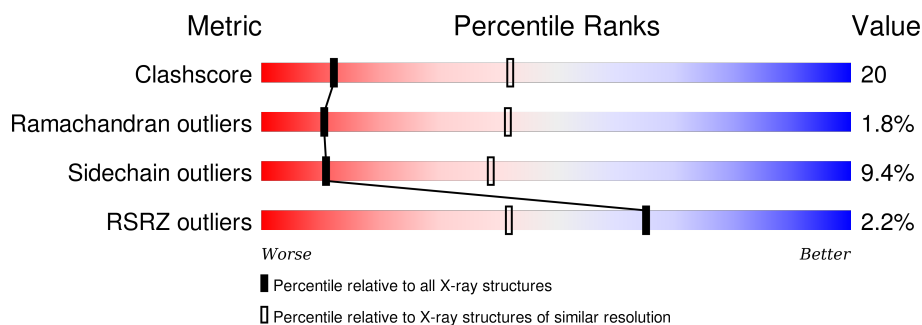
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 ≥ 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>49%</div> <div>35%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	510	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>38%</div> <div>10%</div> <div>5%</div> </div> </div>
1	C	510	<div> <div></div> <div> <div></div> <div>53%</div> <div>37%</div> <div>5%</div> <div></div> </div> </div>
2	D	482	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>38%</div> <div>6%</div> <div></div> </div> </div>
2	E	482	<div> <div>4%</div> <div> <div></div> <div>43%</div> <div>40%</div> <div>11%</div> <div></div> </div> </div>
2	F	482	<div> <div></div> <div> <div></div> <div>55%</div> <div>34%</div> <div>7%</div> <div></div> </div> </div>
3	G	272	<div> <div>7%</div> <div> <div></div> <div>25%</div> <div>15%</div> <div>5%</div> <div></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 8 unique types of molecules in this entry. The entry contains 23462 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	0	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	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			

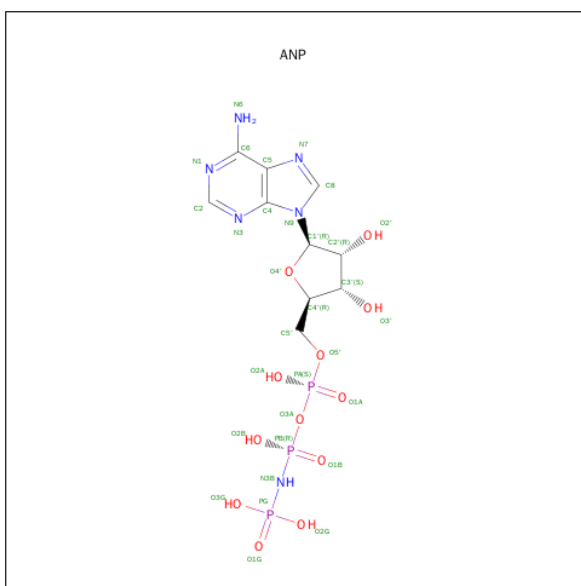
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

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 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: $C_{10}H_{17}N_6O_{12}P_3$).



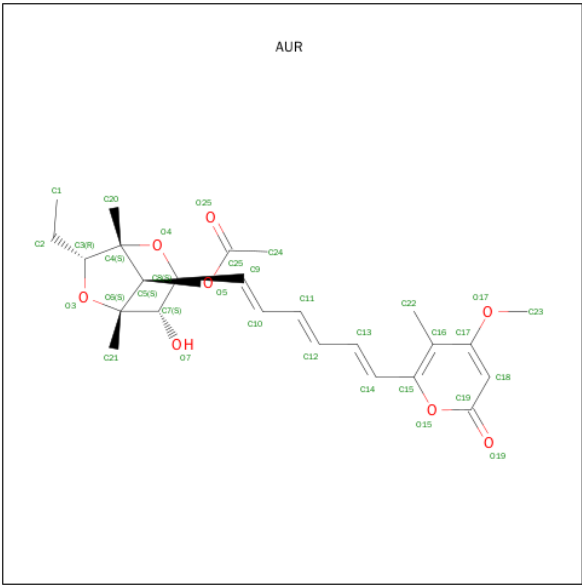
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 6 12 3	0	0
5	B	1	Total C N O P 31 10 6 12 3	0	0
5	C	1	Total C N O P 31 10 6 12 3	0	0
5	F	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is AUROVERTIN B (three-letter code: AUR) (formula: C₂₅H₃₂O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			33	25	8		
7	E	1	Total	C	O	0	0
			33	25	8		

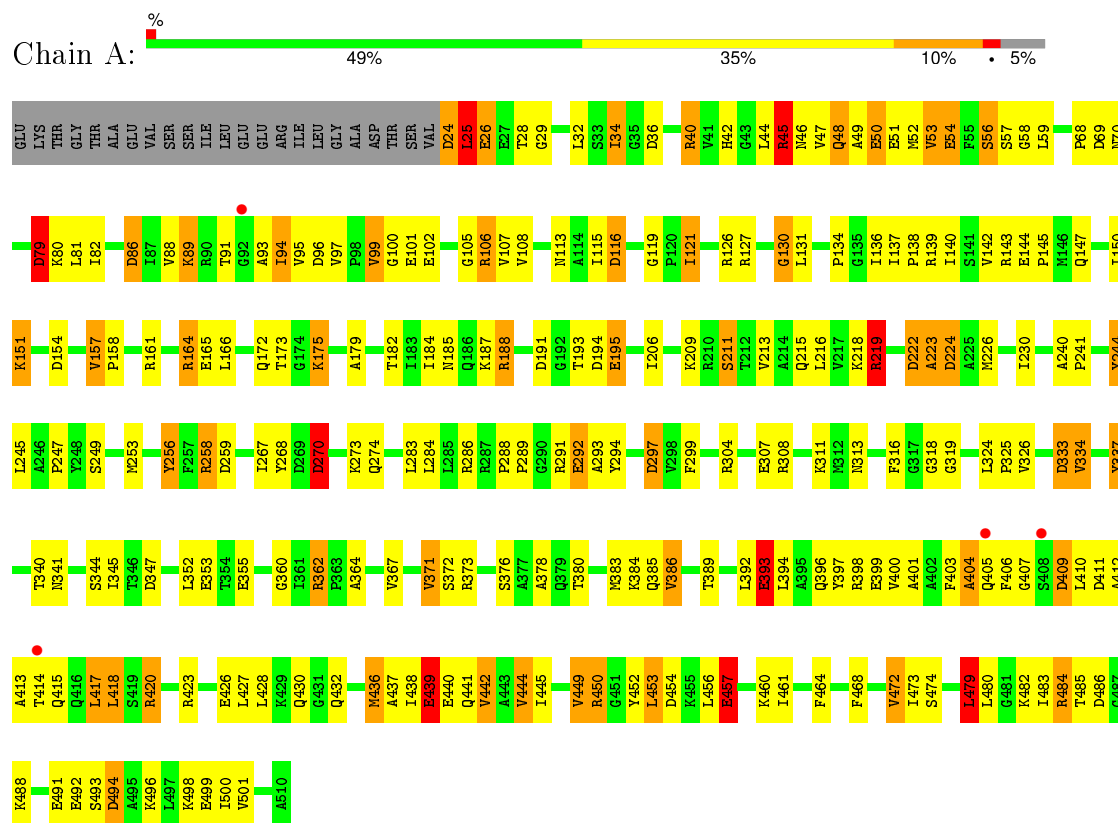
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	80	Total 80	O 80	0	0
8	B	84	Total 84	O 84	0	0
8	C	98	Total 98	O 98	0	0
8	D	94	Total 94	O 94	0	0
8	E	47	Total 47	O 47	0	0
8	F	92	Total 92	O 92	0	0
8	G	23	Total 23	O 23	0	0

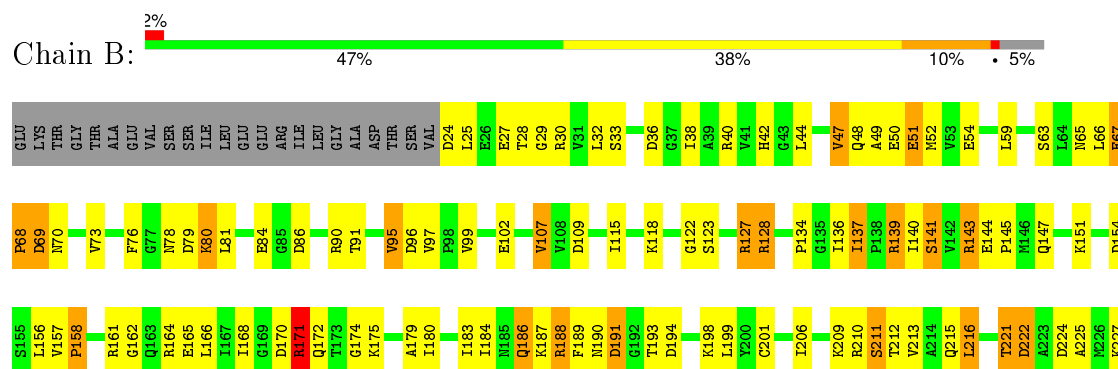
3 Residue-property plots

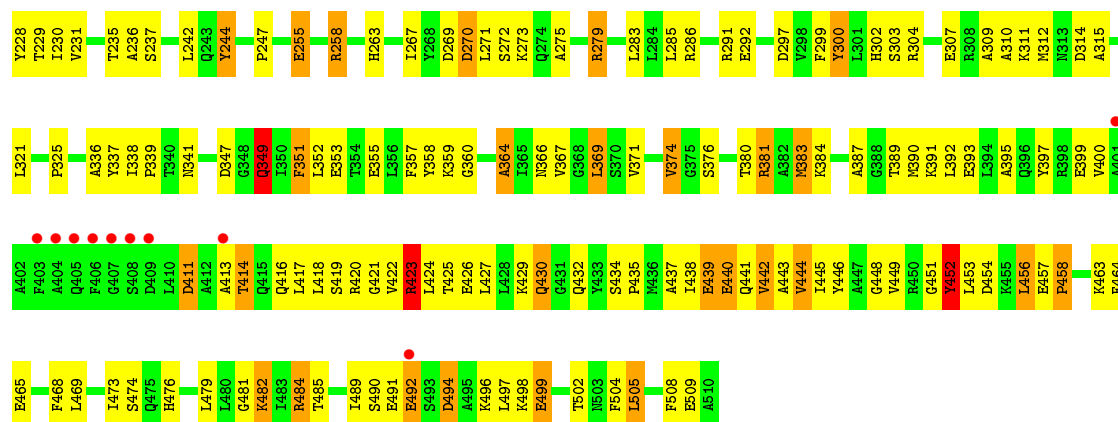
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

