



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:42 AM GMT

PDB ID : 2WPD  
Title : THE MG.ADP INHIBITED STATE OF THE YEAST F1C10 ATP SYN-  
THASE  
Authors : Dautant, A.; Velours, J.; Giraud, M.-F.  
Deposited on : 2009-08-05  
Resolution : 3.43 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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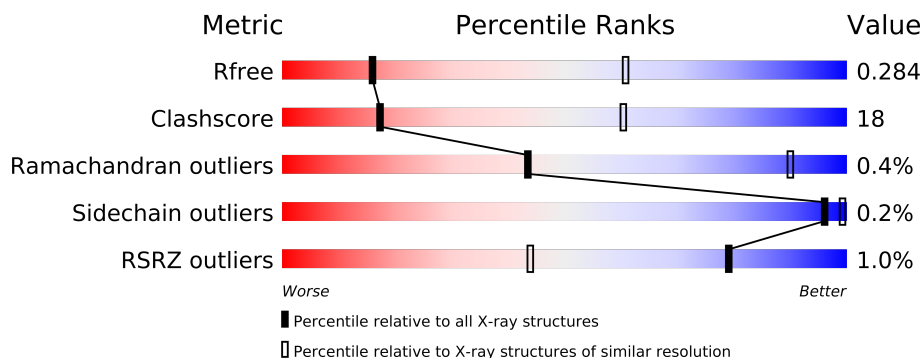
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.43 Å.

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








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1032 (3.58-3.30)
Clashscore	79885	1296 (3.58-3.30)
Ramachandran outliers	78287	1256 (3.58-3.30)
Sidechain outliers	78261	1256 (3.58-3.30)
RSRZ outliers	66119	1032 (3.58-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	478	
2	E	478	
2	F	478	
3	G	278	
4	H	138	
5	I	61	
6	J	76	
6	K	76	
6	L	76	
6	M	76	
6	N	76	

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Mol	Chain	Length	Quality of chain
6	O	76	
6	P	76	
6	Q	76	
6	R	76	
6	S	76	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 30826 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3692	2334	651	704	3			
1	B	485	Total	C	N	O	S	0	0	0
			3685	2328	651	703	3			
1	C	485	Total	C	N	O	S	0	0	0
			3692	2334	651	704	3			

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	473	Total	C	N	O	S	0	0	0
			3572	2262	608	696	6			
2	F	472	Total	C	N	O	S	0	0	0
			3566	2259	607	694	6			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	269	Total	C	N	O	S	0	0	0
			2086	1309	362	405	10			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	132	Total	C	N	O	S	0	0	0
			990	624	165	199	2			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	59	Total	C	N	O	0	0	0
			392	243	71	78			

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	K	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	L	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	M	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	N	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	O	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	P	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	Q	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	R	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			
6	S	76	Total	C	N	O	S	0	0	0
			545	364	84	93	4			

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

Image for chem-comp ATP is not available.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

Image for chem-comp ADP is not available.

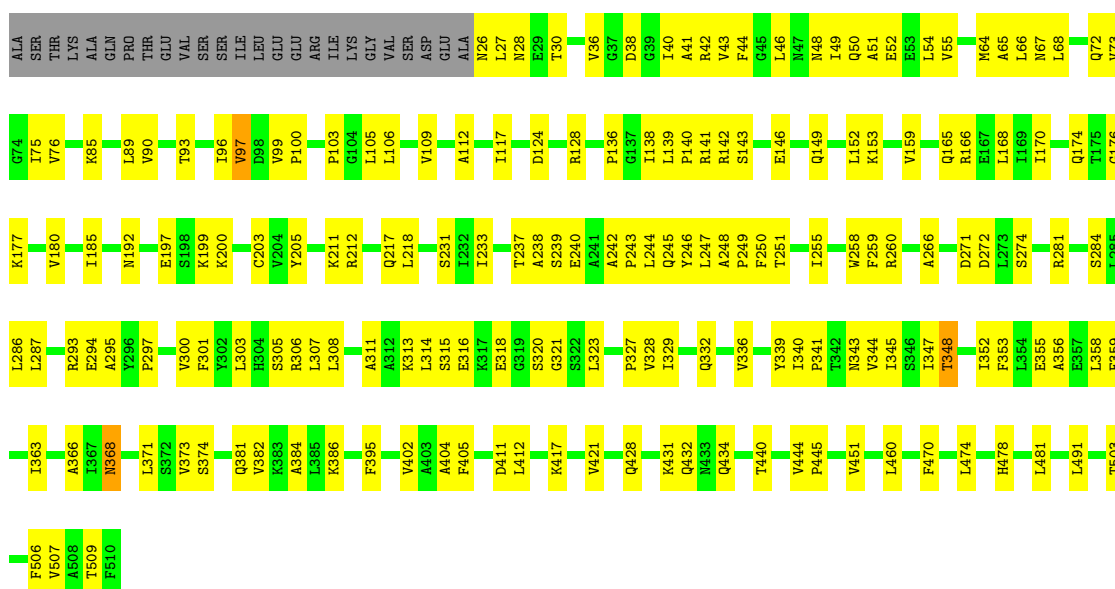
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C N O P 27 10 5 10 2	0	0
9	F	1	Total C N O P 27 10 5 10 2	0	0

### 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.

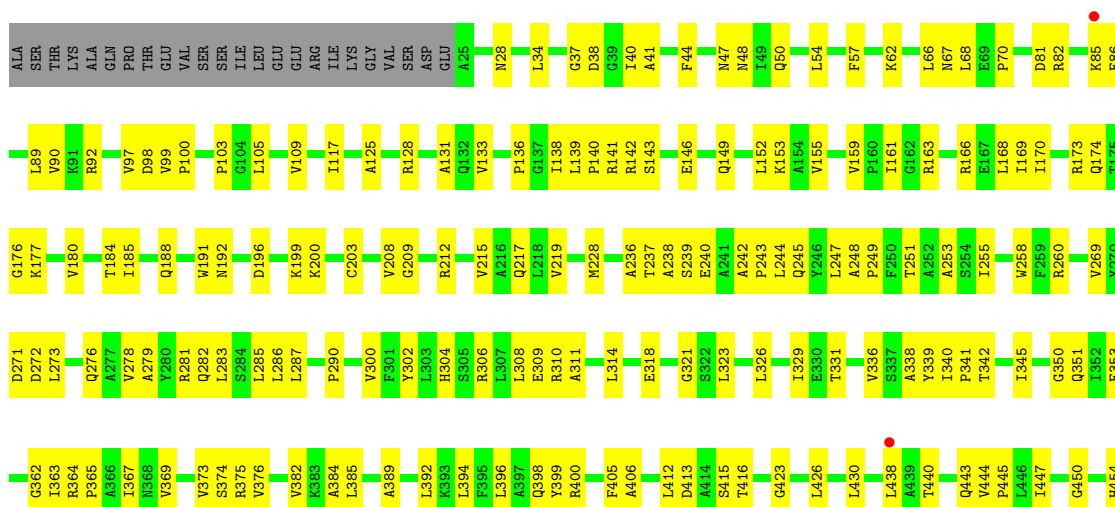
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

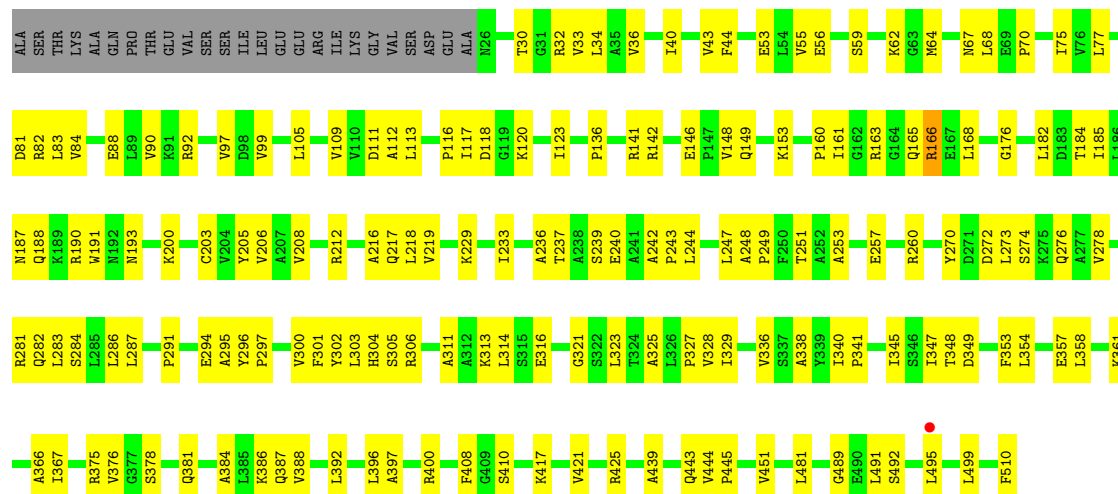
Chain B:





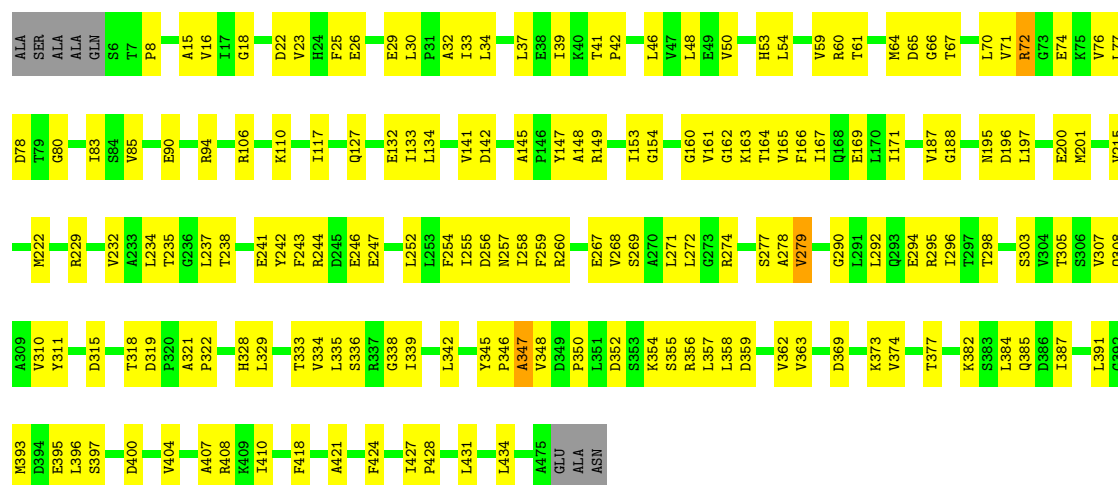
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain C:



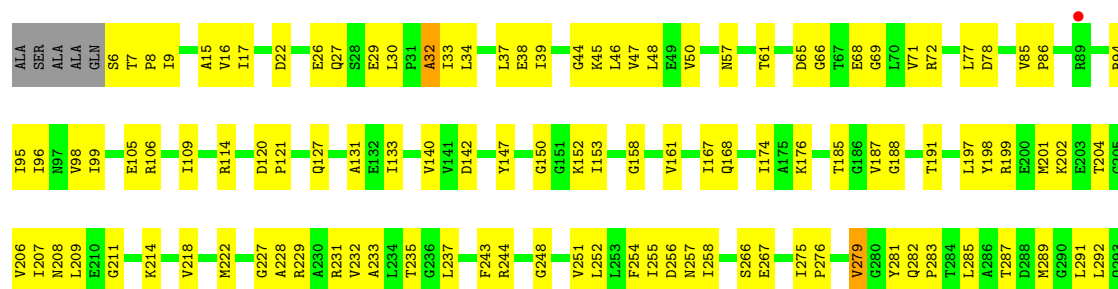
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:

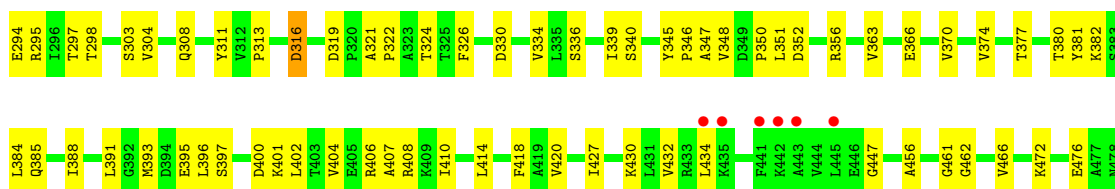


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:

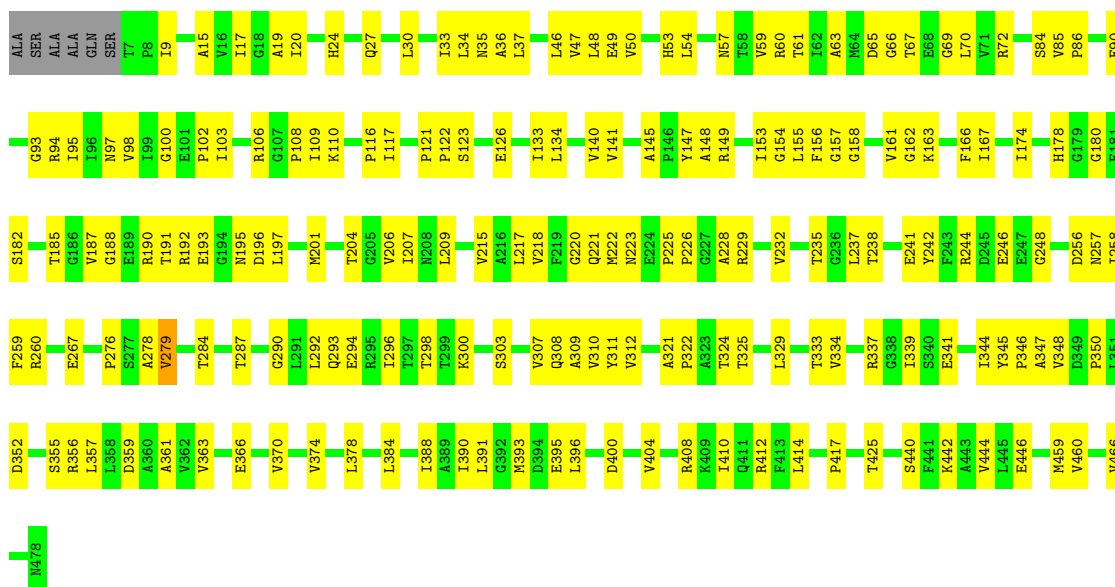






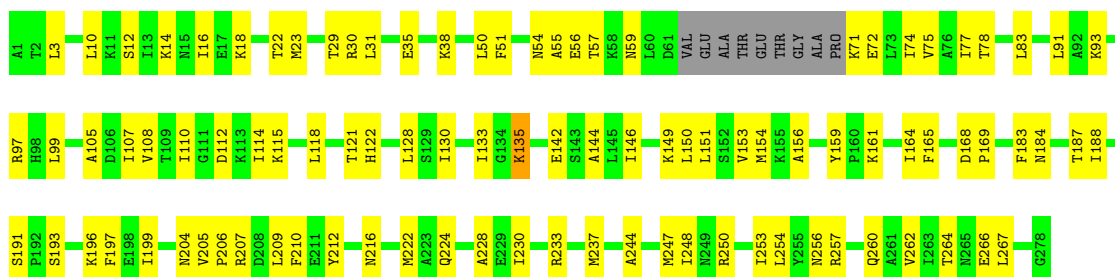
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:



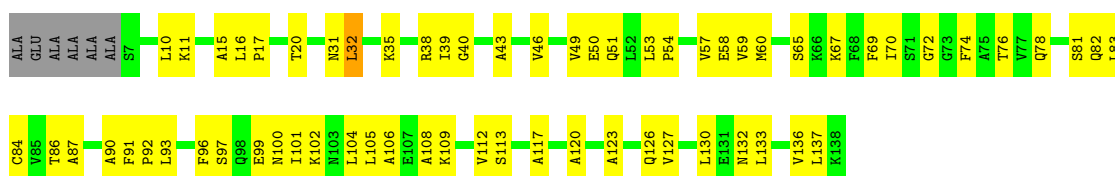
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:



• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

Chain H:



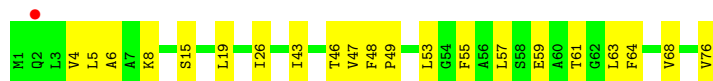
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:



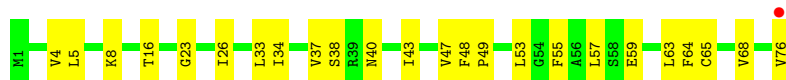
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain J:



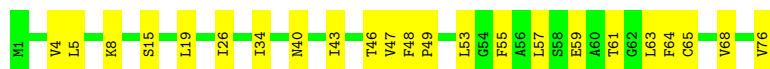
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain K:



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain L:



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain M:



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain N:



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain O:



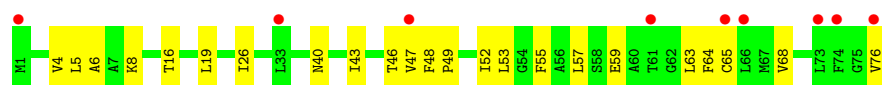
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain P:



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain Q: 



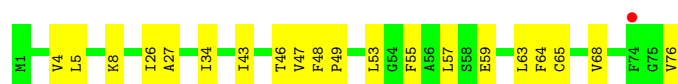
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain R: 



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain S: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.99Å 173.94Å 137.02Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	39.77 – 3.43 39.77 – 3.43	Depositor EDS
% Data completeness (in resolution range)	88.1 (39.77-3.43) 88.1 (39.77-3.43)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.286 , 0.297 0.280 , 0.284	Depositor DCC
$R_{free}$ test set	3741 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 31.5	EDS
Estimated twinning fraction	0.069 for l,k,-h 0.079 for h,-k,-l 0.105 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 74417 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	30826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	0.27	0/3749	0.43	0/5073
1	B	0.24	0/3741	0.39	0/5064
1	C	0.27	0/3749	0.43	0/5073
2	D	0.27	0/3605	0.44	0/4889
2	E	0.24	0/3628	0.41	0/4919
2	F	0.26	0/3622	0.43	0/4911
3	G	0.24	0/2111	0.39	0/2838
4	H	0.24	0/1004	0.39	0/1359
5	I	0.22	0/398	0.34	0/547
6	J	0.22	0/553	0.35	0/747
6	K	0.24	0/553	0.37	0/747
6	L	0.22	0/553	0.35	0/747
6	M	0.23	0/553	0.35	0/747
6	N	0.22	0/553	0.35	0/747
6	O	0.23	0/553	0.35	0/747
6	P	0.23	0/553	0.35	0/747
6	Q	0.22	0/553	0.34	0/747
6	R	0.22	0/553	0.34	0/747
6	S	0.23	0/553	0.35	0/747
All	All	0.25	0/31137	0.41	0/42143