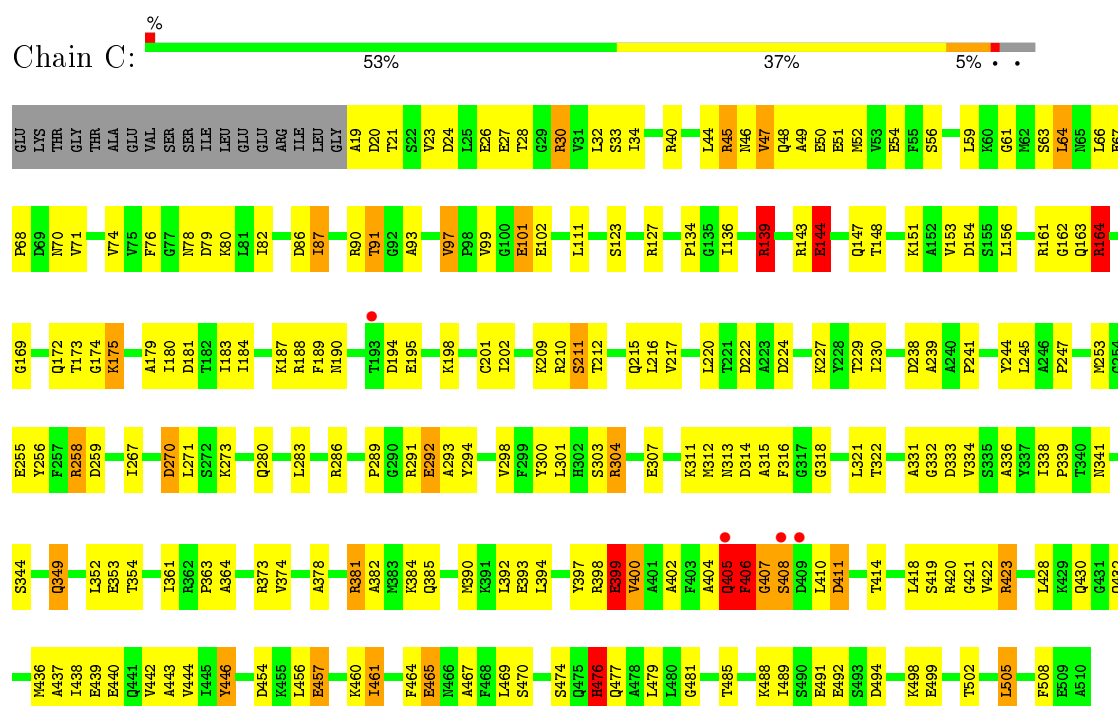


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

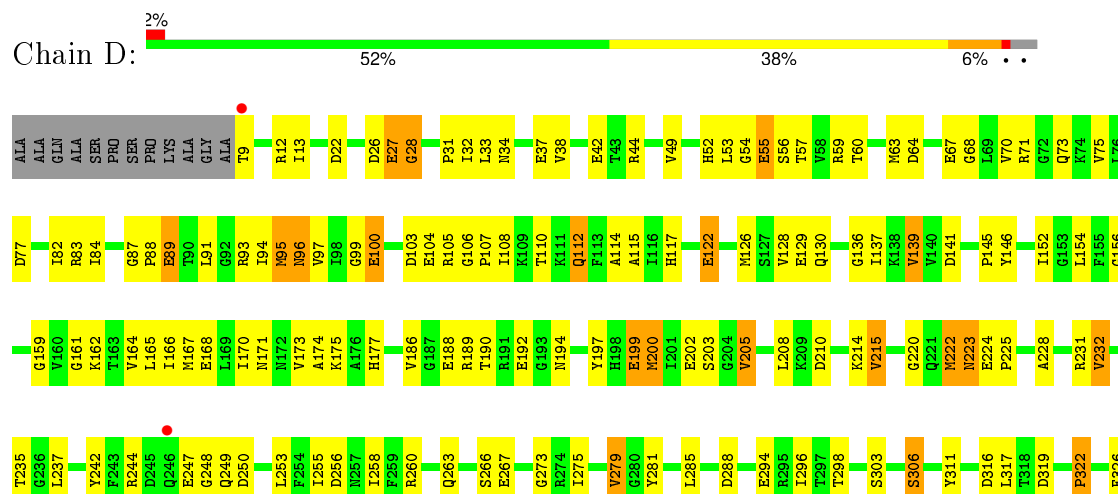


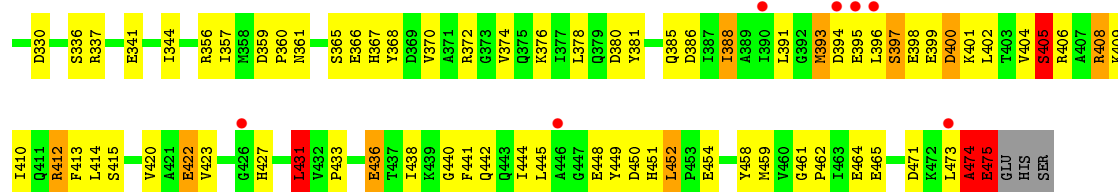


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

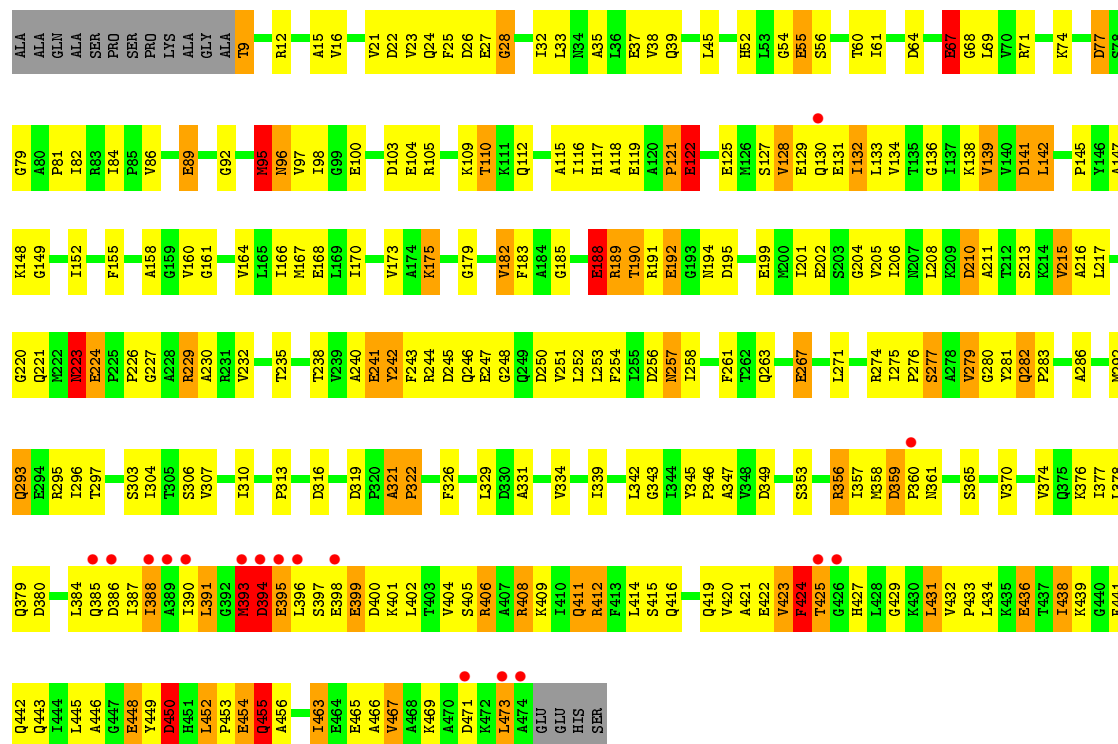


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

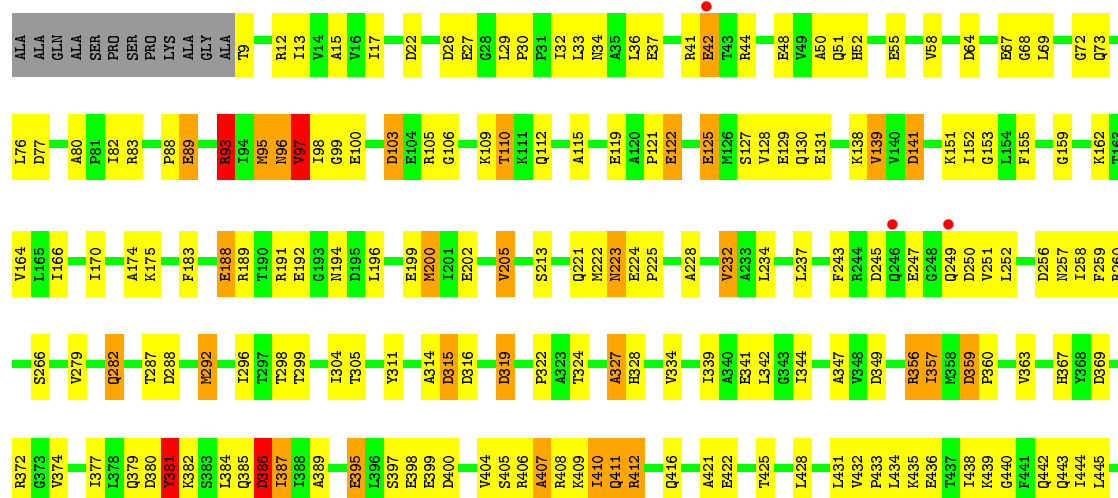




• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	283.40 Å 107.60 Å 140.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 99.4 (20.00-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.44 (at 3.09 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , 0.280 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 91.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 77818 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23462	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, AUR, 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	0.99	17/3766 (0.5%)	1.38	45/5080 (0.9%)
1	B	1.00	16/3766 (0.4%)	1.40	41/5080 (0.8%)
1	C	1.00	19/3799 (0.5%)	1.38	39/5126 (0.8%)
2	D	1.01	24/3596 (0.7%)	1.40	41/4879 (0.8%)
2	E	1.02	25/3587 (0.7%)	1.36	47/4867 (1.0%)
2	F	1.07	26/3587 (0.7%)	1.39	55/4867 (1.1%)
3	G	0.99	7/949 (0.7%)	1.42	18/1266 (1.4%)
All	All	1.01	134/23050 (0.6%)	1.39	286/31165 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
2	D	0	1
2	E	0	2
3	G	1	3
All	All	1	11

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	CD-OE1	8.28	1.34	1.25
2	F	42	GLU	CD-OE2	8.05	1.34	1.25
2	F	224	GLU	CD-OE2	7.94	1.34	1.25
2	D	436	GLU	CD-OE2	7.43	1.33	1.25
1	A	491	GLU	CD-OE1	7.19	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	131	GLU	CD-OE1	7.00	1.33	1.25
2	F	454	GLU	CD-OE2	-6.96	1.18	1.25
2	E	119	GLU	CD-OE2	6.96	1.33	1.25
2	D	89	GLU	CD-OE2	6.89	1.33	1.25
2	F	202	GLU	CD-OE2	6.77	1.33	1.25
2	D	475	GLU	CD-OE2	6.71	1.33	1.25
2	E	27	GLU	CD-OE1	6.69	1.33	1.25
2	E	241	GLU	CD-OE2	6.68	1.32	1.25
2	E	67	GLU	CD-OE2	6.64	1.32	1.25
2	D	55	GLU	CD-OE2	6.63	1.32	1.25
2	E	395	GLU	CD-OE1	6.63	1.32	1.25
2	F	122	GLU	CD-OE2	6.63	1.32	1.25
3	G	22	SER	CA-CB	-6.62	1.43	1.52
2	E	267	GLU	CD-OE2	6.58	1.32	1.25
2	F	247	GLU	CG-CD	-6.50	1.42	1.51
2	F	465	GLU	CD-OE2	6.48	1.32	1.25
2	E	224	GLU	CD-OE1	6.47	1.32	1.25
1	B	399	GLU	CD-OE2	6.40	1.32	1.25
1	A	355	GLU	CD-OE2	6.39	1.32	1.25
2	D	104	GLU	CD-OE2	6.36	1.32	1.25
1	C	353	GLU	CD-OE2	6.33	1.32	1.25
1	C	465	GLU	CD-OE2	6.28	1.32	1.25
1	C	491	GLU	CD-OE2	6.28	1.32	1.25
1	C	439	GLU	CD-OE2	6.27	1.32	1.25
2	D	202	GLU	CD-OE2	6.26	1.32	1.25
2	E	398	GLU	CD-OE2	6.26	1.32	1.25
1	C	492	GLU	CD-OE1	6.25	1.32	1.25
2	D	67	GLU	CD-OE2	6.20	1.32	1.25
1	C	54	GLU	CD-OE1	6.20	1.32	1.25
1	B	51	GLU	CD-OE2	6.19	1.32	1.25
1	C	292	GLU	CD-OE2	6.18	1.32	1.25
3	G	264	GLU	CD-OE2	6.16	1.32	1.25
1	C	399	GLU	CD-OE2	-6.13	1.19	1.25
2	F	247	GLU	CD-OE1	-6.12	1.19	1.25
2	D	294	GLU	CD-OE2	6.09	1.32	1.25
1	B	439	GLU	CD-OE2	6.08	1.32	1.25
2	E	202	GLU	CD-OE2	6.06	1.32	1.25
1	C	101	GLU	CD-OE1	6.04	1.32	1.25
1	A	492	GLU	CD-OE2	6.03	1.32	1.25
2	F	27	GLU	CD-OE2	6.03	1.32	1.25
2	D	399	GLU	CD-OE2	6.02	1.32	1.25
1	A	195	GLU	CD-OE1	6.02	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	341	GLU	CD-OE2	6.02	1.32	1.25
2	F	129	GLU	CD-OE2	6.01	1.32	1.25
2	E	89	GLU	CD-OE1	5.98	1.32	1.25
1	B	67	GLU	CD-OE2	5.96	1.32	1.25
1	B	355	GLU	CD-OE2	5.96	1.32	1.25
1	C	399	GLU	CD-OE1	5.94	1.32	1.25
2	F	395	GLU	CD-OE2	5.93	1.32	1.25
2	D	37	GLU	CD-OE2	5.89	1.32	1.25
2	D	129	GLU	CD-OE2	5.89	1.32	1.25
1	C	393	GLU	CD-OE1	5.86	1.32	1.25
1	A	439	GLU	CD-OE2	5.85	1.32	1.25
2	E	199	GLU	CD-OE1	5.85	1.32	1.25
2	E	122	GLU	CD-OE1	5.84	1.32	1.25
2	F	188	GLU	CD-OE2	5.83	1.32	1.25
2	F	55	GLU	CD-OE2	5.82	1.32	1.25
1	C	499	GLU	CD-OE2	5.82	1.32	1.25
2	D	224	GLU	CD-OE2	5.81	1.32	1.25
2	F	125	GLU	CD-OE2	5.81	1.32	1.25
1	A	353	GLU	CD-OE2	5.80	1.32	1.25
3	G	35	GLU	CD-OE2	5.78	1.32	1.25
1	A	292	GLU	CD-OE2	5.78	1.32	1.25
1	B	54	GLU	CD-OE1	5.76	1.31	1.25
3	G	241	GLU	CD-OE2	5.76	1.31	1.25
2	E	129	GLU	CD-OE2	5.75	1.31	1.25
1	B	440	GLU	CD-OE2	5.75	1.31	1.25
2	E	131	GLU	CD-OE1	5.73	1.31	1.25
3	G	40	PRO	N-CD	5.73	1.55	1.47
1	C	307	GLU	CD-OE1	5.70	1.31	1.25
2	E	192	GLU	CD-OE2	5.70	1.31	1.25
2	F	399	GLU	CD-OE1	5.70	1.31	1.25
2	F	37	GLU	CD-OE2	5.67	1.31	1.25
2	D	464	GLU	CD-OE2	5.65	1.31	1.25
2	D	247	GLU	CD-OE2	5.64	1.31	1.25
1	B	307	GLU	CD-OE2	5.64	1.31	1.25
1	C	457	GLU	CD-OE1	5.62	1.31	1.25
2	E	399	GLU	CD-OE2	5.61	1.31	1.25
2	D	448	GLU	CD-OE2	5.60	1.31	1.25
2	D	199	GLU	CD-OE2	5.58	1.31	1.25
1	C	144	GLU	CD-OE2	5.56	1.31	1.25
1	A	51	GLU	CD-OE2	5.54	1.31	1.25
2	F	192	GLU	CD-OE2	5.54	1.31	1.25
1	A	165	GLU	CD-OE2	5.54	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	188	GLU	CD-OE2	5.53	1.31	1.25
2	D	395	GLU	CD-OE2	5.53	1.31	1.25
2	E	436	GLU	CD-OE2	5.47	1.31	1.25
2	D	27	GLU	CD-OE2	5.46	1.31	1.25
2	E	55	GLU	CD-OE2	5.46	1.31	1.25
2	D	422	GLU	CD-OE2	5.45	1.31	1.25
2	D	122	GLU	CD-OE2	5.45	1.31	1.25
2	F	48	GLU	CD-OE1	-5.45	1.19	1.25
1	B	491	GLU	CD-OE1	5.43	1.31	1.25
1	A	144	GLU	CD-OE1	5.43	1.31	1.25
1	A	399	GLU	CD-OE1	5.43	1.31	1.25
2	F	448	GLU	CD-OE2	5.42	1.31	1.25
1	B	292	GLU	CD-OE1	-5.41	1.19	1.25
2	F	119	GLU	CD-OE2	5.41	1.31	1.25
1	B	84	GLU	CD-OE2	5.39	1.31	1.25
1	B	509	GLU	CD-OE2	5.39	1.31	1.25
2	F	422	GLU	CD-OE2	5.39	1.31	1.25
1	A	426	GLU	CD-OE2	5.38	1.31	1.25
1	C	432	GLN	CB-CG	-5.34	1.38	1.52
2	E	37	GLU	CD-OE2	5.32	1.31	1.25
1	A	393	GLU	CD-OE2	5.29	1.31	1.25
1	B	492	GLU	CD-OE2	5.29	1.31	1.25
1	B	255	GLU	CD-OE2	5.27	1.31	1.25
2	D	341	GLU	CD-OE1	5.27	1.31	1.25
3	G	11	LYS	CE-NZ	5.27	1.62	1.49
1	A	457	GLU	CD-OE1	5.26	1.31	1.25
2	D	42	GLU	CD-OE2	5.24	1.31	1.25
2	D	100	GLU	CD-OE2	5.24	1.31	1.25
2	F	398	GLU	CD-OE2	5.22	1.31	1.25
1	A	54	GLU	CD-OE2	5.21	1.31	1.25
1	A	499	GLU	CD-OE2	5.18	1.31	1.25
1	C	440	GLU	CD-OE2	5.16	1.31	1.25
2	E	168	GLU	CD-OE2	5.15	1.31	1.25
2	D	465	GLU	CD-OE2	5.12	1.31	1.25
2	F	199	GLU	CD-OE1	5.11	1.31	1.25
2	E	448	GLU	CD-OE2	5.11	1.31	1.25
1	B	499	GLU	CD-OE2	5.08	1.31	1.25
2	E	104	GLU	CD-OE2	5.08	1.31	1.25
1	C	26	GLU	CD-OE2	5.06	1.31	1.25
2	E	247	GLU	CD-OE2	5.04	1.31	1.25
1	C	67	GLU	CD-OE2	5.03	1.31	1.25
3	G	219	GLU	CD-OE2	5.02	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	GLU	CD-OE2	5.01	1.31	1.25
2	F	89	GLU	CD-OE2	5.01	1.31	1.25
2	E	465	GLU	CD-OE2	5.00	1.31	1.25