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3692	0	3773	155	0
1	B	3685	0	3768	139	0
1	C	3692	0	3772	127	0
2	D	3549	0	3621	127	0
2	E	3572	0	3638	155	0
2	F	3566	0	3633	158	0
3	G	2086	0	2156	82	0
4	H	990	0	999	62	0
5	I	392	0	306	9	0
6	J	545	0	591	16	0
6	K	545	0	591	24	0
6	L	545	0	591	28	0
6	M	545	0	591	33	0
6	N	545	0	591	29	0
6	O	545	0	591	30	0
6	P	545	0	591	27	0
6	Q	545	0	591	24	0
6	R	545	0	591	19	0
6	S	545	0	591	18	0
7	A	31	0	12	5	0
7	B	31	0	12	1	0
7	C	31	0	12	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	D	27	0	12	2	0
9	F	27	0	12	2	0
All	All	30826	0	31636	1094	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (1094) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:Q:4:VAL:HG21	6:R:5:LEU:HD23	1.16	1.16
6:O:4:VAL:HG21	6:P:5:LEU:HD23	1.25	1.12
6:N:4:VAL:HG21	6:O:5:LEU:HD23	1.19	1.10
6:K:4:VAL:HG21	6:L:5:LEU:HD23	1.15	1.07
6:M:4:VAL:HG21	6:N:5:LEU:HD23	1.28	1.06
6:L:4:VAL:HG21	6:M:5:LEU:HD23	1.03	1.03
6:P:4:VAL:HG21	6:Q:5:LEU:HD23	1.02	1.01
6:J:4:VAL:HG21	6:K:5:LEU:HD23	1.41	1.01
4:H:10:LEU:HD21	4:H:83:LEU:H	1.28	0.98
6:L:4:VAL:HG21	6:M:5:LEU:CD2	1.92	0.97
6:L:4:VAL:CG2	6:M:5:LEU:HD23	1.95	0.97
2:E:50:VAL:HA	2:E:61:THR:HG22	1.41	0.97
1:C:212:ARG:HG2	1:C:237:THR:HG21	1.43	0.97
6:P:4:VAL:HG21	6:Q:5:LEU:CD2	1.95	0.97
1:A:142:ARG:HG3	1:A:315:SER:HA	1.48	0.94
6:P:4:VAL:CG2	6:Q:5:LEU:HD23	1.96	0.94
1:C:116:PRO:HD3	1:C:123:ILE:HG12	1.50	0.92
1:A:42:ARG:HD2	1:A:72:GLN:NE2	1.86	0.90
1:B:398:GLN:HE22	2:F:412:ARG:HE	1.16	0.90
1:A:404:ALA:HB2	3:G:18:LYS:HE2	1.51	0.90
3:G:247:MET:HG3	3:G:250:ARG:HH21	1.37	0.90
1:B:174:GLN:HE21	2:E:356:ARG:HH11	1.16	0.90
1:C:239:SER:HB3	2:F:294:GLU:HG3	1.50	0.90
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.54	0.89
1:A:42:ARG:HD2	1:A:72:GLN:HE22	1.38	0.89
1:B:217:GLN:HE22	2:E:131:ALA:HB2	1.36	0.89
2:F:153:ILE:HD12	2:F:307:VAL:HG22	1.52	0.89
2:E:388:ILE:HG23	2:E:393:MET:HG2	1.55	0.87
6:R:4:VAL:HG21	6:S:5:LEU:HD23	1.56	0.87
1:B:217:GLN:NE2	2:E:131:ALA:HB2	1.90	0.86
2:D:142:ASP:HB3	2:D:434:LEU:HD13	1.59	0.84
1:B:389:ALA:HB2	1:B:447:ILE:HG21	1.59	0.84
1:B:174:GLN:HE21	2:E:356:ARG:NH1	1.75	0.84
2:F:37:LEU:HB2	2:F:48:LEU:HB2	1.59	0.83
1:C:249:PRO:HG2	1:C:276:GLN:OE1	1.79	0.82
6:J:5:LEU:HD23	6:S:4:VAL:HG21	1.62	0.82
2:F:298:THR:HG23	2:F:303:SER:HA	1.62	0.82
3:G:93:LYS:HE2	3:G:97:ARG:HH21	1.43	0.81
1:C:378:SER:HB2	1:C:386:LYS:HE2	1.63	0.81
1:C:273:LEU:HB3	1:C:304:HIS:CE1	2.16	0.81
6:K:4:VAL:HG21	6:L:5:LEU:CD2	2.06	0.81
6:K:4:VAL:CG2	6:L:5:LEU:HD23	2.07	0.81
3:G:110:ILE:HG23	3:G:130:ILE:HB	1.64	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:LYS:HE2	2:D:32:ALA:HB2	1.63	0.80
2:D:321:ALA:HB3	2:D:322:PRO:HD3	1.64	0.80
3:G:50:LEU:HG	4:H:78:GLN:HE21	1.47	0.79
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.63	0.79
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.46	0.79
2:E:98:VAL:HG11	2:E:228:ALA:HB1	1.64	0.78
2:F:50:VAL:HA	2:F:61:THR:HG22	1.66	0.78
4:H:38:ARG:HD2	6:M:41:PRO:HG3	1.66	0.77
6:Q:4:VAL:CG2	6:R:5:LEU:HD23	2.09	0.77
1:B:398:GLN:HE22	2:F:412:ARG:NE	1.83	0.77
2:D:26:GLU:HB2	2:D:29:GLU:OE1	1.84	0.77
6:K:40:ASN:HD22	6:K:43:ILE:HG22	1.48	0.76
2:E:336:SER:HB3	2:E:339:ILE:HG12	1.67	0.76
1:C:417:LYS:O	1:C:421:VAL:HG23	1.87	0.75
2:E:174:ILE:HG21	2:E:252:LEU:HD11	1.68	0.75
1:B:239:SER:HB2	2:E:121:PRO:HG3	1.69	0.75
1:B:240:GLU:HB3	1:B:244:LEU:HD12	1.67	0.74
1:A:103:PRO:HD3	1:A:258:TRP:CH2	2.22	0.74
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.68	0.74
1:C:217:GLN:HE22	2:F:356:ARG:HD2	1.52	0.74
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.69	0.74
6:O:4:VAL:HA	6:P:6:ALA:HB2	1.70	0.73
6:Q:4:VAL:HG21	6:R:5:LEU:CD2	2.09	0.73
1:B:249:PRO:HG3	1:B:276:GLN:NE2	2.04	0.73
1:B:152:LEU:HD12	1:B:180:VAL:HG13	1.70	0.72
1:C:68:LEU:HD12	2:D:16:VAL:HB	1.71	0.72
1:A:159:VAL:HG13	1:A:374:SER:HB2	1.70	0.72
2:F:257:ASN:HD21	2:F:311:TYR:N	1.88	0.72
1:B:103:PRO:HD3	1:B:258:TRP:CH2	2.24	0.72
4:H:49:VAL:HG22	4:H:76:THR:HG23	1.71	0.72
1:A:143:SER:HB3	2:E:199:ARG:HH22	1.55	0.72
2:D:391:LEU:HB3	2:D:395:GLU:HG3	1.72	0.72
6:K:40:ASN:ND2	6:K:43:ILE:HG22	2.05	0.71
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.72	0.71
2:E:106:ARG:NH1	2:E:209:LEU:HD22	2.05	0.71
2:F:310:VAL:HG21	2:F:325:THR:HG21	1.71	0.71
1:A:240:GLU:HB3	1:A:244:LEU:HD12	1.73	0.71
2:E:402:LEU:O	2:E:406:ARG:HG3	1.91	0.71
2:E:206:VAL:HG23	2:E:207:ILE:HG13	1.72	0.71
1:A:168:LEU:HB2	1:A:348:THR:HG21	1.72	0.71
4:H:60:MET:HA	4:H:65:SER:CB	2.20	0.71
1:B:243:PRO:HG3	1:B:283:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:106:ARG:NE	2:F:209:LEU:HD22	2.06	0.70
1:B:219:VAL:HG13	1:B:228:MET:HE3	1.73	0.70
2:D:134:LEU:HD13	2:D:149:ARG:HE	1.55	0.70
1:B:138:ILE:HD11	2:F:95:ILE:HG21	1.73	0.70
6:M:40:ASN:HD21	6:M:43:ILE:HG12	1.56	0.70
1:C:56:GLU:HG2	1:C:62:LYS:HG2	1.72	0.70
2:F:30:LEU:HD21	2:F:57:ASN:HA	1.74	0.70
2:E:298:THR:HG23	2:E:303:SER:HB3	1.73	0.70
6:M:57:LEU:HD22	6:N:55:PHE:CZ	2.26	0.69
1:B:338:ALA:HB3	1:B:341:PRO:HG2	1.73	0.69
3:G:108:VAL:HG13	3:G:128:LEU:HB3	1.75	0.69
1:C:444:VAL:HB	1:C:445:PRO:HD3	1.73	0.69
1:C:336:VAL:HG11	1:C:353:PHE:HE2	1.57	0.69
1:A:314:LEU:HD22	1:A:318:GLU:HG2	1.75	0.69
1:C:99:VAL:HG11	1:C:251:THR:HB	1.75	0.69
2:D:397:SER:HB3	2:D:400:ASP:OD2	1.92	0.69
1:A:311:ALA:HB1	1:A:323:LEU:O	1.93	0.69
2:E:106:ARG:HH12	2:E:209:LEU:HD22	1.58	0.68
1:C:240:GLU:HB3	1:C:244:LEU:HD12	1.75	0.68
2:F:102:PRO:HG3	2:F:109:ILE:HG13	1.75	0.68
2:E:430:LYS:HG3	2:E:461:GLY:HA3	1.74	0.68
1:A:50:GLN:HA	2:E:71:VAL:HG22	1.74	0.68
4:H:60:MET:HA	4:H:65:SER:HB3	1.75	0.68
1:C:142:ARG:HH22	1:C:316:GLU:HB2	1.57	0.68
1:A:166:ARG:HD2	1:A:308:LEU:HB3	1.76	0.68
4:H:91:PHE:CE1	4:H:96:PHE:HB3	2.28	0.68
2:F:417:PRO:HG3	2:F:459:MET:HG3	1.75	0.68
2:F:36:ALA:O	2:F:37:LEU:HD23	1.95	0.67
1:A:168:LEU:HD12	1:A:327:PRO:O	1.94	0.67
2:F:258:ILE:HG22	2:F:309:ALA:O	1.94	0.67
1:B:174:GLN:NE2	2:E:356:ARG:HH11	1.90	0.67
1:C:349:ASP:HA	1:C:375:ARG:HD2	1.76	0.67
3:G:204:ASN:HD22	3:G:207:ARG:HG3	1.60	0.67
2:F:153:ILE:HB	2:F:307:VAL:HA	1.75	0.67
1:C:67:ASN:ND2	1:C:287:LEU:HB3	2.10	0.67
2:F:134:LEU:HD13	2:F:149:ARG:HD2	1.77	0.67
6:N:57:LEU:HD22	6:O:55:PHE:CZ	2.29	0.67
1:C:510:PHE:HD1	1:C:510:PHE:OXT	1.78	0.66
2:F:190:ARG:HD2	2:F:193:GLU:OE2	1.95	0.66
1:C:176:GLY:HA2	7:C:600:ATP:O1A	1.96	0.66
3:G:55:ALA:HB2	3:G:197:PHE:HE2	1.59	0.66
1:B:454:HIS:HB3	1:B:507:VAL:HG21	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:86:PRO:HD3	2:E:114:ARG:HH12	1.61	0.66
1:A:138:ILE:HD13	2:E:191:THR:HG23	1.77	0.66
1:A:211:LYS:HD3	2:D:328:HIS:HA	1.78	0.66
2:E:244:ARG:HD3	2:E:304:VAL:HG23	1.78	0.66
1:A:217:GLN:HG2	2:D:356:ARG:HH12	1.60	0.65
4:H:69:PHE:HB3	4:H:91:PHE:HB3	1.78	0.65
1:B:444:VAL:HB	1:B:445:PRO:HD3	1.79	0.65
1:A:51:ALA:HB3	2:E:69:GLY:H	1.60	0.65
6:J:47:VAL:CG1	6:K:34:ILE:HG23	2.25	0.65
2:D:187:VAL:HG22	2:D:232:VAL:HG13	1.79	0.65
6:M:4:VAL:HA	6:N:6:ALA:HB2	1.79	0.65
1:B:89:LEU:HD23	1:B:90:VAL:N	2.12	0.65
1:C:510:PHE:OXT	1:C:510:PHE:CD1	2.49	0.64
2:F:140:VAL:HG21	2:F:348:VAL:HG21	1.80	0.64
3:G:93:LYS:HE2	3:G:97:ARG:NH2	2.13	0.64
1:C:336:VAL:HG11	1:C:353:PHE:CE2	2.33	0.64
6:J:55:PHE:CZ	6:S:57:LEU:HD22	2.33	0.64
2:D:298:THR:HG23	2:D:303:SER:HA	1.79	0.64
1:C:166:ARG:HD2	1:C:166:ARG:H	1.63	0.64
1:A:358:LEU:HB2	1:A:366:ALA:HB1	1.78	0.64
1:A:404:ALA:HB3	3:G:22:THR:HG21	1.80	0.64
4:H:46:VAL:HG21	6:K:38:SER:O	1.98	0.64
1:C:392:LEU:O	1:C:396:LEU:HD13	1.98	0.64
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.80	0.63
2:E:346:PRO:HB3	2:E:418:PHE:HZ	1.62	0.63
2:F:201:MET:CE	2:F:215:VAL:HG11	2.28	0.63
4:H:10:LEU:HD21	4:H:83:LEU:N	2.08	0.63
1:B:340:ILE:HB	1:B:341:PRO:HD3	1.80	0.63
2:D:153:ILE:HD12	2:D:307:VAL:HG22	1.80	0.63
1:A:153:LYS:HG3	1:A:432:GLN:OE1	1.99	0.63
2:F:9:ILE:HG23	2:F:27:GLN:OE1	1.98	0.63
6:Q:57:LEU:HD22	6:R:55:PHE:CZ	2.33	0.63
1:A:43:VAL:HG11	1:A:90:VAL:HG11	1.81	0.63
4:H:83:LEU:HD23	4:H:84:CYS:N	2.13	0.63
1:C:248:ALA:HB3	1:C:249:PRO:HD3	1.81	0.63
3:G:78:THR:HG22	3:G:91:LEU:HD23	1.81	0.63
2:E:127:GLN:HE22	2:E:297:THR:HG21	1.64	0.63
2:D:23:VAL:HG11	2:D:76:VAL:HG21	1.80	0.63
1:A:371:LEU:O	1:A:373:VAL:HG13	1.99	0.63
1:B:67:ASN:HB2	2:F:17:ILE:HG12	1.81	0.62
6:R:43:ILE:CG2	6:R:46:THR:HB	2.30	0.62
6:L:57:LEU:HD22	6:M:55:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:P:40:ASN:HD21	6:P:43:ILE:HG12	1.63	0.62
1:A:212:ARG:HB2	2:D:127:GLN:HE21	1.64	0.62
1:B:50:GLN:HB3	2:F:69:GLY:HA2	1.81	0.62
6:L:43:ILE:HG22	6:L:47:VAL:HG23	1.80	0.62
3:G:199:ILE:HD11	3:G:205:VAL:HB	1.82	0.62
2:E:237:LEU:HD22	2:E:292:LEU:HD12	1.80	0.62
3:G:54:ASN:HD22	4:H:78:GLN:NE2	1.97	0.62
2:E:142:ASP:HB3	2:E:434:LEU:HD13	1.80	0.62
2:F:229:ARG:NH2	2:F:267:GLU:OE2	2.33	0.62
6:O:57:LEU:HD22	6:P:55:PHE:CZ	2.35	0.62
2:F:106:ARG:HE	2:F:209:LEU:HD22	1.62	0.62
6:R:43:ILE:HG23	6:R:46:THR:HB	1.81	0.62
1:A:176:GLY:HA2	7:A:600:ATP:O1A	2.00	0.62
1:A:340:ILE:HB	1:A:341:PRO:HD3	1.81	0.62
1:A:28:ASN:HB3	1:A:48:ASN:ND2	2.13	0.62
2:D:188:GLY:HA3	2:D:260:ARG:HG3	1.81	0.62
1:B:153:LYS:HG2	1:B:443:GLN:HG2	1.82	0.62
2:F:185:THR:HA	2:F:218:VAL:O	1.99	0.62
1:A:212:ARG:CG	1:A:237:THR:HG21	2.30	0.61
2:E:30:LEU:HD21	2:E:57:ASN:HA	1.80	0.61
2:E:176:LYS:NZ	2:E:214:LYS:HE2	2.15	0.61
2:D:255:ILE:HD12	2:D:308:GLN:HE21	1.65	0.61
2:D:145:ALA:HB1	2:D:355:SER:HB2	1.82	0.61
2:D:336:SER:HB2	2:D:339:ILE:HG12	1.81	0.61
1:C:185:ILE:HG23	1:C:203:CYS:SG	2.41	0.61
6:K:40:ASN:HD22	6:K:43:ILE:CG2	2.12	0.61
1:B:131:ALA:HB1	1:B:247:LEU:HD11	1.82	0.61
1:C:338:ALA:HB3	1:C:341:PRO:HG2	1.82	0.61
6:M:43:ILE:HG22	6:M:47:VAL:HG23	1.83	0.61
2:D:257:ASN:ND2	2:D:259:PHE:HB3	2.16	0.61
4:H:112:VAL:HG12	4:H:120:ALA:HA	1.82	0.61
4:H:97:SER:HB2	4:H:102:LYS:HE3	1.83	0.61
1:A:217:GLN:CD	2:D:356:ARG:HH22	2.03	0.61
1:A:239:SER:CB	2:D:294:GLU:HG3	2.31	0.60
2:F:374:VAL:O	2:F:378:LEU:HG	2.01	0.60
2:F:197:LEU:O	2:F:201:MET:HG2	2.01	0.60
2:E:243:PHE:HB2	2:E:251:VAL:HG21	1.82	0.60
2:E:402:LEU:HG	2:E:406:ARG:HE	1.65	0.60
6:M:43:ILE:HG23	6:M:46:THR:HB	1.83	0.60
1:A:300:VAL:HG11	1:A:339:TYR:HE2	1.66	0.60
2:D:154:GLY:HA3	2:D:329:LEU:HD13	1.82	0.60
1:A:99:VAL:HG21	1:A:251:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:67:ASN:HD21	1:C:287:LEU:HB3	1.66	0.60
1:A:54:LEU:HD23	1:A:64:MET:HB3	1.83	0.60
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.84	0.60
3:G:3:LEU:HD23	3:G:3:LEU:O	2.01	0.60
1:C:341:PRO:O	1:C:345:ILE:HG13	2.02	0.60
2:E:282:GLN:CD	2:E:282:GLN:H	2.04	0.60
2:D:163:LYS:HB2	9:D:600:ADP:O1B	2.01	0.60
1:B:242:ALA:HB3	1:B:243:PRO:HD3	1.83	0.60
1:B:503:THR:O	1:B:507:VAL:HG23	2.01	0.60
2:D:257:ASN:ND2	2:D:259:PHE:H	2.00	0.60
2:F:388:ILE:HD11	2:F:396:LEU:HD11	1.83	0.60
1:C:302:TYR:HA	1:C:305:SER:OG	2.01	0.60
1:B:57:PHE:HD1	1:B:90:VAL:HG22	1.66	0.60
1:B:405:PHE:HZ	2:F:393:MET:SD	2.25	0.60
2:E:388:ILE:HD11	2:E:396:LEU:HD11	1.84	0.59
1:C:381:GLN:HE21	1:C:386:LYS:HA	1.68	0.59
1:A:314:LEU:HD13	1:A:318:GLU:HG3	1.82	0.59
1:C:205:TYR:HB3	1:C:233:ILE:HD12	1.84	0.59
2:D:334:VAL:HG21	2:D:352:ASP:OD2	2.02	0.59
2:D:279:VAL:HG12	2:D:279:VAL:O	2.03	0.59
6:R:47:VAL:CG1	6:S:34:ILE:HG23	2.32	0.59
2:F:157:GLY:H	2:F:312:VAL:HG23	1.67	0.59
2:F:106:ARG:NH1	2:F:106:ARG:HB3	2.18	0.59
2:E:26:GLU:HB2	2:E:29:GLU:OE1	2.02	0.59
6:N:65:CYS:SG	6:O:19:LEU:HD12	2.42	0.59
1:B:38:ASP:O	1:B:286:LEU:HD13	2.03	0.59
4:H:105:LEU:O	4:H:109:LYS:HG2	2.03	0.59
6:R:43:ILE:HG22	6:R:47:VAL:HG23	1.84	0.59
3:G:184:ASN:HA	3:G:210:PHE:CD1	2.37	0.59
4:H:99:GLU:OE2	4:H:137:LEU:HD13	2.03	0.59
1:B:398:GLN:NE2	2:F:412:ARG:HE	1.93	0.59
2:E:340:SER:HB3	2:E:347:ALA:HB2	1.85	0.59
3:G:50:LEU:HG	4:H:78:GLN:NE2	2.16	0.58
6:O:65:CYS:SG	6:P:19:LEU:HD12	2.43	0.58
1:B:48:ASN:O	1:B:92:ARG:NH1	2.36	0.58
6:N:43:ILE:HG23	6:N:46:THR:HB	1.85	0.58
1:B:138:ILE:CD1	2:F:95:ILE:HG21	2.32	0.58
2:E:366:GLU:O	2:E:370:VAL:HG23	2.03	0.58
6:Q:40:ASN:HD21	6:Q:43:ILE:HG12	1.69	0.58
2:E:319:ASP:O	2:E:322:PRO:HG2	2.03	0.58
2:F:102:PRO:HG2	2:F:108:PRO:HA	1.86	0.58
3:G:144:ALA:HB1	5:I:11:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:J:48:PHE:N	6:J:49:PRO:HD2	2.19	0.58
1:A:428:GLN:NE2	1:A:431:LYS:HD2	2.19	0.58
1:A:444:VAL:HB	1:A:445:PRO:HD3	1.86	0.58
1:A:146:GLU:OE1	1:A:313:LYS:HE2	2.04	0.58
4:H:59:VAL:O	4:H:65:SER:HB2	2.04	0.58
2:D:163:LYS:NZ	2:D:311:TYR:HA	2.19	0.58
1:B:290:PRO:HB3	2:F:276:PRO:HG3	1.84	0.58
4:H:16:LEU:HD11	4:H:90:ALA:HB2	1.85	0.58
1:B:212:ARG:HG2	2:E:294:GLU:OE1	2.04	0.57
2:E:140:VAL:HG11	2:E:348:VAL:HB	1.85	0.57
6:N:48:PHE:N	6:N:49:PRO:HD2	2.19	0.57
4:H:35:LYS:HB2	4:H:51:GLN:HG3	1.85	0.57
4:H:91:PHE:HE1	4:H:96:PHE:HB3	1.68	0.57
6:R:48:PHE:N	6:R:49:PRO:HD2	2.19	0.57
1:B:153:LYS:HD3	1:B:438:LEU:HD12	1.85	0.57
1:A:281:ARG:HG3	1:A:295:ALA:O	2.03	0.57
2:D:348:VAL:O	2:D:350:PRO:HD3	2.04	0.57
6:P:43:ILE:HG22	6:P:47:VAL:HG23	1.85	0.57
4:H:15:ALA:HB1	4:H:20:THR:HG22	1.86	0.57
6:O:48:PHE:N	6:O:49:PRO:HD2	2.19	0.57
2:D:243:PHE:HA	2:D:247:GLU:HB3	1.86	0.57
3:G:212:TYR:OH	4:H:86:THR:HG22	2.04	0.57
6:M:48:PHE:N	6:M:49:PRO:HD2	2.19	0.57
6:P:48:PHE:N	6:P:49:PRO:HD2	2.19	0.57
4:H:60:MET:HA	4:H:65:SER:HB2	1.86	0.57
2:F:201:MET:HE3	2:F:215:VAL:HG11	1.87	0.57
1:A:293:ARG:HD3	1:A:339:TYR:CD1	2.40	0.57
6:K:48:PHE:N	6:K:49:PRO:HD2	2.19	0.57
4:H:32:LEU:HD12	4:H:32:LEU:O	2.05	0.57
4:H:72:GLY:HA3	5:I:14:LEU:HD22	1.85	0.57
1:C:273:LEU:HD12	1:C:273:LEU:N	2.20	0.56
1:A:177:LYS:HB2	7:A:600:ATP:O1B	2.05	0.56
2:F:178:HIS:CD2	2:F:180:GLY:H	2.23	0.56
6:L:48:PHE:N	6:L:49:PRO:HD2	2.19	0.56
6:S:48:PHE:N	6:S:49:PRO:HD2	2.19	0.56
2:F:106:ARG:HH11	2:F:106:ARG:HB3	1.68	0.56
2:F:187:VAL:HG12	2:F:260:ARG:HB2	1.86	0.56
3:G:78:THR:CG2	3:G:91:LEU:HD23	2.34	0.56
4:H:69:PHE:CB	4:H:91:PHE:HD2	2.19	0.56
1:B:212:ARG:HD3	1:B:237:THR:HG21	1.88	0.56
1:A:382:VAL:HG12	1:A:384:ALA:H	1.70	0.56
1:B:248:ALA:N	1:B:249:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:391:LEU:HD21	3:G:23:MET:HE3	1.87	0.56
2:F:162:GLY:O	2:F:166:PHE:HB2	2.05	0.56
2:F:293:GLN:HE22	2:F:308:GLN:HE22	1.54	0.56
1:A:68:LEU:HD23	1:A:73:VAL:HG13	1.87	0.56
4:H:106:ALA:HA	4:H:130:LEU:HD13	1.86	0.56
6:Q:48:PHE:N	6:Q:49:PRO:HD2	2.19	0.56
2:D:90:GLU:HG3	2:D:110:LYS:O	2.06	0.56
1:C:481:LEU:HD21	1:C:499:LEU:HB2	1.86	0.56
6:P:65:CYS:SG	6:Q:19:LEU:HD12	2.46	0.56
1:C:358:LEU:HB2	1:C:366:ALA:HB1	1.88	0.56
6:K:57:LEU:HD22	6:L:55:PHE:CZ	2.40	0.56
1:A:301:PHE:HB3	2:E:267:GLU:OE2	2.06	0.56
2:D:133:ILE:HA	2:D:357:LEU:CD1	2.36	0.56
1:C:148:VAL:HB	1:C:161:ILE:HB	1.88	0.56
1:C:270:TYR:HB2	1:C:273:LEU:HD11	1.88	0.56
6:L:43:ILE:HG23	6:L:46:THR:HB	1.86	0.56
1:B:184:THR:O	1:B:188:GLN:HG2	2.05	0.56
6:N:4:VAL:HG21	6:O:5:LEU:CD2	2.13	0.55
2:E:199:ARG:HA	2:E:202:LYS:HE2	1.87	0.55
2:F:85:VAL:HG13	2:F:86:PRO:HD2	1.89	0.55
6:R:47:VAL:HG11	6:S:34:ILE:HG23	1.88	0.55
2:E:27:GLN:O	2:E:29:GLU:HG3	2.06	0.55
1:A:301:PHE:HD2	2:E:229:ARG:HH12	1.54	0.55
1:B:139:LEU:N	1:B:140:PRO:HD2	2.21	0.55
3:G:212:TYR:HB2	5:I:10:TYR:HD2	1.71	0.55
1:A:36:VAL:HG23	1:A:41:ALA:HB2	1.87	0.55
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.88	0.55
2:E:330:ASP:HA	2:E:356:ARG:HD3	1.87	0.55
2:D:382:LYS:HA	2:D:385:GLN:HG2	1.89	0.55
1:C:291:PRO:HB2	1:C:295:ALA:HA	1.89	0.55
6:R:57:LEU:HD22	6:S:55:PHE:CZ	2.41	0.55
1:A:212:ARG:HB3	2:D:127:GLN:HG3	1.87	0.55
2:E:319:ASP:HA	3:G:260:GLN:HE22	1.71	0.55
1:C:149:GLN:HG3	1:C:191:TRP:CH2	2.41	0.55
2:F:90:GLU:HG3	2:F:109:ILE:HG23	1.89	0.55
1:C:109:VAL:O	1:C:117:ILE:HG12	2.07	0.55
2:E:147:TYR:CD2	2:E:153:ILE:HG12	2.42	0.55
2:E:197:LEU:O	2:E:201:MET:HG3	2.07	0.55