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	NE-CZ-NH2	-16.74	111.93	120.30
2	D	408	ARG	NE-CZ-NH1	15.40	128.00	120.30
1	A	143	ARG	NE-CZ-NH2	-13.38	113.61	120.30
2	D	408	ARG	CD-NE-CZ	11.78	140.09	123.60
3	G	9	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	B	279	ARG	NE-CZ-NH1	10.49	125.55	120.30
2	D	231	ARG	NE-CZ-NH1	9.97	125.28	120.30
2	D	459	MET	CG-SD-CE	-9.87	84.41	100.20
1	C	161	ARG	NE-CZ-NH1	9.85	125.22	120.30
2	D	316	ASP	CB-CG-OD1	9.73	127.06	118.30
1	A	450	ARG	NE-CZ-NH2	-9.48	115.56	120.30
2	F	356	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	B	484	ARG	NE-CZ-NH1	9.12	124.86	120.30
2	D	316	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	A	45	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	C	258	ARG	NE-CZ-NH1	8.64	124.62	120.30
2	E	408	ARG	NE-CZ-NH2	-8.52	116.04	120.30
2	F	93	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	D	431	LEU	CB-CG-CD1	8.45	125.37	111.00
3	G	254	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	F	80	ALA	N-CA-CB	-8.24	98.56	110.10
1	B	36	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	F	96	ASN	CB-CA-C	-8.17	94.07	110.40
1	C	294	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	B	270	ASP	CB-CA-C	-8.06	94.29	110.40
1	B	36	ASP	CB-CG-OD1	8.00	125.50	118.30
1	B	222	ASP	CB-CG-OD1	7.93	125.44	118.30
1	B	484	ARG	NE-CZ-NH2	-7.91	116.34	120.30
3	G	44	TYR	CB-CG-CD2	7.89	125.73	121.00
1	B	279	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	B	139	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	F	356	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	222	ASP	CB-CG-OD2	-7.67	111.40	118.30
2	E	64	ASP	CB-CG-OD2	-7.66	111.41	118.30
2	F	256	ASP	CB-CG-OD1	7.53	125.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	71	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	194	ASP	CB-CG-OD2	-7.38	111.65	118.30
3	G	44	TYR	CB-CG-CD1	-7.38	116.57	121.00
1	A	494	ASP	CB-CG-OD2	-7.35	111.68	118.30
3	G	2	THR	N-CA-CB	7.35	124.26	110.30
1	C	423	ARG	NE-CZ-NH2	-7.33	116.64	120.30
2	D	475	GLU	N-CA-CB	7.33	123.79	110.60
2	E	26	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	A	157	VAL	CA-CB-CG2	7.32	121.88	110.90
2	E	408	ARG	CD-NE-CZ	7.30	133.83	123.60
1	A	224	ASP	CB-CG-OD1	7.30	124.87	118.30
2	E	195	ASP	CB-CG-OD2	-7.27	111.76	118.30
2	E	229	ARG	NE-CZ-NH1	7.27	123.93	120.30
2	E	408	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	106	ARG	NE-CZ-NH1	7.21	123.90	120.30
2	F	359	ASP	CB-CG-OD1	7.17	124.76	118.30
3	G	44	TYR	CG-CD1-CE1	7.16	127.03	121.30
1	B	194	ASP	CB-CG-OD1	7.16	124.74	118.30
2	F	77	ASP	CB-CG-OD1	7.15	124.74	118.30
1	B	300	TYR	CB-CG-CD2	-7.14	116.71	121.00
1	C	181	ASP	CB-CG-OD2	-7.09	111.92	118.30
2	D	200	MET	CA-CB-CG	6.99	125.19	113.30
1	A	219	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	143	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	222	ASP	CB-CG-OD2	-6.92	112.07	118.30
2	F	77	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	450	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	C	270	ASP	CB-CG-OD2	-6.85	112.13	118.30
3	G	9	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	128	ARG	NE-CZ-NH1	6.81	123.71	120.30
2	F	110	THR	CA-CB-CG2	6.81	121.94	112.40
1	A	297	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	106	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	258	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	406	PHE	CG-CD1-CE1	6.73	128.20	120.80
2	F	386	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	479	LEU	CB-CG-CD2	6.70	122.39	111.00
1	B	381	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	406	PHE	CB-CG-CD1	6.67	125.47	120.80
2	F	41	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	F	381	TYR	CD1-CG-CD2	-6.66	110.58	117.90
1	A	45	ARG	NE-CZ-NH1	6.65	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	ASP	CB-CG-OD2	6.61	124.25	118.30
2	D	215	VAL	CA-CB-CG1	-6.60	101.00	110.90
1	C	423	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	D	210	ASP	CB-CG-OD1	6.59	124.23	118.30
2	E	22	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	F	381	TYR	CB-CG-CD1	6.55	124.93	121.00
1	A	53	VAL	CG1-CB-CG2	-6.54	100.43	110.90
2	E	195	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C	494	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	259	ASP	CB-CG-OD2	-6.50	112.45	118.30
2	F	41	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	297	ASP	CB-CG-OD1	6.45	124.11	118.30
2	E	359	ASP	CB-CG-OD1	6.44	124.10	118.30
3	G	254	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	E	386	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	24	ASP	CB-CG-OD1	6.42	124.08	118.30
2	F	250	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	40	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	270	ASP	CB-CA-C	-6.40	97.60	110.40
1	B	244	TYR	CB-CG-CD2	-6.39	117.16	121.00
1	B	171	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	E	471	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	C	161	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	30	ARG	NE-CZ-NH1	6.31	123.45	120.30
2	D	103	ASP	CB-CG-OD2	-6.28	112.64	118.30
2	F	406	ARG	NE-CZ-NH2	-6.27	117.16	120.30
2	F	292	MET	CG-SD-CE	-6.27	90.17	100.20
2	F	400	ASP	CB-CG-OD2	-6.24	112.68	118.30
2	F	386	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	79	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	C	291	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	164	ARG	NE-CZ-NH1	-6.21	117.19	120.30
2	E	210	ASP	CB-CG-OD2	6.21	123.89	118.30
2	E	473	LEU	CB-CG-CD2	6.20	121.54	111.00
1	B	494	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	116	ASP	CB-CG-OD2	-6.18	112.73	118.30
2	D	44	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	154	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	210	ARG	N-CA-CB	6.13	121.64	110.60
2	D	256	ASP	CB-CG-OD1	6.12	123.81	118.30
2	E	189	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	158	PRO	N-CD-CG	6.12	112.38	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	321	ALA	N-CA-CB	6.12	118.66	110.10
2	E	274	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	E	450	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	A	24	ASP	CB-CG-OD1	-6.09	112.82	118.30
2	D	22	ASP	CB-CG-OD1	6.09	123.78	118.30
2	F	139	VAL	CB-CA-C	-6.09	99.83	111.40
2	D	231	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	E	141	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	446	TYR	CB-CG-CD2	6.06	124.64	121.00
2	F	141	ASP	CB-CG-OD1	6.06	123.75	118.30
1	C	164	ARG	CD-NE-CZ	-6.05	115.13	123.60
2	D	413	PHE	CG-CD2-CE2	6.05	127.45	120.80
2	F	282	GLN	CB-CG-CD	6.04	127.31	111.60
2	E	64	ASP	CB-CG-OD1	6.04	123.74	118.30
2	D	380	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	F	412	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	D	380	ASP	CB-CG-OD1	6.01	123.71	118.30
3	G	5	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	C	24	ASP	CB-CG-OD2	-5.98	112.91	118.30
1	B	349	GLN	N-CA-CB	5.96	121.33	110.60
2	D	64	ASP	CB-CG-OD1	5.96	123.66	118.30
2	F	407	ALA	CB-CA-C	5.95	119.02	110.10
1	C	304	ARG	N-CA-CB	-5.95	99.90	110.60
2	F	103	ASP	CB-CG-OD2	-5.94	112.95	118.30
2	F	279	VAL	CA-CB-CG2	5.94	119.81	110.90
1	A	454	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	109	ASP	CB-CG-OD1	5.93	123.64	118.30
2	D	222	MET	CB-CA-C	-5.93	98.55	110.40
1	B	452	TYR	CZ-CE2-CD2	5.92	125.13	119.80
1	B	337	TYR	CB-CG-CD1	5.91	124.55	121.00
2	F	22	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	405	GLN	C-N-CA	5.90	136.46	121.70
2	E	356	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	333	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	D	250	ASP	CB-CG-OD2	-5.88	113.01	118.30
2	D	412	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	F	93	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	E	386	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	194	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	432	GLN	N-CA-CB	-5.85	100.08	110.60
1	C	194	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	69	ASP	CB-CG-OD2	-5.84	113.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	386	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	371	VAL	CB-CA-C	-5.82	100.34	111.40
1	B	109	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	154	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	C	494	ASP	CB-CG-OD1	-5.79	113.09	118.30
2	E	394	ASP	CB-CG-OD1	-5.79	113.09	118.30
2	F	381	TYR	CB-CG-CD2	5.79	124.47	121.00
1	C	454	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	381	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	244	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	F	400	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	88	VAL	CG1-CB-CG2	-5.71	101.76	110.90
2	E	110	THR	CA-CB-CG2	5.70	120.38	112.40
2	E	277	SER	N-CA-CB	5.69	119.03	110.50
2	F	359	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	191	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	F	369	ASP	CB-CG-OD1	5.68	123.41	118.30
2	E	223	ASN	CB-CA-C	-5.67	99.07	110.40
1	B	423	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	D	394	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	E	406	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	245	LEU	CB-CA-C	-5.63	99.50	110.20
1	C	20	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	E	359	ASP	CB-CG-OD2	-5.61	113.25	118.30
3	G	5	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	154	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	314	ASP	CB-CG-OD1	-5.58	113.28	118.30
2	E	103	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	F	96	ASN	N-CA-CB	-5.58	100.56	110.60
2	F	22	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	D	260	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	D	474	ALA	C-N-CA	5.57	135.63	121.70
2	E	431	LEU	CB-CA-C	5.57	120.79	110.20
1	A	79	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	139	ARG	NE-CZ-NH2	-5.57	117.52	120.30
3	G	44	TYR	CD1-CE1-CZ	-5.56	114.79	119.80
2	F	381	TYR	CG-CD1-CE1	5.55	125.74	121.30
2	F	245	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	222	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	371	VAL	CA-CB-CG2	5.53	119.19	110.90
1	B	337	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	A	154	ASP	CB-CG-OD1	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	471	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	244	TYR	CB-CG-CD1	5.52	124.31	121.00
2	F	93	ARG	CD-NE-CZ	5.50	131.30	123.60
1	B	24	ASP	C-N-CA	5.45	135.33	121.70
2	E	26	ASP	CB-CG-OD1	5.45	123.20	118.30
3	G	211	ASN	N-CA-CB	-5.41	100.87	110.60
2	F	319	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	127	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	F	315	ASP	CB-CG-OD1	5.39	123.15	118.30
2	F	245	ASP	CB-CG-OD1	5.39	123.15	118.30
2	F	380	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	D	190	THR	CA-CB-CG2	-5.38	104.86	112.40
1	C	259	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	259	ASP	CB-CG-OD1	5.36	123.13	118.30
2	D	141	ASP	CB-CG-OD1	5.36	123.12	118.30
2	E	96	ASN	N-CA-CB	-5.33	101.01	110.60
1	C	238	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	258	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	194	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	F	311	TYR	CG-CD2-CE2	5.31	125.55	121.30
2	D	26	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	223	ALA	CB-CA-C	5.31	118.06	110.10
2	E	356	ARG	NE-CZ-NH2	-5.29	117.65	120.30
3	G	237	LYS	CB-CA-C	5.29	120.98	110.40
2	F	460	VAL	CA-CB-CG1	5.28	118.83	110.90
1	A	194	ASP	CB-CG-OD2	-5.28	113.55	118.30
2	D	64	ASP	CB-CG-OD2	-5.28	113.55	118.30
2	F	205	VAL	CB-CA-C	5.28	121.43	111.40
2	F	183	PHE	CB-CG-CD1	5.28	124.49	120.80
1	A	372	SER	N-CA-CB	5.27	118.41	110.50
1	B	107	VAL	CG1-CB-CG2	-5.27	102.47	110.90
2	E	245	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	C	411	ASP	CB-CG-OD1	-5.25	113.57	118.30
2	D	12	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	F	260	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	F	64	ASP	CB-CG-OD2	-5.25	113.58	118.30
2	F	250	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	C	314	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	476	HIS	N-CA-C	5.23	125.12	111.00
2	F	80	ALA	CB-CA-C	5.23	117.94	110.10
2	F	97	VAL	CA-CB-CG1	-5.23	103.06	110.90
2	D	450	ASP	CB-CG-OD2	-5.21	113.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	22	ASP	CB-CG-OD1	5.21	122.98	118.30
2	F	316	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	E	431	LEU	CB-CG-CD1	5.20	119.84	111.00
2	D	256	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	D	96	ASN	CB-CA-C	-5.20	100.00	110.40
1	C	349	GLN	CB-CA-C	-5.19	100.02	110.40
2	E	77	ASP	CB-CG-OD1	5.18	122.96	118.30
2	E	380	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	C	28	THR	CA-CB-CG2	5.16	119.62	112.40
1	B	353	GLU	CB-CA-C	-5.15	100.11	110.40
2	D	22	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	D	288	ASP	CB-CG-OD1	5.14	122.93	118.30
3	G	40	PRO	CA-N-CD	-5.14	104.31	111.50
3	G	22	SER	CA-CB-OG	5.12	125.01	111.20
1	B	494	ASP	CB-CG-OD1	5.11	122.90	118.30
2	F	349	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	D	311	TYR	CG-CD2-CE2	5.11	125.39	121.30
1	A	304	ARG	CG-CD-NE	5.10	122.52	111.80
3	G	209	LEU	N-CA-CB	5.10	120.60	110.40
1	A	230	ILE	CB-CA-C	-5.09	101.41	111.60
2	E	77	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	334	VAL	CG1-CB-CG2	5.09	119.04	110.90
1	C	259	ASP	CB-CG-OD1	5.09	122.88	118.30
2	E	349	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	91	THR	CA-CB-CG2	5.08	119.52	112.40
2	E	95	MET	CA-CB-CG	5.07	121.93	113.30
2	F	288	ASP	CB-CG-OD2	-5.07	113.73	118.30
2	D	103	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	300	TYR	CB-CG-CD2	-5.04	117.97	121.00
2	E	242	TYR	CB-CG-CD1	5.04	124.03	121.00
2	E	141	ASP	CB-CG-OD2	-5.04	113.77	118.30
2	F	26	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	A	86	ASP	CB-CG-OD1	5.03	122.83	118.30
2	E	128	VAL	CG1-CB-CG2	-5.03	102.86	110.90
2	E	322	PRO	N-CD-CG	5.03	110.74	103.20
3	G	233	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	B	349	GLN	CA-CB-CG	5.01	124.43	113.40
3	G	20	THR	CA-CB-CG2	-5.01	105.38	112.40
2	D	77	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	96	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	219	ARG	CD-NE-CZ	5.00	130.61	123.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	209	LEU	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	PHE	Mainchain
1	B	369	LEU	Mainchain
1	B	432	GLN	Mainchain
1	C	363	PRO	Mainchain
1	C	405	GLN	Mainchain
2	D	431	LEU	Mainchain
2	E	346	PRO	Mainchain
2	E	411	GLN	Sidechain
3	G	17	GLN	Sidechain,Mainchain
3	G	250	PHE	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	3815	162	0
1	B	3715	0	3814	168	0
1	C	3748	0	3845	137	0
2	D	3539	0	3593	140	0
2	E	3530	0	3587	184	0
2	F	3530	0	3587	137	0
3	G	945	0	1019	39	0
4	A	1	0	0	0	0
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	1	0
5	B	31	0	13	8	0
5	C	31	0	13	4	0
5	F	31	0	12	2	0
6	D	27	0	12	3	0
7	E	33	0	32	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	33	0	32	6	0
8	A	80	0	0	6	0
8	B	84	0	0	12	0
8	C	98	0	0	11	0
8	D	94	0	0	11	0
8	E	47	0	0	9	0
8	F	92	0	0	11	0
8	G	23	0	0	2	0
All	All	23462	0	23387	914	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 20.