6:O:15:SER:HA	6:P:16:THR:OG1	2.07	0.55
3:G:169:PRO:HD3	3:G:228:ALA:HB2	1.89	0.55
6:L:47:VAL:CG1	6:M:34:ILE:HG23	2.37	0.54
2:E:316:ASP:OD2	3:G:256:ASN:HB3	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:344:ILE:HD11	2:F:412:ARG:HD3	1.89	0.54
2:F:220:GLY:N	2:F:232:VAL:HG21	2.22	0.54
3:G:244:ALA:O	3:G:248:ILE:HG13	2.07	0.54
3:G:193:SER:HB3	3:G:196:LYS:NZ	2.23	0.54
2:F:257:ASN:HD21	2:F:311:TYR:H	1.54	0.54
2:F:85:VAL:HG21	2:F:235:THR:HG23	1.90	0.54
2:D:94:ARG:NH2	2:D:106:ARG:HB2	2.22	0.54
2:D:421:ALA:HB1	2:D:424:PHE:HD2	1.72	0.54
1:B:351:GLN:H	1:B:373:VAL:HG13	1.71	0.54
1:C:205:TYR:HB3	1:C:233:ILE:CD1	2.38	0.54
2:E:370:VAL:O	2:E:374:VAL:HG23	2.08	0.54
2:E:319:ASP:HA	3:G:260:GLN:NE2	2.22	0.54
1:B:269:VAL:HG22	1:B:326:LEU:HB2	1.89	0.54
2:E:86:PRO:HD3	2:E:114:ARG:NH1	2.22	0.54
1:A:212:ARG:HG3	1:A:237:THR:HG21	1.88	0.54
2:D:37:LEU:HD12	2:D:61:THR:HG21	1.88	0.54
2:E:37:LEU:HB2	2:E:48:LEU:HB2	1.89	0.54
1:A:99:VAL:HG21	1:A:251:THR:CG2	2.38	0.54
1:C:272:ASP:HB2	1:C:328:VAL:O	2.08	0.54
4:H:102:LYS:NZ	4:H:133:LEU:HB3	2.23	0.54
2:F:345:TYR:HA	2:F:346:PRO:C	2.27	0.54
2:F:98:VAL:HG22	2:F:232:VAL:HB	1.90	0.54
1:C:149:GLN:HG3	1:C:191:TRP:HH2	1.72	0.54
2:D:162:GLY:O	2:D:166:PHE:HB2	2.08	0.54
1:A:36:VAL:HG12	2:D:53:HIS:HB2	1.90	0.54
1:B:68:LEU:HD23	2:F:72:ARG:HG3	1.89	0.54
6:K:43:ILE:O	6:K:43:ILE:HG23	2.07	0.54
4:H:11:LYS:HD2	4:H:82:GLN:HE21	1.73	0.54
1:B:450:GLY:HA2	1:B:455:LEU:HD12	1.90	0.54
2:F:134:LEU:HD13	2:F:149:ARG:CD	2.38	0.53
2:D:242:TYR:CE1	2:D:246:GLU:HG3	2.43	0.53
1:C:217:GLN:NE2	2:F:356:ARG:HD2	2.23	0.53
2:E:406:ARG:HH12	2:E:447:GLY:HA2	1.73	0.53
1:B:283:LEU:O	1:B:287:LEU:HG	2.07	0.53
1:C:142:ARG:HB3	1:C:313:LYS:HG3	1.90	0.53
1:B:109:VAL:HG12	1:B:117:ILE:HD11	1.90	0.53
1:C:82:ARG:HD3	2:F:34:LEU:HD12	1.90	0.53
2:E:27:GLN:HA	2:E:57:ASN:OD1	2.08	0.53
1:B:309:GLU:HG3	2:F:223:ASN:HB3	1.91	0.53
2:E:33:ILE:O	2:E:34:LEU:HB2	2.07	0.53
2:D:400:ASP:O	2:D:404:VAL:HG23	2.09	0.53
3:G:142:GLU:O	3:G:146:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:71:VAL:O	2:D:74:GLU:HG3	2.09	0.53
1:B:278:VAL:O	1:B:281:ARG:HG2	2.08	0.53
3:G:204:ASN:HB3	3:G:207:ARG:HB2	1.90	0.53
1:A:106:LEU:HD11	1:A:259:PHE:HZ	1.74	0.53
6:L:65:CYS:SG	6:M:19:LEU:HD12	2.48	0.53
2:F:258:ILE:HD11	2:F:292:LEU:CD2	2.39	0.53
1:A:212:ARG:HG2	1:A:237:THR:HG21	1.91	0.53
1:B:253:ALA:HB3	1:B:310:ARG:NH2	2.24	0.53
1:B:406:ALA:HB2	1:B:412:LEU:HD11	1.90	0.53
6:N:15:SER:HA	6:O:16:THR:OG1	2.09	0.53
1:C:296:TYR:CD2	1:C:340:ILE:HD11	2.44	0.53
2:E:96:ILE:HB	2:E:218:VAL:HG22	1.90	0.53
1:A:239:SER:HB3	2:D:294:GLU:CG	2.38	0.53
6:N:43:ILE:HG22	6:N:47:VAL:HG23	1.91	0.53
1:B:426:LEU:O	1:B:430:LEU:HG	2.09	0.53
6:M:65:CYS:SG	6:N:19:LEU:HD12	2.49	0.53
2:E:140:VAL:HG22	2:E:414:LEU:HB3	1.91	0.53
1:A:65:ALA:HB2	1:A:75:ILE:HG12	1.91	0.53
1:C:272:ASP:OD2	1:C:274:SER:HB2	2.09	0.52
2:E:168:GLN:NE2	2:E:201:MET:HG2	2.22	0.52
1:C:64:MET:CE	1:C:97:VAL:HG21	2.39	0.52
2:D:234:LEU:HD23	2:D:292:LEU:HD13	1.91	0.52
2:F:400:ASP:O	2:F:404:VAL:HG23	2.08	0.52
2:E:152:LYS:HD2	2:E:152:LYS:N	2.23	0.52
1:C:168:LEU:HA	1:C:327:PRO:HG2	1.92	0.52
1:C:67:ASN:ND2	1:C:287:LEU:HD13	2.25	0.52
2:D:339:ILE:HB	2:D:347:ALA:HB1	1.91	0.52
1:B:302:TYR:HE2	1:B:306:ARG:HH21	1.54	0.52
2:D:252:LEU:HD23	2:D:305:THR:HB	1.90	0.52
1:A:67:ASN:ND2	1:A:287:LEU:HD13	2.24	0.52
3:G:83:LEU:O	3:G:233:ARG:HG3	2.09	0.52
1:C:160:PRO:HG3	1:C:381:GLN:HB2	1.91	0.52
1:C:274:SER:OG	1:C:329:ILE:HG23	2.10	0.52
6:L:47:VAL:HG22	6:M:37:VAL:HG21	1.90	0.52
1:C:302:TYR:O	1:C:306:ARG:HG2	2.09	0.52
2:E:37:LEU:N	2:E:37:LEU:HD12	2.25	0.52
1:A:272:ASP:OD2	1:A:274:SER:HB2	2.10	0.52
2:F:53:HIS:ND1	2:F:59:VAL:HG12	2.25	0.52
1:C:273:LEU:HD23	1:C:304:HIS:ND1	2.25	0.52
1:A:368:ASN:ND2	1:A:371:LEU:HG	2.24	0.52
2:F:19:ALA:O	2:F:20:ILE:HD13	2.10	0.52
1:C:253:ALA:O	1:C:257:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:95:ILE:HD11	2:E:198:TYR:CD1	2.44	0.52
2:E:276:PRO:HB2	3:G:267:LEU:HD21	1.92	0.52
1:C:242:ALA:HB3	1:C:243:PRO:HD3	1.90	0.52
4:H:100:ASN:O	4:H:104:LEU:HG	2.10	0.52
1:C:182:LEU:HD13	1:C:218:LEU:HD11	1.91	0.52
2:E:400:ASP:O	2:E:404:VAL:HG23	2.09	0.52
2:F:348:VAL:O	2:F:350:PRO:HD3	2.10	0.52
1:C:166:ARG:HG2	1:C:348:THR:HA	1.92	0.52
2:F:187:VAL:HG22	2:F:232:VAL:HG13	1.91	0.52
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.40	0.52
2:E:208:ASN:ND2	2:E:211:GLY:H	2.08	0.52
1:B:209:GLY:HA2	1:B:245:GLN:NE2	2.25	0.52
6:N:4:VAL:HA	6:O:6:ALA:HB2	1.92	0.52
1:B:217:GLN:NE2	2:E:131:ALA:CB	2.70	0.52
1:A:159:VAL:CG1	1:A:374:SER:HB2	2.39	0.52
1:C:439:ALA:O	1:C:443:GLN:HG3	2.10	0.52
2:D:229:ARG:NH2	2:D:267:GLU:OE1	2.43	0.52
2:E:404:VAL:O	2:E:408:ARG:HG3	2.10	0.51
6:P:15:SER:HA	6:Q:16:THR:OG1	2.11	0.51
1:C:381:GLN:NE2	1:C:386:LYS:HA	2.25	0.51
1:B:152:LEU:CD1	1:B:180:VAL:HG13	2.38	0.51
3:G:112:ASP:OD1	3:G:115:LYS:HE3	2.11	0.51
1:C:294:GLU:O	1:C:295:ALA:HB3	2.11	0.51
1:A:205:TYR:CE2	1:A:218:LEU:HD13	2.45	0.51
6:P:57:LEU:HD22	6:Q:55:PHE:CZ	2.45	0.51
1:C:260:ARG:O	1:C:321:GLY:HA3	2.10	0.51
6:J:61:THR:HG21	6:K:23:GLY:N	2.25	0.51
3:G:91:LEU:HD11	3:G:165:PHE:HB3	1.93	0.51
2:F:393:MET:HA	2:F:396:LEU:HG	1.93	0.51
1:B:40:ILE:HG12	1:B:41:ALA:N	2.24	0.51
2:D:46:LEU:HD23	2:D:70:LEU:HD21	1.91	0.51
6:P:4:VAL:HA	6:Q:6:ALA:HB2	1.92	0.51
2:D:290:GLY:O	2:D:294:GLU:HG2	2.10	0.51
3:G:188:ILE:HD13	3:G:209:LEU:HD23	1.93	0.51
6:K:47:VAL:CG1	6:L:34:ILE:HG23	2.41	0.51
2:D:358:LEU:O	2:D:358:LEU:HG	2.11	0.51
1:A:139:LEU:HB3	1:A:140:PRO:HD3	1.92	0.51
1:A:99:VAL:HG23	1:A:100:PRO:HD2	1.92	0.51
1:B:143:SER:HB2	2:F:196:ASP:OD1	2.10	0.51
7:A:600:ATP:O2G	7:A:600:ATP:O2B	2.29	0.51
1:B:70:PRO:HD3	2:F:15:ALA:HB2	1.93	0.51
1:B:236:ALA:HA	1:B:240:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:P:43:ILE:HG23	6:P:46:THR:HB	1.93	0.51
3:G:12:SER:O	3:G:16:ILE:HG13	2.10	0.51
6:S:43:ILE:HG23	6:S:46:THR:HB	1.93	0.51
6:S:43:ILE:CG2	6:S:46:THR:HB	2.41	0.51
2:F:442:LYS:O	2:F:446:GLU:HG3	2.11	0.51
2:F:141:VAL:HG11	2:F:147:TYR:CE2	2.45	0.51
2:F:370:VAL:O	2:F:374:VAL:HG23	2.11	0.51
1:A:250:PHE:CD1	1:A:307:LEU:HD13	2.46	0.51
6:Q:65:CYS:SG	6:R:19:LEU:HD12	2.51	0.51
4:H:97:SER:HA	5:I:25:LEU:HA	1.93	0.50
6:Q:43:ILE:HG22	6:Q:47:VAL:HG23	1.94	0.50
1:B:455:LEU:HA	1:B:458:ILE:HD12	1.92	0.50
2:F:148:ALA:HB2	2:F:357:LEU:HD11	1.92	0.50
2:E:133:ILE:HG13	2:E:363:VAL:HG12	1.94	0.50
2:F:67:THR:HB	2:F:70:LEU:HD12	1.93	0.50
1:C:34:LEU:HD11	1:C:44:PHE:HB2	1.92	0.50
1:A:30:THR:HB	1:A:89:LEU:HD11	1.94	0.50
2:F:388:ILE:CD1	2:F:396:LEU:HD11	2.40	0.50
2:E:208:ASN:HD22	2:E:211:GLY:HA3	1.76	0.50
3:G:59:ASN:HD22	3:G:183:PHE:HE1	1.60	0.50
2:D:169:GLU:OE1	2:D:418:PHE:HB3	2.10	0.50
2:F:46:LEU:C	2:F:46:LEU:HD23	2.32	0.50
2:E:96:ILE:O	2:E:218:VAL:HA	2.12	0.50
2:F:54:LEU:HD21	2:F:60:ARG:HE	1.77	0.50
1:A:470:PHE:O	1:A:474:LEU:HD13	2.10	0.50
2:F:140:VAL:HG12	2:F:414:LEU:HB3	1.92	0.50
1:C:77:LEU:HD12	1:C:81:ASP:HB3	1.94	0.50
2:E:167:ILE:HG23	2:E:254:PHE:CE2	2.46	0.50
2:F:33:ILE:HA	2:F:50:VAL:CG1	2.41	0.50
2:E:406:ARG:HH12	2:E:447:GLY:CA	2.24	0.50
1:A:40:ILE:HD13	1:A:287:LEU:CD2	2.42	0.50
2:D:258:ILE:HG13	2:D:258:ILE:O	2.12	0.50
6:O:43:ILE:HG23	6:O:46:THR:HB	1.93	0.50
6:N:43:ILE:CG2	6:N:46:THR:HB	2.41	0.50
3:G:253:ILE:HG22	3:G:257:ARG:NH1	2.26	0.50
1:C:397:ALA:HA	1:C:400:ARG:NH2	2.27	0.50
2:F:324:THR:O	2:F:324:THR:HG22	2.11	0.50
1:A:306:ARG:HG2	1:A:306:ARG:O	2.12	0.50
5:I:48:LYS:CB	5:I:52:ALA:HB3	2.42	0.50
1:A:100:PRO:HD3	1:A:128:ARG:NH1	2.27	0.50
1:B:350:GLY:HA2	1:B:373:VAL:HG13	1.94	0.50
1:A:67:ASN:HD22	1:A:287:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:278:ALA:O	2:F:279:VAL:HB	2.12	0.50
2:F:279:VAL:HG12	2:F:279:VAL:O	2.12	0.50
1:C:53:GLU:OE2	1:C:92:ARG:HD2	2.12	0.50
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.94	0.49
1:A:68:LEU:O	2:E:15:ALA:HA	2.11	0.49
2:F:188:GLY:HA2	2:F:222:MET:N	2.27	0.49
1:C:64:MET:HE2	1:C:97:VAL:HG21	1.94	0.49
2:E:204:THR:HG23	2:E:206:VAL:H	1.76	0.49
2:D:222:MET:HA	2:D:229:ARG:HD3	1.94	0.49
2:D:197:LEU:O	2:D:201:MET:HG2	2.12	0.49
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.95	0.49
2:F:258:ILE:HD11	2:F:292:LEU:HD21	1.94	0.49
2:E:153:ILE:N	2:E:153:ILE:HD12	2.27	0.49
1:B:146:GLU:HB2	1:B:163:ARG:HB2	1.94	0.49
1:A:105:LEU:HD12	1:A:255:ILE:HG23	1.95	0.49
2:E:334:VAL:HG21	2:E:352:ASP:HB3	1.94	0.49
3:G:247:MET:HA	3:G:250:ARG:HE	1.78	0.49
2:D:132:GLU:OE1	2:D:149:ARG:HG2	2.11	0.49
3:G:56:GLU:O	3:G:191:SER:HB3	2.12	0.49
1:A:43:VAL:HG11	1:A:90:VAL:CG1	2.42	0.49
6:S:43:ILE:HG22	6:S:47:VAL:HG23	1.95	0.49
2:D:65:ASP:CG	2:D:66:GLY:H	2.15	0.49
2:E:158:GLY:O	2:E:161:VAL:HG22	2.13	0.49
1:B:382:VAL:HG12	1:B:384:ALA:H	1.77	0.49
2:F:201:MET:HE1	2:F:215:VAL:HG11	1.93	0.49
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.94	0.49
2:D:39:ILE:HG23	2:D:46:LEU:HB3	1.93	0.49
2:E:311:TYR:O	2:E:313:PRO:HD3	2.13	0.49
6:L:40:ASN:HD21	6:L:43:ILE:HG12	1.78	0.49
6:L:15:SER:HA	6:M:16:THR:OG1	2.12	0.49
3:G:262:VAL:O	3:G:266:GLU:HG2	2.13	0.49
1:A:395:PHE:HE2	1:A:451:VAL:HG13	1.78	0.49
1:B:480:GLU:O	1:B:484:GLU:HG2	2.12	0.49
1:A:444:VAL:HG11	1:A:491:LEU:HD11	1.94	0.49
3:G:135:LYS:NZ	5:I:41:ASP:HB2	2.28	0.49
1:C:282:GLN:CD	2:F:284:THR:HG22	2.33	0.49
2:F:287:THR:O	2:F:290:GLY:N	2.46	0.49
1:A:46:LEU:HD13	1:A:49:ILE:HD12	1.95	0.49
3:G:207:ARG:HB3	5:I:4:ARG:HH21	1.78	0.49
1:A:217:GLN:HG2	2:D:356:ARG:NH1	2.27	0.49
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.95	0.49
1:A:142:ARG:HG3	1:A:315:SER:CA	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:24:HIS:ND1	2:F:57:ASN:O	2.46	0.49
2:D:71:VAL:H	2:D:74:GLU:CD	2.16	0.49
2:D:359:ASP:O	2:D:363:VAL:HG22	2.13	0.49
2:D:393:MET:SD	2:D:396:LEU:HD12	2.53	0.49
1:B:170:ILE:HD11	1:B:331:THR:HG21	1.94	0.48
1:A:381:GLN:NE2	1:A:386:LYS:HA	2.27	0.48
4:H:39:ILE:HG13	4:H:50:GLU:OE1	2.12	0.48
2:E:72:ARG:HH11	2:E:72:ARG:HG3	1.78	0.48
2:D:50:VAL:HA	2:D:61:THR:HG22	1.94	0.48
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.94	0.48
1:C:421:VAL:HG13	1:C:425:ARG:NH1	2.28	0.48
1:C:408:PHE:CD2	1:C:410:SER:HB2	2.47	0.48
2:E:185:THR:HG21	2:E:233:ALA:HA	1.96	0.48
2:E:410:ILE:O	2:E:414:LEU:HG	2.13	0.48
1:A:96:ILE:HG21	2:E:68:GLU:OE2	2.13	0.48
1:C:270:TYR:CB	1:C:273:LEU:HD11	2.43	0.48
1:A:411:ASP:O	3:G:29:THR:HG21	2.13	0.48
4:H:108:ALA:O	4:H:112:VAL:HG23	2.13	0.48
1:B:345:ILE:HG23	1:B:351:GLN:CD	2.34	0.48
3:G:118:LEU:HA	3:G:121:THR:HG22	1.95	0.48
1:A:109:VAL:O	1:A:117:ILE:HG12	2.13	0.48
2:F:334:VAL:HG21	2:F:352:ASP:OD2	2.13	0.48
1:C:236:ALA:HA	1:C:240:GLU:OE1	2.14	0.48
1:A:170:ILE:HD12	1:A:345:ILE:HD11	1.95	0.48
2:D:18:GLY:O	2:D:67:THR:HG21	2.12	0.48
1:C:68:LEU:HB3	2:D:72:ARG:HD3	1.95	0.48
1:C:191:TRP:O	1:C:200:LYS:HG2	2.13	0.48
1:C:165:GLN:OE1	1:C:376:VAL:HG21	2.13	0.48
3:G:31:LEU:O	3:G:35:GLU:HG2	2.14	0.48
2:F:225:PRO:HB3	2:F:226:PRO:HD2	1.94	0.48
6:M:47:VAL:CG1	6:N:34:ILE:HG23	2.43	0.48
6:J:47:VAL:HG11	6:K:34:ILE:HG23	1.95	0.48
2:F:157:GLY:HA3	2:F:161:VAL:HG21	1.95	0.48
2:D:169:GLU:HG2	2:D:418:PHE:CD1	2.49	0.48
1:B:169:ILE:HG21	1:B:177:LYS:O	2.13	0.48
1:B:149:GLN:HB2	1:B:191:TRP:HH2	1.79	0.48
2:E:174:ILE:HG13	2:E:252:LEU:HD21	1.96	0.48
2:D:145:ALA:CB	2:D:355:SER:HB2	2.44	0.48
6:Q:43:ILE:CG2	6:Q:46:THR:HB	2.43	0.48
2:F:242:TYR:CZ	2:F:246:GLU:HG2	2.49	0.48
2:F:408:ARG:O	2:F:412:ARG:HG2	2.14	0.47
4:H:69:PHE:HB2	4:H:91:PHE:HD2	1.78	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:266:SER:HA	2:E:282:GLN:OE1	2.13	0.47
3:G:78:THR:HG21	3:G:114:ILE:HB	1.95	0.47
1:B:97:VAL:HG11	1:B:247:LEU:HD21	1.97	0.47
1:B:405:PHE:CZ	2:F:393:MET:SD	3.06	0.47
1:B:300:VAL:HG11	1:B:339:TYR:HE2	1.77	0.47
2:E:427:ILE:HD12	2:E:427:ILE:N	2.29	0.47
2:D:346:PRO:O	2:D:348:VAL:N	2.48	0.47
2:E:39:ILE:HB	2:E:46:LEU:HB3	1.96	0.47
2:E:38:GLU:OE1	2:E:45:LYS:HD2	2.15	0.47
3:G:10:LEU:HG	3:G:14:LYS:HE3	1.96	0.47
2:D:78:ASP:OD1	2:D:80:GLY:N	2.46	0.47
1:C:33:VAL:HG22	1:C:43:VAL:HG22	1.96	0.47
4:H:105:LEU:HB3	4:H:109:LYS:HE3	1.96	0.47
1:B:37:GLY:O	1:B:40:ILE:HG22	2.14	0.47
2:E:168:GLN:HB3	2:E:206:VAL:HG11	1.95	0.47
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.95	0.47
1:B:238:ALA:HA	1:B:245:GLN:NE2	2.30	0.47
1:C:387:GLN:OE1	1:C:491:LEU:HB2	2.14	0.47
6:Q:8:LYS:HD3	6:Q:76:VAL:HG21	1.97	0.47
1:B:273:LEU:HB3	1:B:304:HIS:CD2	2.49	0.47
6:M:8:LYS:HD3	6:M:76:VAL:HG21	1.97	0.47
1:B:57:PHE:CD1	1:B:90:VAL:HG22	2.49	0.47
2:D:133:ILE:HA	2:D:357:LEU:HD13	1.97	0.47
2:D:234:LEU:CD2	2:D:292:LEU:HD13	2.44	0.47
1:A:105:LEU:HD13	1:A:255:ILE:HD13	1.97	0.47
2:F:182:SER:HB2	2:F:215:VAL:HB	1.97	0.47
2:D:255:ILE:HB	2:D:308:GLN:HG2	1.97	0.47
1:A:99:VAL:HG11	1:A:251:THR:HG23	1.96	0.47
2:E:6:SER:C	2:E:8:PRO:HD3	2.35	0.47
1:C:141:ARG:HB2	2:D:195:ASN:CG	2.35	0.47
6:L:61:THR:HG21	6:M:23:GLY:N	2.29	0.47
1:A:478:HIS:HB3	1:A:481:LEU:HD12	1.96	0.47
2:E:432:VAL:HG22	2:E:461:GLY:O	2.14	0.47
2:D:54:LEU:HD11	2:D:60:ARG:HH21	1.79	0.47
1:C:59:SER:OG	1:C:83:LEU:HB3	2.15	0.47
1:C:278:VAL:HG13	1:C:281:ARG:NH2	2.29	0.47
2:F:366:GLU:O	2:F:370:VAL:HG23	2.14	0.47
2:E:402:LEU:HG	2:E:406:ARG:NE	2.29	0.47
6:M:47:VAL:HG11	6:N:34:ILE:HG23	1.97	0.47
4:H:69:PHE:HB3	4:H:91:PHE:HD2	1.80	0.47
1:C:392:LEU:HD13	1:C:451:VAL:HG12	1.97	0.47
6:O:43:ILE:CG2	6:O:46:THR:HB	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:R:8:LYS:HD3	6:R:76:VAL:HG21	1.97	0.47
6:M:43:ILE:CG2	6:M:47:VAL:HG23	2.45	0.47
4:H:101:ILE:HG21	5:I:25:LEU:O	2.15	0.47
1:A:341:PRO:O	1:A:345:ILE:HG13	2.15	0.47
2:E:176:LYS:HZ2	2:E:214:LYS:HE2	1.79	0.47
1:B:99:VAL:HG11	1:B:251:THR:HB	1.97	0.47
2:E:456:ALA:O	2:E:466:VAL:HG13	2.15	0.47
1:A:149:GLN:NE2	1:A:440:THR:OG1	2.42	0.47
6:L:8:LYS:HD3	6:L:76:VAL:HG21	1.97	0.47
1:C:274:SER:O	1:C:278:VAL:HG23	2.15	0.46
2:E:252:LEU:N	2:E:252:LEU:HD12	2.30	0.46
7:A:600:ATP:O2A	7:A:600:ATP:O2B	2.33	0.46
1:B:400:ARG:HH22	2:F:341:GLU:CD	2.17	0.46
6:O:8:LYS:HD3	6:O:76:VAL:HG21	1.97	0.46
2:E:381:TYR:O	2:E:385:GLN:HG2	2.15	0.46
1:A:336:VAL:HG11	1:A:353:PHE:HE2	1.80	0.46
2:F:238:THR:HA	2:F:241:GLU:OE2	2.15	0.46
6:J:15:SER:HA	6:K:16:THR:OG1	2.15	0.46
2:D:196:ASP:O	2:D:200:GLU:HG2	2.15	0.46
6:P:8:LYS:HD3	6:P:76:VAL:HG21	1.97	0.46
2:E:281:TYR:CE2	2:E:321:ALA:HB2	2.51	0.46
6:N:8:LYS:HD3	6:N:76:VAL:HG21	1.97	0.46
2:F:93:GLY:O	2:F:94:ARG:HD2	2.15	0.46
4:H:91:PHE:CE1	4:H:97:SER:HB3	2.51	0.46
2:D:258:ILE:HG21	2:D:310:VAL:HG22	1.96	0.46
1:A:329:ILE:HD11	1:A:344:VAL:HG21	1.96	0.46
6:J:8:LYS:HD3	6:J:76:VAL:HG21	1.96	0.46
2:E:255:ILE:HB	2:E:308:GLN:HB3	1.96	0.46
4:H:91:PHE:HZ	4:H:97:SER:HG	1.60	0.46
1:A:356:ALA:O	1:A:359:PHE:HB3	2.15	0.46
2:E:397:SER:O	2:E:401:LYS:HG2	2.15	0.46
2:F:390:ILE:HD11	3:G:247:MET:HE1	1.96	0.46
2:F:90:GLU:HG2	2:F:110:LYS:O	2.16	0.46
2:F:190:ARG:HB2	2:F:193:GLU:HG3	1.97	0.46
1:B:212:ARG:HB3	2:E:127:GLN:HG3	1.96	0.46
2:E:33:ILE:HG22	2:E:34:LEU:HG	1.97	0.46
1:A:52:GLU:HG2	1:A:66:LEU:HD23	1.98	0.46
2:F:154:GLY:HA3	2:F:329:LEU:HD13	1.98	0.46
2:F:163:LYS:O	2:F:167:ILE:HG13	2.16	0.46
6:O:43:ILE:HG22	6:O:47:VAL:HG23	1.97	0.46
2:D:8:PRO:HB2	2:D:77:LEU:HD11	1.96	0.46
1:B:311:ALA:HB1	1:B:323:LEU:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:K:8:LYS:HD3	6:K:76:VAL:HG21	1.96	0.46
1:B:364:ARG:HA	1:B:365:PRO:C	2.35	0.46
2:D:319:ASP:O	2:D:322:PRO:HD2	2.15	0.46
2:F:257:ASN:HD22	2:F:259:PHE:HB3	1.80	0.46
1:C:62:LYS:NZ	1:C:113:LEU:HD13	2.30	0.46
6:Q:43:ILE:HG23	6:Q:46:THR:HB	1.96	0.46
2:D:50:VAL:HG13	2:D:59:VAL:CG1	2.46	0.46
2:F:37:LEU:O	2:F:47:VAL:HA	2.15	0.46
2:E:402:LEU:HD21	2:E:406:ARG:HH21	1.80	0.46
1:A:506:PHE:HA	1:A:509:THR:HG22	1.97	0.46