All (914) 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:215:GLN:HG3	2:F:356:ARG:HH22	1.07	1.15
1:C:127:ARG:HH12	1:C:255:GLU:HB2	0.97	1.07
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.24	1.01
2:F:223:ASN:HD22	2:F:223:ASN:H	1.06	1.00
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.80	0.96
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.80	0.95
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.82	0.93
2:E:223:ASN:H	2:E:223:ASN:HD22	0.92	0.92
1:B:456:LEU:HD12	1:B:457:GLU:H	1.37	0.90
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.54	0.89
2:E:223:ASN:H	2:E:223:ASN:ND2	1.70	0.89
2:E:411:GLN:NE2	7:E:479:AUR:H5	1.86	0.89
1:B:172:GLN:HA	5:B:600:ANP:HNB1	1.37	0.88
2:D:223:ASN:H	2:D:223:ASN:HD22	1.21	0.85
2:E:223:ASN:HD22	2:E:223:ASN:N	1.74	0.85
2:F:93:ARG:HH11	2:F:93:ARG:HG2	1.40	0.84
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.61	0.82
2:F:89:GLU:HG3	2:F:109:LYS:O	1.81	0.81
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.64	0.80
2:E:96:ASN:HB3	2:E:100:GLU:H	1.47	0.80
1:A:26:GLU:HG2	1:A:46:ASN:ND2	1.97	0.79
2:F:225:PRO:HB2	8:F:632:HOH:O	1.81	0.79
1:B:211:SER:HB2	8:B:664:HOH:O	1.83	0.78
1:C:40:ARG:HH11	1:C:70:ASN:HD21	1.32	0.78
1:A:360:GLY:HA2	1:A:362:ARG:NH1	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.49	0.77
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.66	0.77
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.84	0.77
1:B:187:LYS:HE3	1:B:191:ASP:OD2	1.85	0.77
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.49	0.77
2:E:89:GLU:HG3	2:E:109:LYS:O	1.85	0.76
2:E:326:PHE:HB3	8:E:497:HOH:O	1.85	0.76
2:F:411:GLN:HG2	7:F:602:AUR:H7	1.67	0.76
2:F:324:THR:HA	8:F:608:HOH:O	1.86	0.76
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.68	0.76
1:B:63:SER:HA	1:B:73:VAL:HG12	1.68	0.76
2:D:93:ARG:HH12	2:D:105:ARG:HB2	1.52	0.75
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.00	0.75
2:D:93:ARG:HH11	2:D:93:ARG:HG2	1.51	0.74
1:C:99:VAL:HG22	1:C:253:MET:HA	1.70	0.74
2:D:223:ASN:N	2:D:223:ASN:HD22	1.80	0.74
1:A:25:LEU:HD23	1:A:25:LEU:H	1.51	0.74
1:C:52:MET:O	1:C:91:THR:HB	1.88	0.74
1:A:440:GLU:O	1:A:444:VAL:HG13	1.87	0.74
2:E:342:LEU:O	7:E:479:AUR:H14	1.88	0.73
2:E:411:GLN:OE1	7:E:479:AUR:H9	1.87	0.73
1:A:297:ASP:HA	8:A:627:HOH:O	1.88	0.73
1:C:443:ALA:O	1:C:446:TYR:HB3	1.87	0.73
2:F:223:ASN:N	2:F:223:ASN:HD22	1.82	0.73
2:F:407:ALA:O	2:F:411:GLN:HB2	1.87	0.73
1:B:141:SER:O	1:B:143:ARG:HD2	1.88	0.73
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.71	0.72
1:A:136:ILE:HG22	8:A:610:HOH:O	1.88	0.72
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.89	0.72
2:E:224:GLU:HG2	8:E:499:HOH:O	1.88	0.72
1:C:399:GLU:OE2	2:D:408:ARG:NH2	2.23	0.72
2:E:378:LEU:O	7:E:479:AUR:H241	1.89	0.71
1:C:40:ARG:NH1	1:C:70:ASN:HD21	1.87	0.71
2:E:408:ARG:NH2	2:E:412:ARG:NH2	2.38	0.71
1:C:398:ARG:HG2	8:C:625:HOH:O	1.90	0.71
1:A:333:ASP:HB3	8:A:630:HOH:O	1.91	0.71
2:D:225:PRO:HB2	8:D:646:HOH:O	1.91	0.71
1:C:404:ALA:C	1:C:406:PHE:H	1.93	0.71
2:E:411:GLN:NE2	7:E:479:AUR:O25	2.24	0.70
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.91	0.70
1:C:40:ARG:HH11	1:C:70:ASN:ND2	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:O	1:A:47:VAL:HG22	1.92	0.70
2:E:441:PHE:O	2:E:445:LEU:HG	1.92	0.70
2:E:411:GLN:HE22	7:E:479:AUR:H5	1.55	0.70
2:E:149:GLY:HA2	2:E:304:ILE:O	1.91	0.70
3:G:2:THR:HG22	3:G:4:LYS:H	1.57	0.70
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.71	0.69
2:E:279:VAL:HG12	8:E:481:HOH:O	1.92	0.69
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.58	0.69
2:D:223:ASN:ND2	2:D:223:ASN:H	1.89	0.69
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.74	0.69
2:D:404:VAL:O	2:D:408:ARG:HG3	1.91	0.69
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.74	0.69
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.73	0.68
2:E:319:ASP:O	2:E:322:PRO:HD2	1.94	0.68
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.75	0.68
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.74	0.68
1:B:102:GLU:HG3	1:B:122:GLY:O	1.94	0.68
1:C:44:LEU:O	1:C:47:VAL:HG22	1.94	0.68
1:A:417:LEU:HD23	1:A:417:LEU:H	1.59	0.68
2:E:408:ARG:NH2	2:E:412:ARG:HH21	1.92	0.68
2:F:319:ASP:O	2:F:322:PRO:HD2	1.93	0.68
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.74	0.68
1:B:393:GLU:OE1	1:B:424:LEU:HD11	1.94	0.67
2:F:159:GLY:HA2	5:F:600:ANP:HNB1	1.58	0.67
2:D:175:LYS:N	8:D:606:HOH:O	2.27	0.67
1:A:94:ILE:HG12	1:A:95:VAL:N	2.10	0.67
1:C:139:ARG:HB3	1:C:311:LYS:O	1.93	0.67
1:A:385:GLN:OE1	1:A:488:LYS:HB2	1.95	0.67
1:A:270:ASP:OD1	1:A:273:LYS:HG3	1.95	0.67
2:E:138:LYS:HG3	2:E:416:GLN:OE1	1.95	0.67
2:F:395:GLU:OE2	3:G:77:LEU:HA	1.95	0.67
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.78	0.66
2:E:267:GLU:O	2:E:271:LEU:HG	1.96	0.66
1:C:210:ARG:NH1	2:F:121:PRO:O	2.30	0.65
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.78	0.65
1:B:422:VAL:O	1:B:426:GLU:HG2	1.97	0.65
1:B:151:LYS:HG3	1:B:430:GLN:HE21	1.60	0.65
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.96	0.65
1:A:341:ASN:O	1:A:345:ILE:HG13	1.97	0.65
1:A:175:LYS:HG3	1:A:352:LEU:HD12	1.78	0.65
3:G:254:ARG:NH2	8:G:273:HOH:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:OE1	1:A:438:ILE:HD13	1.97	0.65
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.60	0.65
2:E:455:GLN:O	2:E:469:LYS:HD3	1.97	0.64
1:B:381:ARG:O	1:B:384:LYS:HB2	1.96	0.64
2:F:93:ARG:NH2	2:F:106:GLY:O	2.31	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.63	0.63
2:F:372:ARG:NH2	8:F:683:HOH:O	2.28	0.63
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.81	0.63
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.63
2:D:162:LYS:N	6:D:600:ADP:O1B	2.30	0.63
1:B:175:LYS:NZ	8:B:649:HOH:O	2.30	0.63
1:B:151:LYS:NZ	1:B:429:LYS:O	2.32	0.62
2:E:449:TYR:HB3	2:E:452:LEU:HB2	1.81	0.62
2:E:425:THR:O	2:E:427:HIS:ND1	2.27	0.62
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.64	0.62
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.28	0.62
2:F:223:ASN:ND2	2:F:223:ASN:H	1.88	0.62
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.80	0.62
1:A:150:ILE:HA	1:A:430:GLN:HE22	1.63	0.62
1:A:485:THR:HG22	1:A:486:ASP:N	2.14	0.62
2:E:224:GLU:O	2:E:229:ARG:NH1	2.30	0.62
3:G:221:THR:HG22	8:G:295:HOH:O	1.99	0.62
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.81	0.62
2:D:473:LEU:O	2:D:475:GLU:N	2.33	0.62
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.82	0.62
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.80	0.62
1:A:82:ILE:HA	1:A:86:ASP:OD2	1.99	0.62
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.00	0.61
2:D:96:ASN:HB2	2:D:100:GLU:H	1.64	0.61
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.65	0.61
1:A:106:ARG:NH2	1:A:119:GLY:O	2.29	0.61
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.82	0.61
2:E:412:ARG:NH1	7:E:479:AUR:O19	2.32	0.61
1:A:414:THR:O	1:A:418:LEU:HD22	2.00	0.61
1:A:164:ARG:NH1	1:A:347:ASP:OD2	2.33	0.61
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.82	0.61
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.65	0.61
2:E:142:LEU:HD23	2:E:414:LEU:HD21	1.82	0.61
2:D:173:VAL:N	8:D:606:HOH:O	2.33	0.61
2:E:455:GLN:NE2	2:E:469:LYS:NZ	2.49	0.61
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLN:O	1:B:445:ILE:HG12	2.00	0.61
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.81	0.60
1:B:499:GLU:O	1:B:502:THR:HB	2.00	0.60
2:D:53:LEU:HD11	2:D:59:ARG:HB2	1.83	0.60
1:B:400:VAL:HB	1:B:418:LEU:HD13	1.83	0.60
2:D:406:ARG:O	2:D:410:ILE:HG13	2.00	0.60
1:C:172:GLN:HA	5:C:600:ANP:HNB1	1.65	0.60
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.63	0.60
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.84	0.60
2:F:151:LYS:HA	8:F:609:HOH:O	2.00	0.60
1:C:211:SER:O	1:C:215:GLN:HG2	2.00	0.60
2:F:93:ARG:NH1	2:F:93:ARG:HG2	2.09	0.60
1:A:151:LYS:H	1:A:430:GLN:NE2	1.99	0.60
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.81	0.60
1:B:151:LYS:CG	1:B:430:GLN:HE21	2.15	0.60
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.83	0.60
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.60
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.01	0.60
2:E:39:GLN:HB2	2:E:74:LYS:HB2	1.84	0.60
1:C:419:SER:O	1:C:423:ARG:HG2	2.02	0.60
1:B:118:LYS:NZ	8:B:628:HOH:O	2.34	0.60
2:D:93:ARG:NH2	2:D:106:GLY:O	2.34	0.59
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.67	0.59
1:B:151:LYS:NZ	1:B:427:LEU:O	2.31	0.59
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.84	0.59
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.18	0.59
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.36	0.59
2:D:473:LEU:C	2:D:475:GLU:H	2.04	0.59
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.84	0.59
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.85	0.59
2:D:402:LEU:O	2:D:406:ARG:HG3	2.03	0.59
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.02	0.59
2:F:252:LEU:HD23	2:F:305:THR:HB	1.85	0.59
2:F:243:PHE:O	2:F:249:GLN:HB2	2.03	0.59
2:F:162:LYS:HE3	8:F:627:HOH:O	2.03	0.58
2:E:421:ALA:O	2:E:425:THR:HB	2.03	0.58
1:B:349:GLN:NE2	8:B:615:HOH:O	2.35	0.58
1:A:48:GLN:HB3	2:E:68:GLY:O	2.03	0.58
2:D:156:GLY:HA2	8:D:651:HOH:O	2.02	0.58
2:E:316:ASP:OD2	3:G:254:ARG:NH1	2.36	0.58
2:F:234:LEU:O	2:F:237:LEU:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:438:ILE:O	2:E:442:GLN:HB2	2.03	0.58
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.69	0.58
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.58
1:A:130:GLY:HA2	1:A:308:ARG:NH1	2.19	0.58
1:A:145:PRO:O	1:A:161:ARG:HD2	2.03	0.58
2:E:246:GLN:NE2	2:E:246:GLN:HA	2.19	0.58
1:A:313:ASN:O	1:A:316:PHE:N	2.29	0.58
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.02	0.58
1:B:27:GLU:O	1:B:90:ARG:HG3	2.04	0.58
2:E:92:GLY:N	2:E:215:VAL:O	2.32	0.58
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.86	0.58
2:E:61:ILE:O	2:E:61:ILE:HG13	2.02	0.58
1:A:142:VAL:HG22	1:A:161:ARG:O	2.04	0.58
2:E:279:VAL:O	2:E:279:VAL:HG12	2.04	0.57
1:A:130:GLY:H	1:A:308:ARG:HH12	1.52	0.57
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.86	0.57
2:D:170:ILE:O	2:D:174:ALA:HB3	2.05	0.57
2:D:359:ASP:OD1	2:D:360:PRO:HD2	2.05	0.57
2:E:408:ARG:O	2:E:412:ARG:HG3	2.05	0.57
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.86	0.57
2:D:391:LEU:HD21	3:G:16:ILE:HG23	1.86	0.57
1:B:151:LYS:HG3	1:B:430:GLN:HG3	1.87	0.57
1:A:215:GLN:NE2	2:D:128:VAL:HB	2.20	0.57
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.70	0.57
2:F:374:VAL:O	2:F:377:ILE:HG22	2.04	0.57
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.85	0.57
3:G:38:LEU:HD11	3:G:42:ARG:NE	2.20	0.57
2:D:83:ARG:HA	2:D:114:ALA:O	2.04	0.57
2:E:167:MET:HE3	2:E:420:VAL:HG11	1.86	0.57
1:B:383:MET:O	1:B:387:ALA:N	2.34	0.57
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.85	0.57
2:E:9:THR:HG21	2:E:28:GLY:O	2.05	0.57
1:B:171:ARG:NH1	1:B:171:ARG:HG3	2.19	0.56
1:C:175:LYS:HE3	5:C:600:ANP:O1B	2.05	0.56
2:E:400:ASP:O	2:E:404:VAL:HG23	2.04	0.56
2:F:314:ALA:O	2:F:315:ASP:HB2	2.05	0.56
1:A:121:ILE:H	1:A:121:ILE:HD13	1.70	0.56
2:D:93:ARG:NH1	2:D:93:ARG:HG2	2.19	0.56
1:A:164:ARG:NH2	1:A:345:ILE:O	2.39	0.56
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.71	0.56
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.87	0.56
1:A:134:PRO:O	1:A:139:ARG:NH2	2.29	0.56
2:E:25:PHE:O	2:E:56:SER:HB3	2.06	0.56
1:C:143:ARG:N	8:C:646:HOH:O	2.27	0.56
2:E:258:ILE:O	2:E:261:PHE:HB3	2.05	0.56
1:C:476:HIS:N	1:C:476:HIS:ND1	2.53	0.56
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.19	0.56
1:B:174:GLY:HA2	5:B:600:ANP:PA	2.46	0.56
1:C:91:THR:HG22	1:C:93:ALA:H	1.71	0.56
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.86	0.56
1:A:179:ALA:O	1:A:182:THR:HB	2.06	0.56
1:C:102:GLU:OE1	1:C:123:SER:HA	2.04	0.56
1:B:221:THR:HG22	1:B:222:ASP:N	2.20	0.56
1:B:165:GLU:O	1:B:325:PRO:HD2	2.06	0.56
2:D:84:ILE:HB	2:D:95:MET:HE3	1.86	0.56
2:E:216:ALA:HB1	8:E:490:HOH:O	2.04	0.56
1:C:418:LEU:O	1:C:422:VAL:HG23	2.06	0.56
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.87	0.55
2:E:422:GLU:O	2:E:424:PHE:N	2.39	0.55
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.88	0.55
1:A:389:THR:O	1:A:393:GLU:HG2	2.06	0.55
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.55
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.89	0.55
3:G:20:THR:HG21	3:G:236:SER:N	2.21	0.55
8:A:634:HOH:O	2:D:376:LYS:HB2	2.07	0.55
2:D:38:VAL:HG22	2:D:75:VAL:HG22	1.88	0.55
2:F:93:ARG:NH1	2:F:105:ARG:HB2	2.21	0.55
2:D:397:SER:OG	2:D:400:ASP:HB2	2.07	0.55
1:C:45:ARG:NH2	1:C:68:PRO:O	2.40	0.55
1:B:175:LYS:HE3	5:B:600:ANP:O1B	2.07	0.55
2:E:409:LYS:HE2	2:E:452:LEU:O	2.07	0.55
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.05	0.55
2:E:242:TYR:C	2:E:244:ARG:H	2.10	0.55
2:F:409:LYS:NZ	2:F:452:LEU:O	2.26	0.55
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.89	0.55
2:D:263:GLN:NE2	8:D:618:HOH:O	2.29	0.55
2:D:263:GLN:O	2:D:267:GLU:HG3	2.07	0.55
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.88	0.55
3:G:7:THR:O	3:G:11:LYS:HB2	2.07	0.55
2:E:411:GLN:HG2	7:E:479:AUR:H7	1.88	0.55
2:F:164:VAL:HG23	5:F:600:ANP:O1A	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:ARG:O	2:E:23:VAL:HG13	2.07	0.55
1:C:174:GLY:HA2	5:C:600:ANP:PA	2.47	0.55
2:F:95:MET:HG3	2:F:99:GLY:HA2	1.88	0.55
2:F:251:VAL:HG12	2:F:252:LEU:N	2.22	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.06	0.54
1:C:467:ALA:O	1:C:470:SER:HB2	2.07	0.54
1:C:312:MET:O	1:C:318:GLY:HA2	2.07	0.54
1:A:26:GLU:HG2	1:A:46:ASN:HD21	1.73	0.54
1:A:438:ILE:O	1:A:442:VAL:HG13	2.07	0.54
1:A:213:VAL:O	1:A:216:LEU:HB3	2.08	0.54
1:B:32:LEU:HD11	1:B:42:HIS:HB2	1.89	0.54
2:E:221:GLN:N	2:E:224:GLU:OE1	2.40	0.54
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.72	0.54
2:E:148:LYS:HE3	2:E:250:ASP:OD2	2.07	0.54
2:E:422:GLU:C	2:E:424:PHE:H	2.11	0.54
1:C:406:PHE:O	1:C:408:SER:N	2.40	0.54
2:E:138:LYS:O	2:E:142:LEU:HB3	2.08	0.54
1:B:440:GLU:O	1:B:443:ALA:HB3	2.07	0.54
2:D:440:GLY:O	2:D:444:ILE:HG13	2.07	0.54
2:D:244:ARG:O	2:D:248:GLY:HA2	2.08	0.54
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.54
2:E:185:GLY:HA3	2:E:188:GLU:HG3	1.88	0.54
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.08	0.54
2:F:188:GLU:O	2:F:221:GLN:HB3	2.08	0.54
1:B:302:HIS:ND1	8:B:607:HOH:O	2.33	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.90	0.54
1:C:30:ARG:NE	1:C:87:ILE:HD11	2.08	0.53
3:G:43:VAL:HG12	3:G:43:VAL:O	2.08	0.53
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.23	0.53
1:C:392:LEU:HB3	2:D:458:TYR:OH	2.08	0.53
2:E:152:ILE:HA	2:E:331:ALA:O	2.09	0.53
1:B:300:TYR:O	1:B:304:ARG:HG2	2.08	0.53
2:E:116:ILE:HA	2:E:238:THR:OG1	2.08	0.53
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.90	0.53
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.42	0.53
2:D:366:GLU:O	2:D:370:VAL:HG23	2.09	0.53
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.90	0.53
1:B:456:LEU:HD12	1:B:457:GLU:N	2.16	0.53
2:E:122:GLU:HB2	2:E:125:GLU:HG3	1.91	0.53
1:B:352:LEU:HA	1:B:364:ALA:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:O	1:B:175:LYS:HE2	2.09	0.53
1:A:36:ASP:O	1:A:284:LEU:HD13	2.09	0.53
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.74	0.53
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.74	0.53
1:C:32:LEU:HB2	1:C:40:ARG:O	2.09	0.52
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.90	0.52
1:C:173:THR:HG22	1:C:354:THR:HG22	1.91	0.52
1:B:137:ILE:HD13	2:F:103:ASP:HA	1.90	0.52
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.91	0.52
2:D:88:PRO:O	2:D:91:LEU:HD12	2.08	0.52
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.91	0.52
1:C:215:GLN:CG	2:F:356:ARG:HH22	2.00	0.52
2:F:151:LYS:HD3	2:F:328:HIS:O	2.09	0.52
2:E:439:LYS:O	2:E:442:GLN:HB3	2.09	0.52
1:A:184:ILE:HD12	1:A:223:ALA:HB3	1.91	0.52
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.91	0.52
1:A:108:VAL:HA	1:A:113:ASN:O	2.09	0.52
1:A:224:ASP:HA	8:A:617:HOH:O	2.09	0.52
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.72	0.52
2:F:324:THR:O	2:F:324:THR:HG22	2.07	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.91	0.51
2:F:151:LYS:HG2	8:F:609:HOH:O	2.09	0.51
2:D:208:LEU:HA	8:D:609:HOH:O	2.10	0.51
1:A:268:TYR:HB2	1:A:325:PRO:HA	1.91	0.51
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.92	0.51
1:B:171:ARG:NH2	2:E:326:PHE:CD2	2.78	0.51
1:C:399:GLU:CD	2:D:408:ARG:HH22	2.13	0.51
1:A:48:GLN:HA	2:E:69:LEU:O	2.10	0.51
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.91	0.51
2:E:118:ALA:H	2:E:295:ARG:NH1	2.08	0.51
1:A:49:ALA:O	1:A:50:GLU:HB2	2.11	0.51
2:E:263:GLN:HB3	8:E:493:HOH:O	2.10	0.51
2:E:342:LEU:HB3	7:E:479:AUR:H12	1.92	0.51
2:E:95:MET:HA	2:E:100:GLU:O	2.10	0.51
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.26	0.51
1:B:157:VAL:O	1:B:157:VAL:HG12	2.10	0.51
1:A:215:GLN:NE2	2:D:128:VAL:HG12	2.26	0.51
2:E:359:ASP:OD1	2:E:360:PRO:HD2	2.10	0.51
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.08	0.51
2:E:463:ILE:O	2:E:467:VAL:HG23	2.10	0.51
1:B:162:GLY:HA2	1:B:321:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:384:LEU:O	2:F:387:ILE:HD12	2.10	0.51
1:A:337:TYR:O	1:A:340:THR:HB	2.10	0.51
2:E:397:SER:H	2:E:400:ASP:HB2	1.75	0.51
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.91	0.51
2:F:433:PRO:O	2:F:436:GLU:HB2	2.11	0.51
2:F:266:SER:HB3	2:F:282:GLN:NE2	2.25	0.51
3:G:254:ARG:O	3:G:258:ILE:HG13	2.11	0.51
1:B:59:LEU:HD22	1:B:81:LEU:HD12	1.93	0.51
1:C:71:VAL:HG23	8:C:668:HOH:O	2.10	0.51
1:C:30:ARG:HA	1:C:86:ASP:O	2.10	0.51
1:A:215:GLN:HE22	2:D:128:VAL:HB	1.74	0.51
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.92	0.51
2:F:404:VAL:O	2:F:408:ARG:HG3	2.11	0.51
1:C:151:LYS:HE2	1:C:436:MET:SD	2.50	0.51
2:F:442:GLN:O	2:F:445:LEU:HB2	2.11	0.51
1:B:358:TYR:C	1:B:360:GLY:H	2.13	0.51
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.11	0.51
2:D:356:ARG:HG2	2:D:356:ARG:O	2.11	0.51
2:E:385:GLN:HE22	7:E:479:AUR:H203	1.76	0.51
2:E:339:ILE:HD12	7:E:479:AUR:O7	2.11	0.51
2:D:412:ARG:NH1	8:D:681:HOH:O	2.32	0.51
1:C:390:MET:HE2	1:C:428:LEU:HD11	1.92	0.51
2:E:204:GLY:O	2:E:206:ILE:N	2.44	0.51
1:C:244:TYR:O	1:C:247:PRO:HD2	2.10	0.51
1:C:344:SER:HA	8:C:670:HOH:O	2.10	0.51
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.26	0.51
1:A:460:LYS:HD2	1:A:460:LYS:N	2.26	0.50
1:A:151:LYS:HG2	1:A:430:GLN:HE21	1.74	0.50
1:B:279:ARG:NH1	8:B:624:HOH:O	2.32	0.50
1:A:56:SER:O	1:A:58:GLY:N	2.44	0.50
2:F:97:VAL:HG13	2:F:232:VAL:HA	1.93	0.50
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.94	0.50
2:E:425:THR:C	2:E:427:HIS:H	2.14	0.50
1:A:258:ARG:O	1:A:319:GLY:HA3	2.11	0.50
1:C:143:ARG:HB2	8:C:634:HOH:O	2.11	0.50
2:F:228:ALA:O	2:F:232:VAL:HG22	2.11	0.50
1:B:297:ASP:HA	8:B:622:HOH:O	2.12	0.50
1:A:99:VAL:HG23	1:A:253:MET:HA	1.94	0.50
2:D:122:GLU:HA	2:D:122:GLU:OE1	2.11	0.50
1:B:211:SER:O	1:B:215:GLN:HG3	2.12	0.50
2:E:394:ASP:C	2:E:396:LEU:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ARG:O	1:B:423:ARG:N	2.45	0.50
2:D:54:GLY:O	2:D:55:GLU:HB2	2.12	0.50
2:D:168:GLU:O	2:D:168:GLU:HG3	2.10	0.50
2:E:96:ASN:OD1	2:E:97:VAL:N	2.44	0.50
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.93	0.50
2:E:296:ILE:HD13	2:E:306:SER:HB2	1.92	0.50
1:B:69:ASP:O	1:B:70:ASN:HB3	2.12	0.50
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.94	0.50
1:B:434:SER:N	1:B:435:PRO:HD3	2.26	0.50
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.94	0.50
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.93	0.50
2:F:467:VAL:O	2:F:470:ALA:HB3	2.12	0.49
2:F:196:LEU:O	2:F:200:MET:HB2	2.12	0.49
2:F:304:ILE:HG22	2:F:304:ILE:O	2.12	0.49
1:C:361:ILE:O	1:C:361:ILE:HG22	2.11	0.49
1:B:445:ILE:O	1:B:449:VAL:HG23	2.12	0.49
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.93	0.49
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.94	0.49
2:D:367:HIS:HB2	8:D:641:HOH:O	2.11	0.49
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.94	0.49
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.26	0.49
2:E:469:LYS:O	2:E:473:LEU:HG	2.13	0.49
2:E:408:ARG:HH22	2:E:412:ARG:NH2	2.07	0.49
2:E:455:GLN:NE2	2:E:469:LYS:HZ1	2.10	0.49
1:A:151:LYS:HE2	1:A:427:LEU:O	2.13	0.49
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.93	0.49
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.93	0.49
2:E:244:ARG:O	2:E:248:GLY:HA2	2.10	0.49
2:D:177:HIS:O	2:D:214:LYS:NZ	2.37	0.49
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.94	0.49
1:B:464:PHE:O	1:B:468:PHE:HB3	2.12	0.49
2:E:402:LEU:HD23	2:E:406:ARG:NH2	2.26	0.49
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.95	0.49
3:G:30:LYS:HA	3:G:33:ARG:HE	1.77	0.49
2:D:279:VAL:HG12	2:D:279:VAL:O	2.12	0.49
2:E:227:GLY:O	2:E:230:ALA:HB3	2.12	0.49
1:C:49:ALA:O	1:C:50:GLU:HB2	2.13	0.49
2:E:449:TYR:O	2:E:452:LEU:HB2	2.13	0.49
2:E:292:MET:SD	2:E:293:GLN:NE2	2.86	0.49
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.28	0.49
3:G:10:LEU:HG	3:G:246:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:449:TYR:HD1	2:D:452:LEU:HD21	1.77	0.49
2:F:152:ILE:HG22	2:F:153:GLY:N	2.27	0.49
2:F:342:LEU:HD13	7:F:602:AUR:H10	1.95	0.49
2:D:105:ARG:HH11	2:D:208:LEU:HD22	1.77	0.49
3:G:16:ILE:HA	3:G:19:ILE:HD12	1.95	0.49
2:D:422:GLU:HG2	2:D:427:HIS:O	2.12	0.49
2:F:138:LYS:HE2	2:F:416:GLN:HB2	1.94	0.49
1:B:303:SER:HB2	2:F:222:MET:HB3	1.95	0.49
2:E:414:LEU:HG	2:E:441:PHE:CE2	2.48	0.49
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.94	0.49
1:C:354:THR:HG23	8:C:649:HOH:O	2.12	0.49
1:C:209:LYS:HE2	1:C:212:THR:OG1	2.13	0.49
2:F:44:ARG:NH2	8:F:648:HOH:O	2.38	0.49
1:A:392:LEU:O	1:A:396:GLN:HG3	2.13	0.48
2:F:339:ILE:O	2:F:342:LEU:HB2	2.13	0.48
3:G:9:ARG:HH22	3:G:242:MET:HE1	1.78	0.48
3:G:239:ALA:O	3:G:243:ILE:HG13	2.12	0.48
1:C:331:ALA:O	1:C:333:ASP:N	2.45	0.48
2:D:105:ARG:HH11	2:D:208:LEU:CD2	2.26	0.48
1:B:128:ARG:HD3	8:B:654:HOH:O	2.12	0.48
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.95	0.48
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.77	0.48
1:C:381:ARG:O	1:C:385:GLN:HG3	2.13	0.48
2:E:405:SER:OG	2:E:406:ARG:N	2.46	0.48
1:A:241:PRO:O	1:A:244:TYR:HB3	2.14	0.48
2:E:223:ASN:ND2	2:E:223:ASN:N	2.42	0.48
2:E:385:GLN:NE2	7:E:479:AUR:C20	2.77	0.48
1:B:215:GLN:NE2	2:E:130:GLN:NE2	2.62	0.48
2:D:203:SER:OG	2:D:205:VAL:HG23	2.14	0.48
1:B:136:ILE:HG23	2:F:194:ASN:HA	1.94	0.48
2:D:471:ASP:O	2:D:474:ALA:N	2.47	0.48
1:A:441:GLN:O	1:A:445:ILE:HG12	2.13	0.48
2:D:84:ILE:N	2:D:114:ALA:O	2.41	0.48
2:D:96:ASN:CB	2:D:100:GLU:H	2.26	0.48
1:A:415:GLN:HA	1:A:418:LEU:HD23	1.96	0.48
1:B:134:PRO:O	1:B:139:ARG:NH2	2.35	0.48
1:A:496:LYS:HG2	1:A:500:ILE:HD11	1.96	0.48
2:E:67:GLU:H	2:E:67:GLU:HG3	1.51	0.48
2:F:266:SER:HB3	2:F:282:GLN:HE21	1.79	0.48
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.48
1:C:148:THR:HG21	1:C:153:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:NE2	2:D:128:VAL:CB	2.77	0.48
2:F:93:ARG:HH12	2:F:105:ARG:HB2	1.79	0.48
1:A:151:LYS:HG2	1:A:430:GLN:NE2	2.29	0.48
1:A:267:ILE:HA	1:A:324:LEU:O	2.14	0.48
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.14	0.48
1:A:291:ARG:HA	3:G:262:LEU:HD13	1.96	0.48
1:B:389:THR:HG22	1:B:392:LEU:HD12	1.96	0.48
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.28	0.47
2:E:423:VAL:O	2:E:424:PHE:HB2	2.14	0.47
1:B:212:THR:O	1:B:216:LEU:HB2	2.14	0.47
3:G:36:ARG:O	3:G:40:PRO:HD3	2.14	0.47
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.95	0.47
1:B:172:GLN:CA	5:B:600:ANP:HNB1	2.20	0.47
1:C:352:LEU:HA	1:C:364:ALA:O	2.13	0.47
2:E:166:ILE:O	2:E:170:ILE:HG13	2.14	0.47
2:D:298:THR:HG23	2:D:303:SER:HA	1.97	0.47
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.29	0.47
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.96	0.47
2:E:282:GLN:NE2	2:E:282:GLN:H	2.12	0.47
2:E:16:VAL:HG22	2:E:21:VAL:HG13	1.95	0.47
1:B:183:ILE:O	1:B:186:GLN:HB2	2.14	0.47
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.13	0.47
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.96	0.47
1:A:468:PHE:O	1:A:472:VAL:HG13	2.14	0.47
1:C:304:ARG:NH1	8:C:629:HOH:O	2.47	0.47
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.13	0.47
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.97	0.47
3:G:217:LEU:O	3:G:221:THR:HG23	2.14	0.47
2:F:439:LYS:O	2:F:442:GLN:N	2.48	0.47
2:E:415:SER:O	2:E:416:GLN:HB2	2.14	0.47
2:E:54:GLY:O	2:E:55:GLU:HB2	2.14	0.47
2:E:158:ALA:C	2:E:160:VAL:H	2.18	0.47
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.96	0.47
1:B:479:LEU:HD22	1:B:482:LYS:HD2	1.95	0.47
1:A:218:LYS:HE2	1:A:222:ASP:OD2	2.15	0.47
1:C:402:ALA:O	1:C:405:GLN:HG3	2.14	0.47
1:A:386:VAL:HG21	1:A:442:VAL:HB	1.97	0.47
1:A:415:GLN:O	1:A:415:GLN:HG2	2.14	0.47
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.28	0.47
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.97	0.47
1:A:445:ILE:O	1:A:449:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.97	0.47
2:D:49:VAL:HA	2:D:60:THR:HG22	1.96	0.47
2:E:77:ASP:CG	2:E:79:GLY:H	2.18	0.47
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.50	0.47
1:A:53:VAL:HG13	1:A:89:LYS:O	2.15	0.47
1:A:404:ALA:O	1:A:406:PHE:N	2.48	0.47
2:D:130:GLN:HE22	2:D:356:ARG:CD	2.28	0.47
8:B:627:HOH:O	2:F:189:ARG:HG2	2.14	0.47
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.29	0.47
1:C:336:ALA:HB3	1:C:339:PRO:HG2	1.95	0.47
2:F:205:VAL:O	2:F:213:SER:HA	2.14	0.47
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.97	0.47
2:F:155:PHE:HB2	2:F:334:VAL:HA	1.97	0.47
2:F:385:GLN:HE22	7:F:602:AUR:H202	1.80	0.47
1:B:33:SER:HB2	2:E:52:HIS:O	2.15	0.47
1:C:23:VAL:HG12	1:C:23:VAL:O	2.15	0.47
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.28	0.46
3:G:6:ILE:HG23	3:G:246:LEU:HD22	1.97	0.46
1:C:280:GLN:OE1	2:F:287:THR:HG23	2.15	0.46
2:E:189:ARG:HB2	2:E:192:GLU:HG3	1.97	0.46
2:D:273:GLY:HA2	3:G:272:LEU:HD22	1.98	0.46
1:A:130:GLY:N	1:A:308:ARG:HH12	2.12	0.46
2:F:409:LYS:HD3	2:F:457:PHE:CE1	2.51	0.46
2:D:405:SER:O	2:D:409:LYS:HG3	2.14	0.46
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.98	0.46
1:B:273:LYS:HB3	8:B:666:HOH:O	2.15	0.46
2:D:161:GLY:HA3	8:D:639:HOH:O	2.15	0.46
3:G:2:THR:HG22	3:G:4:LYS:N	2.29	0.46
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.30	0.46
2:E:210:ASP:OD1	2:E:211:ALA:N	2.47	0.46
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.31	0.46
1:B:285:LEU:O	1:B:286:ARG:HB2	2.16	0.46
2:F:381:TYR:CD1	2:F:385:GLN:NE2	2.79	0.46
1:B:440:GLU:O	1:B:444:VAL:HG13	2.15	0.46
2:F:251:VAL:HG12	2:F:252:LEU:H	1.80	0.46
2:F:175:LYS:NZ	8:F:692:HOH:O	2.48	0.46
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.96	0.46
2:D:357:ILE:O	2:D:359:ASP:N	2.48	0.46
1:B:201:CYS:O	1:B:229:THR:HA	2.16	0.46
1:C:400:VAL:HG13	8:C:671:HOH:O	2.15	0.46
1:B:145:PRO:O	1:B:161:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:MET:HE3	2:D:228:ALA:HA	1.98	0.46
1:C:267:ILE:N	1:C:267:ILE:HD12	2.30	0.46
1:B:499:GLU:HA	1:B:502:THR:HB	1.98	0.46
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.97	0.46
2:E:77:ASP:OD1	2:E:79:GLY:N	2.45	0.46
2:E:251:VAL:HG12	2:E:252:LEU:N	2.31	0.46
3:G:212:ILE:HA	3:G:212:ILE:HD13	1.85	0.46
1:B:357:PHE:HZ	5:B:600:ANP:O4'	1.98	0.46
2:F:13:ILE:HD13	2:F:69:LEU:HD13	1.98	0.46
1:C:292:GLU:O	1:C:293:ALA:HB3	2.15	0.46
1:A:52:MET:O	1:A:91:THR:HG23	2.16	0.46
2:D:9:THR:HG21	2:D:28:GLY:O	2.16	0.46
2:F:170:ILE:O	2:F:174:ALA:HB3	2.15	0.46
2:E:98:ILE:HB	8:E:489:HOH:O	2.15	0.46
1:B:452:TYR:O	1:B:453:LEU:HD23	2.15	0.46
1:A:164:ARG:HD3	1:A:347:ASP:OD2	2.15	0.46
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.51	0.46
1:A:286:ARG:NE	8:D:644:HOH:O	2.48	0.46
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.98	0.46
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.98	0.46
2:F:421:ALA:O	2:F:425:THR:HG23	2.15	0.46
2:F:453:PRO:HG2	2:F:473:LEU:HD12	1.98	0.45
1:A:99:VAL:CG2	1:A:253:MET:HA	2.46	0.45
2:E:374:VAL:O	2:E:377:ILE:HG22	2.17	0.45
2:D:105:ARG:NH1	2:D:208:LEU:CD2	2.79	0.45
1:B:437:ALA:O	1:B:440:GLU:N	2.46	0.45
1:B:311:LYS:HD2	1:B:312:MET:O	2.17	0.45
2:D:438:ILE:O	2:D:442:GLN:HB2	2.16	0.45
2:E:423:VAL:O	2:E:423:VAL:HG12	2.16	0.45
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.98	0.45
2:F:455:GLN:H	2:F:455:GLN:CD	2.19	0.45
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.31	0.45
2:F:32:ILE:O	2:F:33:LEU:HB2	2.17	0.45
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.99	0.45
1:A:34:ILE:HD12	1:A:79:ASP:HB3	1.97	0.45
2:E:411:GLN:CG	7:E:479:AUR:H7	2.46	0.45
1:B:65:ASN:HD22	2:F:17:ILE:CG1	2.30	0.45
1:A:53:VAL:HG12	1:A:54:GLU:N	2.32	0.45
1:A:411:ASP:OD1	1:A:413:ALA:HB3	2.16	0.45
1:C:498:LYS:O	1:C:502:THR:OG1	2.30	0.45
1:C:136:ILE:O	2:D:194:ASN:OD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:GLN:N	2:D:112:GLN:OE1	2.49	0.45
1:A:105:GLY:HA2	1:A:226:MET:O	2.16	0.45
1:B:96:ASP:HB2	1:B:127:ARG:O	2.17	0.45
2:F:440:GLY:O	2:F:444:ILE:HG13	2.17	0.45
1:B:413:ALA:O	1:B:417:LEU:HG	2.17	0.45
1:C:162:GLY:HA2	1:C:321:LEU:O	2.17	0.45