2:F:191:THR:HA	2:F:221:GLN:HE21	1.81	0.46
2:E:384:LEU:O	2:E:388:ILE:HG12	2.16	0.46
1:A:43:VAL:HG12	1:A:44:PHE:N	2.31	0.46
2:F:98:VAL:HG21	2:F:228:ALA:HB1	1.98	0.46
2:D:41:THR:HB	2:D:42:PRO:HD2	1.98	0.46
3:G:55:ALA:O	3:G:57:THR:HG23	2.15	0.46
1:B:28:ASN:HB3	1:B:48:ASN:ND2	2.31	0.46
1:A:242:ALA:HB3	1:A:243:PRO:HD3	1.97	0.46
2:F:140:VAL:CG1	2:F:414:LEU:HB3	2.46	0.45
1:B:54:LEU:HD11	1:B:62:LYS:HB3	1.98	0.45
1:A:112:ALA:O	1:A:251:THR:HG21	2.16	0.45
6:O:40:ASN:HD21	6:O:43:ILE:HG12	1.81	0.45
2:E:94:ARG:NH1	2:E:109:ILE:HG12	2.31	0.45
6:S:8:LYS:HD3	6:S:76:VAL:HG21	1.97	0.45
1:C:283:LEU:O	1:C:287:LEU:HG	2.16	0.45
2:F:188:GLY:HA3	2:F:260:ARG:HG3	1.98	0.45
2:D:357:LEU:HD22	2:D:362:VAL:HG11	1.98	0.45
2:F:85:VAL:HG22	2:F:100:GLY:HA3	1.98	0.45
1:A:55:VAL:HA	1:A:93:THR:HG23	1.98	0.45
2:E:256:ASP:HA	2:E:257:ASN:HA	1.58	0.45
2:F:33:ILE:HA	2:F:50:VAL:HG11	1.98	0.45
1:B:133:VAL:O	1:B:310:ARG:HD3	2.15	0.45
1:B:412:LEU:HB3	1:B:416:THR:OG1	2.16	0.45
1:B:105:LEU:HD22	1:B:255:ILE:HG23	1.98	0.45
1:A:284:SER:CB	1:A:297:PRO:HG2	2.47	0.45
6:O:14:ILE:HG21	6:P:14:ILE:HG12	1.98	0.45
1:B:394:LEU:HD11	2:F:425:THR:HG22	1.99	0.45
3:G:205:VAL:HB	3:G:206:PRO:HD3	1.97	0.45
2:D:25:PHE:HB2	2:D:30:LEU:HD23	1.98	0.45
6:M:15:SER:HA	6:N:16:THR:OG1	2.16	0.45
6:O:20:LEU:HB2	6:P:20:LEU:HD22	1.99	0.45
1:B:173:ARG:HH12	2:E:326:PHE:HD2	1.62	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:156:PHE:HB2	2:F:334:VAL:HG22	1.99	0.45
1:A:503:THR:O	1:A:507:VAL:HG23	2.16	0.45
1:B:185:ILE:HG12	1:B:203:CYS:SG	2.56	0.45
2:F:46:LEU:HD23	2:F:47:VAL:N	2.32	0.45
2:F:48:LEU:HD23	2:F:63:ALA:HA	1.99	0.45
3:G:51:PHE:CE1	4:H:49:VAL:HG21	2.52	0.45
2:F:94:ARG:NH2	2:F:102:PRO:HB3	2.32	0.45
1:A:417:LYS:O	1:A:421:VAL:HG23	2.16	0.45
1:C:40:ILE:HD12	1:C:287:LEU:CD2	2.46	0.45
2:F:162:GLY:HA2	9:F:600:ADP:O1A	2.16	0.45
1:A:434:GLN:HB2	7:A:600:ATP:C6	2.52	0.45
6:K:65:CYS:SG	6:L:19:LEU:HD12	2.57	0.45
3:G:75:VAL:HB	3:G:164:ILE:CD1	2.47	0.45
2:E:47:VAL:HG21	2:E:99:ILE:HD12	1.98	0.45
6:O:7:ALA:HB1	6:P:10:ILE:HG13	1.99	0.45
1:C:168:LEU:HD11	1:C:329:ILE:HG13	1.99	0.45
1:B:215:VAL:O	1:B:219:VAL:HG23	2.17	0.45
2:F:140:VAL:CG2	2:F:348:VAL:HG21	2.45	0.45
1:C:111:ASP:O	1:C:112:ALA:C	2.55	0.45
1:C:216:ALA:O	1:C:219:VAL:HG22	2.17	0.45
1:B:196:ASP:OD2	1:B:199:LYS:HG2	2.17	0.45
6:N:26:ILE:HD13	6:N:55:PHE:CE1	2.52	0.45
4:H:91:PHE:HE1	4:H:97:SER:N	2.14	0.45
6:O:26:ILE:HD13	6:O:55:PHE:CE1	2.52	0.45
1:B:66:LEU:HD11	1:B:67:ASN:HD22	1.81	0.45
2:D:165:VAL:HG11	2:D:421:ALA:HB2	1.99	0.45
1:B:82:ARG:HA	2:E:33:ILE:HB	1.99	0.45
1:A:242:ALA:N	1:A:243:PRO:CD	2.80	0.45
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	0.45
2:F:123:SER:HB2	2:F:126:GLU:HG3	1.99	0.45
1:B:285:LEU:HD12	2:E:283:PRO:HB3	1.99	0.45
2:D:164:THR:O	2:D:167:ILE:HG22	2.17	0.45
1:A:402:VAL:HG12	1:A:402:VAL:O	2.16	0.45
1:B:28:ASN:HB3	1:B:48:ASN:HD22	1.82	0.45
1:B:455:LEU:HD23	1:B:458:ILE:HD12	1.98	0.45
1:C:136:PRO:HB2	1:C:141:ARG:HE	1.82	0.45
1:A:305:SER:HA	1:A:347:ILE:HD13	1.99	0.45
1:A:106:LEU:HD11	1:A:259:PHE:CZ	2.51	0.44
2:F:384:LEU:O	2:F:388:ILE:HG12	2.17	0.44
1:B:351:GLN:H	1:B:373:VAL:CG1	2.30	0.44
1:A:67:ASN:HD21	1:A:287:LEU:HD13	1.82	0.44
1:A:96:ILE:HG22	1:A:97:VAL:N	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:176:GLY:HA2	7:B:600:ATP:O1A	2.17	0.44
1:B:279:ALA:O	1:B:282:GLN:HB3	2.17	0.44
1:C:240:GLU:HB3	1:C:244:LEU:CD1	2.46	0.44
2:D:163:LYS:HZ3	2:D:311:TYR:HA	1.81	0.44
6:L:26:ILE:HD13	6:L:55:PHE:CE1	2.52	0.44
2:E:287:THR:O	2:E:291:LEU:HG	2.16	0.44
2:E:65:ASP:CG	2:E:66:GLY:H	2.21	0.44
2:D:141:VAL:HG11	2:D:147:TYR:CE2	2.52	0.44
2:F:204:THR:OG1	2:F:206:VAL:HG23	2.16	0.44
1:C:116:PRO:HB3	1:C:123:ILE:HD11	1.98	0.44
2:F:256:ASP:HA	2:F:257:ASN:HA	1.59	0.44
3:G:108:VAL:CG1	3:G:128:LEU:HB3	2.45	0.44
6:M:26:ILE:HD13	6:M:55:PHE:CE1	2.53	0.44
1:A:212:ARG:CB	2:D:127:GLN:HE21	2.29	0.44
6:S:26:ILE:HD13	6:S:55:PHE:CE1	2.53	0.44
6:Q:26:ILE:HD13	6:Q:55:PHE:CE1	2.52	0.44
2:E:462:GLY:O	2:E:466:VAL:HG23	2.18	0.44
3:G:75:VAL:HB	3:G:164:ILE:HD13	1.98	0.44
1:C:492:SER:H	1:C:495:LEU:HD12	1.81	0.44
6:K:26:ILE:HD13	6:K:55:PHE:CE1	2.53	0.44
1:B:54:LEU:HD13	1:B:97:VAL:HG22	2.00	0.44
4:H:113:SER:HA	4:H:120:ALA:HB1	2.00	0.44
2:D:377:THR:HG22	2:D:407:ALA:HB2	2.00	0.44
3:G:38:LYS:HE2	3:G:224:GLN:HG3	1.98	0.44
2:E:32:ALA:O	2:E:50:VAL:HG11	2.17	0.44
6:R:26:ILE:HD13	6:R:55:PHE:CE1	2.53	0.44
6:P:26:ILE:HD13	6:P:55:PHE:CE1	2.53	0.44
1:B:133:VAL:HB	1:B:310:ARG:HH11	1.83	0.44
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.82	0.44
3:G:254:LEU:HG	3:G:257:ARG:HH22	1.81	0.44
2:D:431:LEU:HD23	2:D:431:LEU:C	2.38	0.44
1:B:440:THR:O	1:B:444:VAL:HG23	2.18	0.44
1:A:99:VAL:CG2	1:A:100:PRO:HD2	2.48	0.44
1:A:272:ASP:HB2	1:A:328:VAL:O	2.17	0.44
1:A:139:LEU:HD23	2:E:105:GLU:OE2	2.17	0.44
1:B:362:GLY:O	1:B:364:ARG:HG3	2.17	0.44
3:G:59:ASN:ND2	3:G:183:PHE:HE1	2.16	0.44
6:J:43:ILE:CG2	6:J:46:THR:HB	2.47	0.44
1:B:168:LEU:HD11	1:B:329:ILE:HG12	2.00	0.44
6:N:53:LEU:O	6:N:57:LEU:HG	2.18	0.44
3:G:50:LEU:HD23	4:H:84:CYS:SG	2.57	0.44
6:M:57:LEU:HD22	6:N:55:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:166:ARG:O	1:C:166:ARG:HG2	2.18	0.44
6:L:47:VAL:HG11	6:M:34:ILE:HG23	2.00	0.44
1:A:67:ASN:OD1	2:E:17:ILE:HG23	2.17	0.44
1:A:205:TYR:CE2	1:A:218:LEU:CD1	3.01	0.44
2:F:391:LEU:HD13	2:F:395:GLU:HG3	2.00	0.44
2:F:65:ASP:CG	2:F:66:GLY:H	2.21	0.44
6:M:64:PHE:O	6:M:68:VAL:HG23	2.18	0.44
3:G:187:THR:O	3:G:187:THR:HG22	2.18	0.44
2:E:244:ARG:O	2:E:248:GLY:HA2	2.17	0.43
6:M:53:LEU:O	6:M:57:LEU:HG	2.18	0.43
6:Q:53:LEU:O	6:Q:57:LEU:HG	2.18	0.43
1:B:247:LEU:HG	1:B:251:THR:HG23	2.00	0.43
6:K:53:LEU:O	6:K:57:LEU:HG	2.18	0.43
6:R:53:LEU:O	6:R:57:LEU:HG	2.18	0.43
1:A:67:ASN:HD21	1:A:287:LEU:HB3	1.83	0.43
1:B:314:LEU:HB3	1:B:318:GLU:HB2	1.99	0.43
6:R:29:VAL:CG2	6:S:27:ALA:HA	2.48	0.43
3:G:71:LYS:HE3	3:G:159:TYR:HA	2.00	0.43
6:J:64:PHE:O	6:J:68:VAL:HG23	2.18	0.43
2:E:77:LEU:HD12	2:E:78:ASP:H	1.83	0.43
1:B:260:ARG:O	1:B:321:GLY:HA3	2.18	0.43
1:A:197:GLU:C	1:A:199:LYS:H	2.20	0.43
4:H:58:GLU:HB2	4:H:67:LYS:HG3	2.00	0.43
1:C:284:SER:OG	1:C:297:PRO:HG3	2.18	0.43
2:E:201:MET:HA	2:E:204:THR:HG22	2.00	0.43
2:F:33:ILE:HG22	2:F:34:LEU:N	2.33	0.43
1:C:388:VAL:O	1:C:451:VAL:HG21	2.18	0.43
6:L:57:LEU:HD22	6:M:55:PHE:CE1	2.53	0.43
6:N:20:LEU:HB2	6:O:20:LEU:HD22	1.98	0.43
6:K:64:PHE:O	6:K:68:VAL:HG23	2.18	0.43
1:C:311:ALA:HB1	1:C:323:LEU:O	2.18	0.43
2:F:145:ALA:HB1	2:F:355:SER:HB3	2.00	0.43
1:C:187:ASN:O	1:C:190:ARG:HG3	2.17	0.43
6:J:26:ILE:HD13	6:J:55:PHE:CE1	2.53	0.43
2:E:282:GLN:NE2	2:E:285:LEU:HD13	2.33	0.43
1:C:305:SER:HA	1:C:347:ILE:HD13	2.01	0.43
4:H:109:LYS:HD2	4:H:126:GLN:OE1	2.18	0.43
2:F:117:ILE:HA	2:F:238:THR:OG1	2.18	0.43
2:E:94:ARG:CZ	2:E:109:ILE:HG12	2.48	0.43
1:A:316:GLU:HA	1:A:320:SER:OG	2.19	0.43
3:G:99:LEU:HD21	3:G:122:HIS:CG	2.52	0.43
2:E:188:GLY:O	2:E:222:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:384:ALA:HB2	1:C:489:GLY:O	2.18	0.43
4:H:10:LEU:C	4:H:10:LEU:HD23	2.39	0.43
2:E:228:ALA:O	2:E:232:VAL:HG23	2.17	0.43
1:A:260:ARG:O	1:A:321:GLY:HA3	2.18	0.43
6:O:53:LEU:O	6:O:57:LEU:HG	2.18	0.43
4:H:123:ALA:O	4:H:127:VAL:HG23	2.19	0.43
6:N:64:PHE:O	6:N:68:VAL:HG23	2.18	0.43
2:D:64:MET:CE	2:D:83:ILE:HD11	2.49	0.43
2:D:117:ILE:HA	2:D:238:THR:OG1	2.19	0.43
2:E:388:ILE:HD12	2:E:393:MET:HA	2.00	0.43
2:F:167:ILE:HD11	2:F:309:ALA:HB2	2.00	0.43
6:S:53:LEU:O	6:S:57:LEU:HG	2.18	0.43
1:C:166:ARG:HD2	1:C:166:ARG:N	2.29	0.43
6:N:59:GLU:O	6:N:63:LEU:HG	2.19	0.43
6:J:59:GLU:O	6:J:63:LEU:HG	2.19	0.43
6:R:64:PHE:O	6:R:68:VAL:HG23	2.18	0.43
4:H:31:ASN:O	4:H:57:VAL:HA	2.19	0.43
1:B:369:VAL:HG21	1:B:396:LEU:HD13	2.01	0.43
6:M:59:GLU:O	6:M:63:LEU:HG	2.19	0.43
1:B:467:GLU:O	1:B:471:LEU:HG	2.18	0.43