2:E:121:PRO:HD3	8:E:502:HOH:O	2.15	0.45
2:E:182:VAL:HG21	2:E:240:ALA:HB2	1.99	0.45
3:G:82:HIS:CD2	3:G:82:HIS:H	2.35	0.45
1:B:187:LYS:HD2	1:B:224:ASP:O	2.16	0.45
1:C:46:ASN:HB2	1:C:90:ARG:HH11	1.82	0.45
1:A:267:ILE:N	1:A:267:ILE:HD12	2.32	0.45
2:D:189:ARG:O	2:D:192:GLU:HB2	2.16	0.45
1:B:492:GLU:O	1:B:496:LYS:HB2	2.17	0.45
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.98	0.45
1:B:443:ALA:O	1:B:446:TYR:HB3	2.17	0.45
3:G:38:LEU:HD11	3:G:42:ARG:HE	1.81	0.45
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.97	0.45
2:E:454:GLU:O	2:E:456:ALA:N	2.50	0.45
1:B:338:ILE:O	1:B:341:ASN:HB2	2.17	0.45
1:B:309:ALA:O	1:B:310:ALA:HB2	2.17	0.45
2:F:327:ALA:HB3	8:F:682:HOH:O	2.16	0.45
1:B:481:GLY:O	1:B:485:THR:HB	2.16	0.45
2:E:256:ASP:HA	2:E:257:ASN:HA	1.61	0.45
1:A:479:LEU:O	1:A:482:LYS:HB2	2.16	0.45
1:C:90:ARG:HB3	1:C:90:ARG:HE	1.58	0.45
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.99	0.45
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.52	0.45
1:A:157:VAL:N	1:A:158:PRO:CD	2.79	0.45
3:G:35:GLU:O	3:G:39:LYS:HG2	2.16	0.45
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.99	0.45
1:C:179:ALA:O	1:C:183:ILE:HG13	2.16	0.45
1:C:442:VAL:O	1:C:446:TYR:HB2	2.17	0.44
2:D:412:ARG:HG3	2:D:412:ARG:HH11	1.81	0.44
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.82	0.44
2:E:387:ILE:HG22	2:E:388:ILE:N	2.32	0.44
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.16	0.44
1:A:240:ALA:N	1:A:241:PRO:HD2	2.32	0.44
2:F:327:ALA:HB2	8:F:681:HOH:O	2.16	0.44
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.52	0.44
2:F:386:ASP:O	2:F:389:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ILE:O	2:D:33:LEU:HB2	2.17	0.44
2:F:379:GLN:O	2:F:382:LYS:HB3	2.18	0.44
1:B:390:MET:HE3	1:B:424:LEU:HD22	1.99	0.44
2:E:384:LEU:O	2:E:388:ILE:HG12	2.17	0.44
1:A:404:ALA:C	1:A:406:PHE:H	2.21	0.44
1:C:97:VAL:HG12	1:C:111:LEU:O	2.18	0.44
1:A:32:LEU:HD21	1:A:42:HIS:HB2	1.99	0.44
2:D:253:LEU:O	2:D:306:SER:HA	2.17	0.44
1:B:206:ILE:HD13	1:B:247:PRO:HG3	1.99	0.44
2:E:86:VAL:O	2:E:110:THR:HG21	2.16	0.44
1:B:389:THR:HA	1:B:392:LEU:HG	1.99	0.44
2:E:189:ARG:O	2:E:192:GLU:N	2.51	0.44
1:A:91:THR:C	1:A:93:ALA:H	2.20	0.44
2:E:32:ILE:O	2:E:33:LEU:HB2	2.18	0.44
2:F:431:LEU:HD12	2:F:431:LEU:HA	1.80	0.44
1:A:137:ILE:N	1:A:138:PRO:CD	2.80	0.44
1:C:382:ALA:O	1:C:385:GLN:HB2	2.18	0.44
1:B:367:VAL:HG12	1:B:391:LYS:HE3	2.00	0.44
3:G:7:THR:O	3:G:11:LYS:HD2	2.16	0.44
1:B:297:ASP:N	1:B:297:ASP:OD1	2.48	0.44
1:A:209:LYS:NZ	2:D:330:ASP:OD1	2.48	0.44
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.99	0.44
2:F:298:THR:HG22	2:F:299:THR:N	2.32	0.44
1:C:397:TYR:CD1	1:C:421:GLY:HA3	2.53	0.44
3:G:213:ILE:HA	3:G:213:ILE:HD13	1.82	0.44
2:F:455:GLN:HA	7:F:602:AUR:O19	2.17	0.44
1:C:139:ARG:HD3	8:C:688:HOH:O	2.17	0.44
1:B:423:ARG:HE	1:B:458:PRO:CD	2.29	0.44
1:C:172:GLN:HA	5:C:600:ANP:N3B	2.32	0.44
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.99	0.44
2:F:410:ILE:HG13	2:F:444:ILE:HG21	2.00	0.44
2:F:463:ILE:HG22	8:F:643:HOH:O	2.18	0.44
1:B:49:ALA:O	1:B:50:GLU:HB2	2.17	0.44
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.60	0.44
2:D:220:GLY:HA3	2:D:232:VAL:HG21	1.99	0.44
1:C:481:GLY:O	1:C:485:THR:HB	2.18	0.44
1:A:423:ARG:NH2	1:A:456:LEU:O	2.51	0.44
2:F:9:THR:O	2:F:76:LEU:HA	2.17	0.44
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.53	0.44
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.81	0.44
1:C:286:ARG:NH1	8:C:632:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.81	0.44
1:A:215:GLN:HG3	2:D:356:ARG:HH11	1.73	0.44
2:D:344:ILE:HG23	2:D:415:SER:HB3	2.00	0.44
2:E:138:LYS:HE2	2:E:432:VAL:HG21	2.00	0.44
2:E:455:GLN:HE21	2:E:469:LYS:NZ	2.16	0.44
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.82	0.44
3:G:13:ILE:HG22	3:G:243:ILE:HG12	2.00	0.44
1:B:465:GLU:O	1:B:469:LEU:HB2	2.18	0.44
2:F:434:LEU:O	2:F:438:ILE:HG12	2.17	0.44
2:E:220:GLY:HA3	2:E:232:VAL:HG21	2.00	0.44
2:E:394:ASP:C	2:E:396:LEU:N	2.71	0.43
1:B:383:MET:O	1:B:387:ALA:HB3	2.18	0.43
1:B:65:ASN:HD22	2:F:17:ILE:HG13	1.82	0.43
1:A:107:VAL:HG12	1:A:115:ILE:HD11	2.00	0.43
2:F:435:LYS:HG3	2:F:436:GLU:N	2.33	0.43
2:E:201:ILE:HD13	2:E:208:LEU:HD11	2.00	0.43
1:A:311:LYS:NZ	1:A:318:GLY:O	2.43	0.43
1:C:27:GLU:O	1:C:90:ARG:HG3	2.18	0.43
2:E:241:GLU:HA	2:E:304:ILE:HD11	2.00	0.43
2:F:296:ILE:HD13	2:F:296:ILE:HG21	1.76	0.43
1:B:358:TYR:O	1:B:360:GLY:N	2.51	0.43
1:B:270:ASP:OD2	1:B:273:LYS:HG3	2.17	0.43
3:G:23:MET:HB2	3:G:232:MET:HE2	2.00	0.43
2:F:282:GLN:HG2	2:F:282:GLN:H	1.23	0.43
1:A:34:ILE:HG22	2:D:52:HIS:HB2	1.99	0.43
1:B:172:GLN:HA	5:B:600:ANP:N3B	2.19	0.43
2:F:445:LEU:HD23	2:F:445:LEU:HA	1.83	0.43
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.33	0.43
2:D:388:ILE:HD12	2:D:393:MET:SD	2.58	0.43
2:E:397:SER:C	2:E:399:GLU:N	2.72	0.43
1:B:358:TYR:C	1:B:360:GLY:N	2.72	0.43
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.53	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.18	0.43
2:F:12:ARG:HG2	2:F:72:GLY:O	2.19	0.43
2:F:453:PRO:HB2	2:F:455:GLN:HG2	2.00	0.43
1:C:399:GLU:O	1:C:402:ALA:N	2.51	0.43
1:A:385:GLN:OE1	1:A:488:LYS:HE3	2.17	0.43
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.43
2:D:83:ARG:HA	2:D:115:ALA:HA	2.00	0.43
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.48	0.43
1:B:341:ASN:HB3	8:B:610:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.53	0.43
1:B:168:ILE:O	1:B:351:PHE:HA	2.18	0.43
2:D:164:VAL:O	2:D:167:MET:HB2	2.17	0.43
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.99	0.43
2:F:83:ARG:HA	2:F:115:ALA:HA	2.01	0.43
1:B:505:LEU:HA	1:B:505:LEU:HD13	1.87	0.43
2:E:139:VAL:HG13	2:E:414:LEU:HD22	2.00	0.43
1:A:376:SER:C	1:A:378:ALA:H	2.21	0.43
1:A:383:MET:O	1:A:386:VAL:HG23	2.18	0.43
1:A:268:TYR:O	1:A:326:VAL:HG23	2.19	0.43
1:A:400:VAL:HG13	1:A:403:PHE:CD2	2.53	0.43
2:F:409:LYS:HG2	2:F:454:GLU:HA	2.00	0.43
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.43
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.53	0.43
1:A:28:THR:CG2	1:A:29:GLY:N	2.81	0.43
2:E:155:PHE:CD1	2:E:155:PHE:N	2.87	0.43
1:B:283:LEU:HD12	2:E:277:SER:HB3	2.00	0.43
2:D:171:ASN:O	8:D:606:HOH:O	2.21	0.43
1:A:400:VAL:HG12	1:A:418:LEU:HD11	2.00	0.43
1:B:271:LEU:HB3	1:B:302:HIS:CE1	2.54	0.43
3:G:13:ILE:HD13	3:G:242:MET:SD	2.58	0.43
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.43
1:C:33:SER:HB2	2:F:52:HIS:O	2.19	0.43
1:B:174:GLY:HA2	5:B:600:ANP:O5'	2.19	0.43
1:B:151:LYS:H	1:B:430:GLN:NE2	2.16	0.43
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.71	0.43
2:F:412:ARG:CD	2:F:454:GLU:HB3	2.48	0.43
1:C:201:CYS:O	1:C:229:THR:HA	2.19	0.43
1:A:376:SER:C	1:A:378:ALA:N	2.72	0.43
1:A:403:PHE:CZ	3:G:22:SER:HB2	2.54	0.43
2:E:434:LEU:O	2:E:438:ILE:HG12	2.18	0.43
1:B:156:LEU:HD13	1:B:367:VAL:HG11	2.01	0.43
1:B:421:GLY:O	1:B:425:THR:OG1	2.30	0.43
1:C:384:LYS:HE3	1:C:384:LYS:HB2	1.91	0.43
1:C:144:GLU:H	1:C:144:GLU:HG3	1.60	0.43
1:B:147:GLN:OE1	1:B:438:ILE:HD13	2.18	0.42
2:E:21:VAL:O	2:E:60:THR:OG1	2.35	0.42
1:B:479:LEU:HD11	1:B:497:LEU:HD13	2.00	0.42
2:D:445:LEU:HD23	2:D:445:LEU:HA	1.84	0.42
1:B:489:ILE:HG22	1:B:494:ASP:HB2	2.00	0.42
1:B:209:LYS:NZ	2:E:356:ARG:NH1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.35	0.42
1:B:423:ARG:O	1:B:426:GLU:N	2.49	0.42
2:D:473:LEU:C	2:D:475:GLU:N	2.72	0.42
2:D:96:ASN:HB2	2:D:100:GLU:N	2.34	0.42
1:C:374:VAL:HG11	1:C:378:ALA:HB2	2.00	0.42
2:D:70:VAL:HG12	2:D:71:ARG:N	2.33	0.42
2:E:242:TYR:C	2:E:244:ARG:N	2.72	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.87	0.42
2:D:33:LEU:HD13	2:D:117:HIS:CG	2.55	0.42
1:B:272:SER:O	1:B:275:ALA:HB3	2.19	0.42
1:C:51:GLU:HG2	1:C:52:MET:N	2.34	0.42
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.42
2:D:412:ARG:O	2:D:415:SER:OG	2.35	0.42
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.42
1:C:190:ASN:O	1:C:198:LYS:HE2	2.20	0.42
1:B:383:MET:SD	1:B:387:ALA:HB2	2.59	0.42
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.40	0.42
1:C:457:GLU:O	1:C:460:LYS:HB2	2.19	0.42
1:A:172:GLN:HA	5:A:600:ANP:N3B	2.34	0.42
2:F:36:LEU:HD23	2:F:36:LEU:N	2.34	0.42
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.70	0.42
2:D:93:ARG:HE	2:D:108:ILE:HG12	1.83	0.42
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.53	0.42
2:F:468:ALA:O	2:F:471:ASP:N	2.52	0.42
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.42
2:D:319:ASP:O	2:D:322:PRO:HD2	2.19	0.42
2:E:443:GLN:O	2:E:446:ALA:HB3	2.20	0.42
2:E:443:GLN:HA	2:E:446:ALA:HB3	2.01	0.42
2:D:159:GLY:N	6:D:600:ADP:O3B	2.49	0.42
1:B:52:MET:HG2	1:B:95:VAL:HG22	2.02	0.42
1:B:235:THR:O	1:B:237:SER:N	2.52	0.42
2:D:200:MET:CE	2:D:215:VAL:HG21	2.50	0.42
1:C:338:ILE:O	1:C:341:ASN:N	2.52	0.42
2:E:343:GLY:O	2:E:345:TYR:HD1	2.02	0.42
2:E:385:GLN:NE2	7:E:479:AUR:H203	2.35	0.42
1:B:175:LYS:H	5:B:600:ANP:PB	2.42	0.42
1:A:293:ALA:HB2	3:G:265:ILE:HD13	2.02	0.42
2:D:188:GLU:O	2:D:222:MET:HG3	2.20	0.42
1:C:398:ARG:NH1	8:C:625:HOH:O	2.50	0.42
1:B:439:GLU:O	1:B:442:VAL:HG23	2.20	0.42
1:B:44:LEU:O	1:B:47:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:OG1	1:A:93:ALA:HB3	2.20	0.42
1:C:303:SER:HB2	2:D:222:MET:HB3	2.02	0.42
1:C:239:ALA:HB1	1:C:241:PRO:HD2	2.02	0.42
2:D:368:TYR:O	2:D:372:ARG:HG2	2.20	0.42
2:F:408:ARG:O	2:F:412:ARG:NH1	2.43	0.42
2:E:253:LEU:O	2:E:306:SER:HA	2.20	0.42
1:B:180:ILE:HD11	1:B:216:LEU:HD21	2.01	0.42
2:F:469:LYS:O	2:F:473:LEU:HG	2.20	0.42
1:A:97:VAL:N	1:A:127:ARG:O	2.38	0.42
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.55	0.42
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.55	0.42
1:B:269:ASP:HA	1:B:270:ASP:HA	1.89	0.42
1:B:291:ARG:HD3	8:B:633:HOH:O	2.19	0.42
1:C:271:LEU:HA	1:C:271:LEU:HD23	1.85	0.42
2:E:454:GLU:C	2:E:456:ALA:H	2.23	0.41
3:G:266:ILE:HD13	3:G:266:ILE:HG21	1.76	0.41
2:F:96:ASN:HB2	2:F:100:GLU:H	1.85	0.41
2:F:432:VAL:HA	2:F:433:PRO:HD3	1.88	0.41
2:E:105:ARG:NH1	8:E:516:HOH:O	2.49	0.41
1:C:74:VAL:HG13	1:C:241:PRO:HG3	2.01	0.41
2:D:105:ARG:NH1	2:D:208:LEU:HD23	2.35	0.41
1:B:438:ILE:HD12	1:B:438:ILE:HA	1.85	0.41
1:A:394:LEU:O	1:A:397:TYR:HB3	2.20	0.41
2:D:165:LEU:HG	2:D:165:LEU:O	2.20	0.41
2:E:456:ALA:HB1	2:E:466:ALA:O	2.20	0.41
1:A:69:ASP:O	1:A:70:ASN:HB3	2.20	0.41
1:A:130:GLY:HA2	1:A:308:ARG:HH12	1.85	0.41
2:F:188:GLU:H	2:F:221:GLN:NE2	2.18	0.41
1:B:76:PHE:O	1:B:242:LEU:HD21	2.20	0.41
1:A:211:SER:N	2:D:126:MET:HE2	2.35	0.41
2:F:12:ARG:HA	2:F:73:GLN:O	2.19	0.41
1:B:230:ILE:HG22	1:B:231:VAL:N	2.35	0.41
1:C:465:GLU:O	1:C:465:GLU:HG2	2.20	0.41
2:D:154:LEU:HD13	2:D:165:LEU:HD23	2.02	0.41
1:C:505:LEU:O	1:C:508:PHE:HB3	2.21	0.41
1:C:76:PHE:CD1	1:C:241:PRO:HB2	2.56	0.41
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.20	0.41
1:C:64:LEU:HD12	1:C:64:LEU:HA	1.90	0.41
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.55	0.41
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.49	0.41
2:D:374:VAL:O	2:D:378:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:ILE:O	2:E:283:PRO:HG3	2.21	0.41
2:F:439:LYS:HE3	2:F:443:GLN:NE2	2.25	0.41
1:B:199:LEU:HA	1:B:263:HIS:O	2.21	0.41
2:F:298:THR:CG2	2:F:299:THR:N	2.83	0.41
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.20	0.41
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.41
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.51	0.41
1:C:134:PRO:CD	1:C:258:ARG:HH12	2.33	0.41
1:C:469:LEU:HD12	1:C:469:LEU:HA	1.93	0.41
1:C:220:LEU:HA	1:C:220:LEU:HD23	1.69	0.41
2:F:342:LEU:HD13	7:F:602:AUR:C10	2.51	0.41
1:C:51:GLU:OE2	1:C:90:ARG:HB3	2.20	0.41
2:E:136:GLY:HA2	2:E:432:VAL:O	2.20	0.41
2:E:393:MET:HE3	2:E:396:LEU:HD12	2.01	0.41
1:A:347:ASP:C	1:A:373:ARG:HH11	2.24	0.41
1:B:66:LEU:O	2:F:15:ALA:HA	2.21	0.41
1:A:185:ASN:O	1:A:188:ARG:HG3	2.20	0.41
2:F:96:ASN:HD22	2:F:100:GLU:CG	2.34	0.41
1:B:67:GLU:O	1:B:69:ASP:N	2.54	0.41
1:A:496:LYS:O	1:A:500:ILE:HG13	2.20	0.41
1:B:213:VAL:O	1:B:216:LEU:HB3	2.21	0.41
2:E:286:ALA:N	8:E:484:HOH:O	2.54	0.41
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.01	0.41
2:E:35:ALA:HB2	2:E:82:ILE:HG13	2.01	0.41
1:A:483:ILE:HA	8:A:680:HOH:O	2.20	0.41
1:C:420:ARG:HG3	1:C:420:ARG:HH11	1.86	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.01	0.41
2:E:173:VAL:HG12	2:E:179:GLY:O	2.20	0.41
2:E:96:ASN:HB3	2:E:100:GLU:N	2.26	0.41
2:D:393:MET:HE3	2:D:404:VAL:HG21	2.03	0.41
2:E:138:LYS:HE3	2:E:416:GLN:HB2	2.02	0.41
1:A:151:LYS:H	1:A:151:LYS:HG2	1.72	0.41
1:B:166:LEU:HD23	1:B:349:GLN:HB3	2.03	0.41
2:E:84:ILE:HD13	2:E:235:THR:HG23	2.02	0.41
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.41
1:B:468:PHE:HB2	1:B:504:PHE:CE2	2.56	0.40
1:A:79:ASP:OD1	1:A:79:ASP:N	2.54	0.40
2:E:281:TYR:CE1	2:E:321:ALA:HB2	2.56	0.40
1:A:307:GLU:OE1	2:E:190:THR:HB	2.21	0.40
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.56	0.40
1:B:48:GLN:HB3	2:F:68:GLY:HA2	2.02	0.40
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.51	0.40
1:C:44:LEU:HA	1:C:44:LEU:HD23	1.94	0.40
1:B:451:GLY:C	1:B:453:LEU:H	2.25	0.40
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.50	0.40
2:D:82:ILE:O	2:D:115:ALA:HA	2.21	0.40
1:B:244:TYR:O	1:B:247:PRO:HD2	2.21	0.40
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.02	0.40
1:B:28:THR:CG2	1:B:29:GLY:N	2.83	0.40
2:E:147:ALA:HB2	2:E:357:ILE:HD13	2.04	0.40
2:F:385:GLN:HE22	7:F:602:AUR:C20	2.34	0.40
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.86	0.40
1:B:157:VAL:N	1:B:158:PRO:CD	2.84	0.40
1:A:411:ASP:OD1	1:A:413:ALA:N	2.54	0.40
1:A:439:GLU:HG2	1:A:484:ARG:HB2	2.04	0.40
3:G:261:GLU:O	3:G:264:GLU:N	2.54	0.40
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.40
2:D:146:TYR:HB3	2:D:152:ILE:HD11	2.03	0.40
1:C:456:LEU:HD23	1:C:461:ILE:HG12	2.03	0.40
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.35	0.40
2:E:422:GLU:C	2:E:424:PHE:N	2.74	0.40
2:D:381:TYR:O	2:D:385:GLN:HG3	2.22	0.40
2:F:50:ALA:O	2:F:51:GLN:HB3	2.19	0.40
1:C:163:GLN:O	1:C:322:THR:HG23	2.21	0.40
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.55	0.40
2:E:334:VAL:HG23	2:E:353:SER:HA	2.04	0.40
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	430 (89%)	44 (9%)	11 (2%)	8	35
1	B	485/510 (95%)	430 (89%)	45 (9%)	10 (2%)	9	37
1	C	490/510 (96%)	438 (89%)	46 (9%)	6 (1%)	16	52
2	D	465/482 (96%)	415 (89%)	45 (10%)	5 (1%)	17	55
2	E	464/482 (96%)	401 (86%)	46 (10%)	17 (4%)	4	23
2	F	464/482 (96%)	422 (91%)	40 (9%)	2 (0%)	39	75
3	G	116/272 (43%)	98 (84%)	16 (14%)	2 (2%)	11	43
All	All	2969/3248 (91%)	2634 (89%)	282 (10%)	53 (2%)	11	42

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	57	SER
1	A	405	GLN
1	B	25	LEU
1	B	364	ALA
1	C	407	GLY
2	E	393	MET
2	E	423	VAL
2	E	424	PHE
1	A	364	ALA
1	B	236	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP
1	C	476	HIS
2	D	28	GLY
2	D	474	ALA
2	E	28	GLY
2	E	161	GLY
2	E	205	VAL
2	E	243	PHE
2	E	455	GLN
3	G	81	ILE
1	A	404	ALA
1	A	409	ASP
1	B	359	LYS
1	B	452	TYR
2	E	347	ALA
2	F	347	ALA

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Mol	Chain	Res	Type
1	A	337	TYR
1	A	484	ARG
1	B	458	PRO
2	E	122	GLU
2	F	327	ALA
1	A	401	ALA
1	A	464	PHE
1	B	315	ALA
1	B	411	ASP
2	E	67	GLU
2	E	175	LYS
2	E	190	THR
2	E	454	GLU
1	B	68	PRO
2	D	405	SER
3	G	43	VAL
1	C	461	ILE
2	E	121	PRO
2	E	279	VAL
1	B	95	VAL
2	D	279	VAL
2	D	107	PRO
2	E	388	ILE
1	A	130	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	341 (87%)	52 (13%)	5	20
1	B	393/412 (95%)	351 (89%)	42 (11%)	8	31
1	C	397/412 (96%)	365 (92%)	32 (8%)	15	47
2	D	377/386 (98%)	348 (92%)	29 (8%)	16	50
2	E	376/386 (97%)	339 (90%)	37 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	376/386 (97%)	349 (93%)	27 (7%)	18	53
3	G	102/230 (44%)	94 (92%)	8 (8%)	16	49
All	All	2414/2624 (92%)	2187 (91%)	227 (9%)	11	39

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	25	LEU
1	A	34	ILE
1	A	40	ARG
1	A	45	ARG
1	A	48	GLN
1	A	50	GLU
1	A	56	SER
1	A	79	ASP
1	A	80	LYS
1	A	89	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	151	LYS
1	A	164	ARG
1	A	173	THR
1	A	175	LYS
1	A	188	ARG
1	A	193	THR
1	A	195	GLU
1	A	206	ILE
1	A	211	SER
1	A	219	ARG
1	A	256	TYR
1	A	270	ASP
1	A	334	VAL
1	A	344	SER
1	A	362	ARG
1	A	367	VAL
1	A	371	VAL

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Mol	Chain	Res	Type
1	A	380	THR
1	A	386	VAL
1	A	393	GLU
1	A	409	ASP
1	A	417	LEU
1	A	418	LEU
1	A	420	ARG
1	A	436	MET
1	A	439	GLU
1	A	442	VAL
1	A	444	VAL
1	A	449	VAL
1	A	453	LEU
1	A	457	GLU
1	A	472	VAL
1	A	473	ILE
1	A	474	SER
1	A	479	LEU
1	B	38	ILE
1	B	47	VAL
1	B	79	ASP
1	B	80	LYS
1	B	97	VAL
1	B	123	SER
1	B	137	ILE
1	B	141	SER
1	B	143	ARG
1	B	164	ARG
1	B	171	ARG
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	221	THR
1	B	227	LYS
1	B	299	PHE
1	B	349	GLN
1	B	351	PHE
1	B	371	VAL
1	B	374	VAL

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Mol	Chain	Res	Type
1	B	376	SER
1	B	380	THR
1	B	383	MET
1	B	414	THR
1	B	416	GLN
1	B	419	SER
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
1	B	454	ASP
1	B	456	LEU
1	B	474	SER
1	B	476	HIS
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	91	THR
1	C	97	VAL
1	C	101	GLU
1	C	139	ARG
1	C	144	GLU
1	C	164	ARG
1	C	175	LYS
1	C	189	PHE
1	C	195	GLU
1	C	211	SER
1	C	217	VAL
1	C	227	LYS
1	C	245	LEU
1	C	298	VAL
1	C	301	LEU
1	C	334	VAL
1	C	349	GLN
1	C	399	GLU

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Mol	Chain	Res	Type
1	C	400	VAL
1	C	406	PHE
1	C	414	THR
1	C	444	VAL
1	C	474	SER
1	C	477	GLN
1	C	479	LEU
1	C	505	LEU
2	D	27	GLU
2	D	56	SER
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	137	ILE
2	D	139	VAL
2	D	166	ILE
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	306	SER
2	D	322	PRO
2	D	336	SER
2	D	337	ARG
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	393	MET
2	D	397	SER
2	D	400	ASP
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

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Mol	Chain	Res	Type
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	142	LEU
2	E	164	VAL
2	E	175	LYS
2	E	182	VAL
2	E	188	GLU
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	358	MET
2	E	365	SER
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	412	ARG
2	E	424	PHE
2	E	425	THR
2	E	431	LEU
2	E	438	ILE
2	E	450	ASP
2	E	452	LEU
2	E	455	GLN
2	E	463	ILE
2	E	467	VAL
2	F	34	ASN
2	F	42	GLU
2	F	67	GLU
2	F	93	ARG
2	F	95	MET
2	F	97	VAL
2	F	112	GLN
2	F	127	SER
2	F	139	VAL
2	F	166	ILE

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Mol	Chain	Res	Type
2	F	191	ARG
2	F	200	MET
2	F	223	ASN
2	F	232	VAL
2	F	258	ILE
2	F	292	MET
2	F	357	ILE
2	F	381	TYR
2	F	386	ASP
2	F	387	ILE
2	F	397	SER
2	F	405	SER
2	F	410	ILE
2	F	411	GLN
2	F	428	LEU
2	F	455	GLN
2	F	467	VAL
3	G	4	LYS
3	G	22	SER
3	G	77	LEU
3	G	82	HIS
3	G	211	ASN
3	G	214	TYR
3	G	221	THR
3	G	254	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	186	GLN
1	A	215	GLN
1	A	396	GLN
1	A	430	GLN
1	A	476	HIS
1	B	48	GLN
1	B	65	ASN
1	B	215	GLN
1	B	430	GLN
1	C	70	ASN
1	C	260	ASN
2	D	194	ASN

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Mol	Chain	Res	Type
2	D	221	GLN
2	D	223	ASN
2	D	442	GLN
2	E	39	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	E	385	GLN
2	E	455	GLN
2	F	34	ASN
2	F	39	GLN
2	F	96	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	443	GLN
3	G	82	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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$
5	ANP	A	600	4	27,33,33	1.53	5 (18%)	30,52,52	2.42	8 (26%)
5	ANP	B	600	4	27,33,33	1.42	7 (25%)	30,52,52	2.14	6 (20%)
5	ANP	C	600	4	27,33,33	1.74	6 (22%)	30,52,52	2.16	7 (23%)
6	ADP	D	600	4	22,29,29	1.09	1 (4%)	27,45,45	1.63	6 (22%)
7	AUR	E	479	-	31,35,35	1.90	6 (19%)	31,52,52	1.88	8 (25%)
5	ANP	F	600	4	27,33,33	1.55	8 (29%)	30,52,52	2.72	10 (33%)
7	AUR	F	602	-	31,35,35	1.54	5 (16%)	31,52,52	2.10	8 (25%)

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	-	1/12/38/38	0/3/3/3
5	ANP	B	600	4	-	1/12/38/38	0/3/3/3
5	ANP	C	600	4	-	1/12/38/38	0/3/3/3
6	ADP	D	600	4	-	0/12/32/32	0/3/3/3
7	AUR	E	479	-	-	0/16/55/55	0/1/3/3
5	ANP	F	600	4	-	0/12/38/38	0/3/3/3
7	AUR	F	602	-	-	0/16/55/55	0/1/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	479	AUR	C7-C8	-5.58	1.47	1.53
7	F	602	AUR	C7-C8	-4.30	1.48	1.53
7	E	479	AUR	O5-C5	-3.92	1.36	1.44
7	F	602	AUR	O5-C5	-3.79	1.36	1.44
5	F	600	ANP	O3'-C3'	-3.24	1.35	1.43
7	F	602	AUR	C18-C17	-3.14	1.34	1.39
6	D	600	ADP	C8-N7	-3.01	1.28	1.34
5	C	600	ANP	PG-O3G	-2.92	1.48	1.56
5	B	600	ANP	PB-O2B	-2.77	1.49	1.56
5	A	600	ANP	PG-O3G	-2.63	1.49	1.56
5	F	600	ANP	C8-N7	-2.59	1.29	1.34
5	C	600	ANP	PG-O2G	-2.50	1.49	1.56
7	E	479	AUR	C18-C17	-2.47	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	ANP	PG-O2G	-2.44	1.49	1.56
5	B	600	ANP	C8-N7	-2.43	1.30	1.34
5	A	600	ANP	PB-O2B	-2.40	1.50	1.56
5	F	600	ANP	PG-O3G	-2.30	1.50	1.56
5	A	600	ANP	C2-N1	-2.16	1.29	1.33
5	C	600	ANP	O5'-C5'	-2.16	1.36	1.44
5	C	600	ANP	C8-N7	-2.15	1.30	1.34
5	B	600	ANP	C5-C4	-2.14	1.35	1.40
5	F	600	ANP	PB-O2B	-2.10	1.50	1.56
5	F	600	ANP	PA-O2A	-2.08	1.46	1.54
5	A	600	ANP	PG-O2G	-2.08	1.50	1.56
5	F	600	ANP	PG-O2G	-2.03	1.51	1.56
5	B	600	ANP	PG-O3G	-2.01	1.51	1.56
5	B	600	ANP	PB-O3A	2.07	1.61	1.59
5	F	600	ANP	PB-O3A	2.16	1.61	1.59
7	F	602	AUR	O3-C6	2.25	1.50	1.45
5	F	600	ANP	PG-O1G	2.43	1.48	1.46
7	E	479	AUR	O3-C6	2.62	1.51	1.45
5	B	600	ANP	PG-O1G	3.06	1.49	1.46
5	C	600	ANP	PG-O1G	3.38	1.50	1.46
7	F	602	AUR	C18-C19	3.50	1.44	1.37
7	E	479	AUR	C18-C19	3.58	1.44	1.37
7	E	479	AUR	O4-C8	4.39	1.48	1.44
5	A	600	ANP	PB-O3A	4.47	1.64	1.59
5	C	600	ANP	PB-O3A	5.09	1.65	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	600	ANP	O1G-PG-N3B	-9.27	97.68	111.90
7	F	602	AUR	O17-C17-C16	-6.76	109.39	115.02
5	A	600	ANP	O1G-PG-N3B	-5.64	103.24	111.90
5	C	600	ANP	PA-O3A-PB	-5.01	115.87	132.67
5	B	600	ANP	O2G-PG-O1G	-4.74	100.89	113.49
5	C	600	ANP	C1'-N9-C4	-4.41	120.29	126.94
7	E	479	AUR	C20-C4-C3	-4.41	106.91	113.84
5	C	600	ANP	O1G-PG-N3B	-4.32	105.28	111.90
5	A	600	ANP	C2'-C1'-N9	-4.12	107.99	114.29
5	B	600	ANP	O1G-PG-N3B	-3.89	105.93	111.90
7	F	602	AUR	O5-C25-O25	-3.82	115.28	122.92
7	F	602	AUR	C5-O5-C25	-3.73	111.37	117.75
6	D	600	ADP	O4'-C1'-N9	-3.57	100.62	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	ANP	O1B-PB-N3B	-3.26	106.89	111.90
5	F	600	ANP	O2G-PG-O1G	-3.16	105.08	113.49
7	F	602	AUR	C20-C4-C3	-3.14	108.91	113.84
7	E	479	AUR	O25-C25-C24	-3.13	113.26	124.85
5	F	600	ANP	PA-O3A-PB	-3.05	122.44	132.67
5	A	600	ANP	O3G-PG-O2G	-2.90	98.98	107.58
5	A	600	ANP	PA-O3A-PB	-2.87	123.04	132.67
5	C	600	ANP	O2G-PG-O1G	-2.80	106.05	113.49
6	D	600	ADP	C2'-C1'-N9	-2.41	110.62	114.29
5	F	600	ANP	O3A-PB-N3B	-2.40	99.84	106.44
5	F	600	ANP	C1'-N9-C4	-2.31	123.45	126.94
5	F	600	ANP	C2'-C1'-N9	-2.24	110.88	114.29
7	F	602	AUR	O5-C5-C4	-2.23	104.81	111.52
7	F	602	AUR	C13-C12-C11	-2.21	119.82	124.94
7	F	602	AUR	O25-C25-C24	-2.18	116.79	124.85
7	E	479	AUR	C19-C18-C17	-2.12	115.25	119.18
7	E	479	AUR	C10-C11-C12	-2.01	120.28	124.94
6	D	600	ADP	C4-C5-N7	2.09	111.40	109.48
5	C	600	ANP	O3A-PA-O5'	2.10	108.51	102.94
7	E	479	AUR	C8-C9-C10	2.27	130.92	125.66
6	D	600	ADP	C1'-N9-C4	2.27	130.37	126.94
5	A	600	ANP	O2'-C2'-C3'	2.28	119.25	111.83
6	D	600	ADP	O2B-PB-O1B	2.57	118.84	110.58
7	E	479	AUR	C5-C6-C7	2.77	114.95	110.75
5	B	600	ANP	O2B-PB-O1B	3.05	116.37	110.00
5	F	600	ANP	O1B-PB-N3B	3.18	116.78	111.90
7	E	479	AUR	C16-C15-C14	3.27	127.57	120.12
5	C	600	ANP	O3G-PG-O2G	3.46	117.83	107.58
5	F	600	ANP	C4-C5-N7	3.67	112.85	109.48
6	D	600	ADP	N3-C2-N1	3.89	131.87	128.89
5	B	600	ANP	N3-C2-N1	3.99	131.95	128.89
7	F	602	AUR	O5-C25-C24	4.07	118.77	111.10
7	E	479	AUR	O7-C7-C8	4.43	118.41	109.64
5	B	600	ANP	O1B-PB-N3B	4.70	119.11	111.90
5	F	600	ANP	O2B-PB-O1B	5.35	121.17	110.00
5	A	600	ANP	O2G-PG-O1G	5.53	128.21	113.49
5	B	600	ANP	O3G-PG-O2G	5.54	124.00	107.58
5	C	600	ANP	O2B-PB-O1B	5.96	122.44	110.00
5	F	600	ANP	O3G-PG-O2G	6.27	126.17	107.58
5	A	600	ANP	O2B-PB-O1B	6.52	123.61	110.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ANP	1	0
5	B	600	ANP	8	0
5	C	600	ANP	4	0
6	D	600	ADP	3	0
7	E	479	AUR	14	0
5	F	600	ANP	2	0
7	F	602	AUR	6	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/510 (95%)	-0.48	4 (0%) 87 75	4, 40, 81, 100	0
1	B	487/510 (95%)	-0.42	10 (2%) 67 44	1, 35, 93, 100	0
1	C	492/510 (96%)	-0.61	4 (0%) 87 75	7, 30, 71, 100	0
2	D	467/482 (96%)	-0.42	9 (1%) 70 48	8, 37, 87, 100	0
2	E	466/482 (96%)	-0.18	17 (3%) 46 23	3, 53, 100, 100	0
2	F	466/482 (96%)	-0.57	3 (0%) 90 80	3, 30, 76, 91	0
3	G	122/272 (44%)	0.61	19 (15%) 3 1	7, 79, 100, 100	0
All	All	2987/3248 (91%)	-0.40	66 (2%) 65 42	1, 38, 92, 100	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	PHE	6.7
3	G	86	ALA	6.0
1	B	408	SER	5.1
2	E	389	ALA	4.5
3	G	25	MET	4.4
3	G	216	SER	4.2
1	C	408	SER	4.1
1	B	405	GLN	4.1
1	A	408	SER	3.9
1	B	407	GLY	3.9
1	B	406	PHE	3.8
3	G	40	PRO	3.6
2	D	394	ASP	3.6
3	G	90	LYS	3.6
3	G	213	ILE	3.5
1	A	405	GLN	3.4
1	C	405	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	395	GLU	3.4
1	C	409	ASP	3.3
2	E	388	ILE	3.3
2	E	390	ILE	3.2
1	A	414	THR	3.1
3	G	29	ALA	3.1
3	G	85	VAL	3.1
2	E	398	GLU	3.0
2	E	385	GLN	3.0
3	G	43	VAL	3.0
3	G	87	LYS	2.9
2	E	471	ASP	2.9
2	E	386	ASP	2.8
1	B	413	ALA	2.8
3	G	41	ALA	2.7
2	E	474	ALA	2.7
2	E	425	THR	2.6
2	D	426	GLY	2.6
1	B	404	ALA	2.6
2	F	249	GLN	2.6
1	B	409	ASP	2.6
3	G	210	ALA	2.5
2	D	473	LEU	2.5
3	G	89	MET	2.5
2	E	395	GLU	2.5
3	G	211	ASN	2.5
2	D	246	GLN	2.5
3	G	214	TYR	2.4
1	B	401	ALA	2.4
3	G	39	LYS	2.4
2	E	426	GLY	2.4
2	D	396	LEU	2.4
3	G	88	GLN	2.4
1	C	193	THR	2.3
2	F	42	GLU	2.3
2	E	393	MET	2.3
1	B	492	GLU	2.2
2	E	130	GLN	2.2
2	D	9	THR	2.2
2	F	246	GLN	2.2
2	E	360	PRO	2.1
2	D	446	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	396	LEU	2.1
2	E	473	LEU	2.1
3	G	218	LYS	2.1
2	E	394	ASP	2.1
1	A	92	GLY	2.1
3	G	82	HIS	2.0
2	D	390	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	D	601	1/1	0.99	0.36	10.37	16,16,16,16	0
4	MG	F	601	1/1	0.92	0.28	8.00	19,19,19,19	0
7	AUR	E	479	33/33	0.80	0.33	0.41	61,64,87,87	33
5	ANP	F	600	31/31	0.96	0.15	0.07	21,25,34,36	0
7	AUR	F	602	33/33	0.95	0.20	0.05	16,22,53,56	33
6	ADP	D	600	27/27	0.96	0.14	-0.30	16,30,34,36	0
5	ANP	A	600	31/31	0.96	0.13	-0.61	17,31,44,45	0
5	ANP	B	600	31/31	0.96	0.14	-0.71	18,37,44,47	0
5	ANP	C	600	31/31	0.97	0.12	-0.73	7,20,25,27	0
4	MG	B	601	1/1	0.88	0.17	-	35,35,35,35	0
4	MG	C	601	1/1	0.95	0.17	-	19,19,19,19	0
4	MG	A	601	1/1	0.97	0.12	-	14,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.