1:C:55:VAL:HG21	1:C:75:ILE:HD13	2.01	0.43
4:H:10:LEU:HG	4:H:81:SER:O	2.19	0.43
2:E:204:THR:OG1	2:E:420:VAL:HB	2.19	0.43
3:G:23:MET:HG2	3:G:237:MET:HE2	1.99	0.43
2:D:404:VAL:O	2:D:408:ARG:HG3	2.19	0.43
3:G:57:THR:HG22	3:G:191:SER:OG	2.18	0.43
1:C:242:ALA:N	1:C:243:PRO:CD	2.81	0.43
6:P:53:LEU:O	6:P:57:LEU:HG	2.18	0.43
1:A:97:VAL:HG11	1:A:247:LEU:HD13	1.98	0.43
1:B:136:PRO:HG2	1:B:141:ARG:HH21	1.84	0.43
2:E:377:THR:HG22	2:E:407:ALA:HB2	2.00	0.43
6:Q:64:PHE:O	6:Q:68:VAL:HG23	2.18	0.43
6:R:59:GLU:O	6:R:63:LEU:HG	2.19	0.43
6:S:64:PHE:O	6:S:68:VAL:HG23	2.18	0.43
2:F:30:LEU:N	2:F:30:LEU:HD12	2.34	0.43
1:C:392:LEU:O	1:C:396:LEU:CD1	2.67	0.43
2:D:257:ASN:HD22	2:D:259:PHE:HB3	1.79	0.43
6:Q:40:ASN:ND2	6:Q:43:ILE:HG12	2.32	0.43
1:B:81:ASP:O	2:E:33:ILE:HD12	2.19	0.43
2:D:241:GLU:OE2	2:D:295:ARG:HB3	2.18	0.43
1:B:392:LEU:O	1:B:396:LEU:HG	2.18	0.43
6:O:64:PHE:O	6:O:68:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:ALA:HA	1:A:245:GLN:NE2	2.34	0.43
2:E:472:LYS:O	2:E:476:GLU:HG3	2.19	0.43
6:K:59:GLU:O	6:K:63:LEU:HG	2.19	0.43
6:L:59:GLU:O	6:L:63:LEU:HG	2.19	0.43
6:L:64:PHE:O	6:L:68:VAL:HG23	2.18	0.43
2:E:380:THR:O	2:E:384:LEU:HG	2.18	0.43
4:H:69:PHE:CE2	4:H:133:LEU:HD23	2.54	0.43
3:G:212:TYR:CE2	3:G:216:ASN:ND2	2.86	0.43
3:G:168:ASP:HA	3:G:169:PRO:HD2	1.90	0.43
4:H:132:ASN:O	4:H:136:VAL:HG23	2.18	0.43
6:P:64:PHE:O	6:P:68:VAL:HG23	2.18	0.43
2:F:155:LEU:HD23	2:F:333:THR:HB	2.01	0.43
2:E:396:LEU:HD13	2:E:404:VAL:HG21	1.99	0.43
3:G:77:ILE:HD12	3:G:222:MET:HG2	2.01	0.43
1:A:368:ASN:HD22	1:A:371:LEU:HB2	1.84	0.43
2:E:30:LEU:HD12	2:E:30:LEU:H	1.84	0.43
6:K:47:VAL:HG11	6:L:34:ILE:HG23	2.01	0.43
1:C:408:PHE:HD2	1:C:410:SER:HB2	1.82	0.43
3:G:149:LYS:O	3:G:153:VAL:HG12	2.18	0.43
1:A:136:PRO:HB2	1:A:141:ARG:HE	1.84	0.43
6:J:53:LEU:O	6:J:57:LEU:HG	2.18	0.43
6:P:59:GLU:O	6:P:63:LEU:HG	2.19	0.43
1:A:142:ARG:CG	1:A:315:SER:HA	2.34	0.42
1:A:103:PRO:HA	1:A:106:LEU:HD13	2.01	0.42
4:H:102:LYS:HZ3	4:H:133:LEU:HB3	1.83	0.42
6:L:53:LEU:O	6:L:57:LEU:HG	2.18	0.42
4:H:112:VAL:HB	4:H:123:ALA:HB2	1.99	0.42
3:G:118:LEU:HD12	3:G:118:LEU:N	2.34	0.42
3:G:150:LEU:O	3:G:154:MET:HB2	2.19	0.42
3:G:74:ILE:HB	3:G:107:ILE:HG12	2.01	0.42
2:D:427:ILE:HG23	2:D:428:PRO:HD2	2.01	0.42
1:C:30:THR:HA	1:C:90:VAL:O	2.19	0.42
6:N:4:VAL:CG2	6:O:5:LEU:HD23	2.13	0.42
1:A:55:VAL:HG21	1:A:75:ILE:HD13	2.00	0.42
1:A:271:ASP:HA	1:A:272:ASP:HA	1.75	0.42
1:A:46:LEU:O	1:A:49:ILE:HG22	2.19	0.42
1:B:336:VAL:HG23	2:F:337:ARG:HH11	1.84	0.42
1:C:146:GLU:HB2	1:C:163:ARG:HB2	2.01	0.42
2:F:84:SER:HA	2:F:116:PRO:HA	2.00	0.42
1:C:354:LEU:HD23	1:C:367:ILE:HA	2.01	0.42
3:G:72:GLU:HG3	3:G:161:LYS:O	2.19	0.42
1:C:153:LYS:HG2	1:C:443:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:39:ILE:HG22	4:H:40:GLY:N	2.34	0.42
1:B:365:PRO:HB2	1:B:367:ILE:HG13	2.00	0.42
2:D:369:ASP:O	2:D:373:LYS:HG3	2.18	0.42
1:B:34:LEU:HD11	1:B:44:PHE:HB2	2.00	0.42
6:O:59:GLU:O	6:O:63:LEU:HG	2.19	0.42
1:B:375:ARG:NH1	2:F:190:ARG:CZ	2.83	0.42
2:E:345:TYR:HA	2:E:346:PRO:C	2.40	0.42
2:D:345:TYR:HA	2:D:346:PRO:C	2.40	0.42
1:A:205:TYR:HB3	1:A:233:ILE:HD13	2.01	0.42
2:E:6:SER:C	2:E:8:PRO:CD	2.88	0.42
6:M:61:THR:HG21	6:N:23:GLY:N	2.34	0.42
3:G:209:LEU:HA	4:H:74:PHE:CE2	2.54	0.42
1:B:141:ARG:NH1	2:F:191:THR:HB	2.35	0.42
1:B:98:ASP:OD2	1:B:128:ARG:HB3	2.20	0.42
6:S:59:GLU:O	6:S:63:LEU:HG	2.19	0.42
2:F:121:PRO:HA	2:F:122:PRO:HD3	1.88	0.42
2:D:271:LEU:HD12	2:D:271:LEU:N	2.34	0.42
1:A:260:ARG:HH11	1:A:314:LEU:HD11	1.84	0.42
1:C:283:LEU:N	1:C:283:LEU:HD12	2.35	0.42
2:F:140:VAL:HG21	2:F:348:VAL:CG2	2.48	0.42
2:D:256:ASP:HA	2:D:257:ASN:HA	1.62	0.42
4:H:16:LEU:HB3	4:H:17:PRO:HD2	2.00	0.42
1:C:118:ASP:OD1	1:C:120:LYS:HG3	2.19	0.42
1:A:174:GLN:HB3	2:D:354:LYS:HD2	2.02	0.42
1:C:273:LEU:N	1:C:273:LEU:CD1	2.82	0.42
3:G:23:MET:HG2	3:G:237:MET:CE	2.49	0.42
2:E:30:LEU:N	2:E:30:LEU:HD12	2.34	0.42
2:F:359:ASP:OD2	2:F:361:ALA:HB3	2.20	0.42
6:Q:59:GLU:O	6:Q:63:LEU:HG	2.19	0.42
1:C:193:ASN:ND2	1:C:229:LYS:NZ	2.68	0.42
2:D:333:THR:O	2:D:333:THR:HG22	2.19	0.42
1:A:405:PHE:O	1:A:412:LEU:HD11	2.19	0.42
2:F:339:ILE:HB	2:F:347:ALA:HB1	2.01	0.42
2:E:282:GLN:NE2	2:E:285:LEU:HB2	2.35	0.42
4:H:109:LYS:NZ	4:H:130:LEU:HD11	2.35	0.42
1:B:399:TYR:CE1	1:B:423:GLY:HA3	2.54	0.42
1:C:116:PRO:HD3	1:C:123:ILE:CG1	2.35	0.42
6:P:43:ILE:CG2	6:P:46:THR:HB	2.49	0.42
2:F:220:GLY:HA3	2:F:232:VAL:HG21	2.02	0.42
2:E:351:LEU:CD1	2:E:382:LYS:HD2	2.50	0.42
1:B:208:VAL:O	1:B:208:VAL:HG23	2.20	0.42
2:D:268:VAL:O	2:D:272:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:33:ILE:HG22	2:D:34:LEU:HG	2.02	0.42
1:C:40:ILE:HG13	1:C:286:LEU:HB3	2.01	0.41
1:C:166:ARG:HA	1:C:325:ALA:O	2.19	0.41
1:B:100:PRO:HB3	1:B:125:ALA:HB2	2.02	0.41
2:D:94:ARG:HH21	2:D:106:ARG:HB2	1.85	0.41
1:B:47:ASN:HA	2:F:72:ARG:NH2	2.35	0.41
2:E:9:ILE:HB	2:E:78:ASP:HB3	2.02	0.41
1:A:38:ASP:HB3	1:A:286:LEU:HD22	2.01	0.41
5:I:31:THR:HG23	5:I:33:SER:HB3	2.02	0.41
2:E:258:ILE:O	2:E:258:ILE:HG13	2.20	0.41
2:F:412:ARG:HG2	2:F:412:ARG:HH11	1.85	0.41
6:M:43:ILE:CG2	6:M:46:THR:HB	2.48	0.41
1:A:266:ALA:O	1:A:323:LEU:HD12	2.20	0.41
1:B:375:ARG:HG2	9:F:600:ADP:H5'1	2.02	0.41
6:L:43:ILE:CG2	6:L:46:THR:HB	2.49	0.41
1:A:28:ASN:HB3	1:A:48:ASN:HD22	1.81	0.41
4:H:117:ALA:HA	4:H:120:ALA:HB3	2.02	0.41
4:H:35:LYS:HD2	4:H:53:LEU:HD11	2.01	0.41
2:D:269:SER:HB2	2:D:274:ARG:HD2	2.02	0.41
2:E:279:VAL:H	3:G:264:THR:HG1	1.63	0.41
2:E:227:GLY:O	2:E:231:ARG:HG2	2.20	0.41
6:J:6:ALA:HB2	6:S:4:VAL:HA	2.01	0.41
4:H:112:VAL:O	4:H:120:ALA:HB2	2.19	0.41
2:F:174:ILE:O	2:F:178:HIS:HB2	2.20	0.41
1:A:46:LEU:HB3	1:A:49:ILE:HB	2.02	0.41
1:A:343:ASN:O	1:A:347:ILE:HG13	2.20	0.41
3:G:72:GLU:HB3	3:G:105:ALA:CB	2.50	0.41
1:B:142:ARG:HA	2:F:195:ASN:HD21	1.85	0.41
1:B:159:VAL:HG12	1:B:374:SER:HB2	2.02	0.41
6:J:19:LEU:HD12	6:S:65:CYS:SG	2.60	0.41
2:D:15:ALA:HB3	2:D:22:ASP:HB2	2.02	0.41
2:F:207:ILE:HD11	2:F:215:VAL:HG13	2.03	0.41
2:D:171:ILE:HG12	2:D:254:PHE:CZ	2.56	0.41
6:N:47:VAL:CG1	6:O:34:ILE:HG23	2.50	0.41
3:G:30:ARG:HB3	3:G:230:ILE:HD13	2.01	0.41
1:A:152:LEU:HD11	1:A:180:VAL:HA	2.01	0.41
1:C:36:VAL:HG21	1:C:84:VAL:HB	2.03	0.41
2:F:460:VAL:HG21	2:F:466:VAL:HG22	2.03	0.41
2:E:244:ARG:HG3	2:E:303:SER:N	2.35	0.41
2:F:220:GLY:CA	2:F:232:VAL:HG21	2.51	0.41
2:E:276:PRO:CB	3:G:267:LEU:HD21	2.51	0.41
1:A:250:PHE:HZ	1:A:303:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:254:LEU:HG	3:G:257:ARG:NH2	2.35	0.41
2:D:241:GLU:O	2:D:244:ARG:HB3	2.20	0.41
2:D:33:ILE:HG22	2:D:34:LEU:N	2.35	0.41
1:B:338:ALA:O	1:B:342:THR:HG23	2.20	0.41
1:A:64:MET:O	1:A:76:VAL:HG22	2.19	0.41
2:E:7:THR:N	2:E:8:PRO:CD	2.83	0.41
2:D:384:LEU:HD22	2:D:387:ILE:HD12	2.03	0.41
3:G:151:LEU:HD23	3:G:156:ALA:HB3	2.02	0.41
1:C:300:VAL:O	1:C:303:LEU:HB3	2.21	0.41
1:B:413:ASP:OD2	1:B:415:SER:HB3	2.21	0.41
1:B:376:VAL:HG11	2:F:192:ARG:NH1	2.35	0.41
1:C:184:THR:O	1:C:188:GLN:HG2	2.20	0.41
2:D:148:ALA:HA	2:D:357:LEU:HD11	2.03	0.41
1:A:381:GLN:HE21	1:A:386:LYS:HA	1.84	0.41
1:A:243:PRO:O	1:A:246:TYR:HB3	2.20	0.41
6:N:29:VAL:CG2	6:O:27:ALA:HA	2.51	0.41
2:D:161:VAL:CG1	2:D:335:LEU:HB3	2.51	0.41
1:A:203:CYS:O	1:A:231:SER:HA	2.21	0.41
2:F:133:ILE:HD13	2:F:363:VAL:HG12	2.03	0.41
1:A:460:LEU:O	1:A:460:LEU:HG	2.21	0.41
1:B:152:LEU:HD12	1:B:155:VAL:HG21	2.03	0.41
2:F:95:ILE:O	2:F:103:ILE:HG12	2.21	0.41
2:D:145:ALA:CA	2:D:355:SER:HB2	2.51	0.41
1:A:353:PHE:HE1	1:A:355:GLU:HG2	1.86	0.41
1:B:271:ASP:HA	1:B:272:ASP:HA	1.79	0.41
1:C:105:LEU:N	1:C:105:LEU:HD12	2.35	0.41
1:A:352:ILE:O	1:A:352:ILE:HG22	2.20	0.41
2:F:244:ARG:O	2:F:248:GLY:HA2	2.21	0.41
1:A:68:LEU:HD12	2:E:16:VAL:HB	2.03	0.41
1:A:294:GLU:O	1:A:295:ALA:HB3	2.20	0.41
2:D:53:HIS:CD2	2:D:59:VAL:HG22	2.56	0.41
6:Q:52:ILE:O	6:Q:55:PHE:HB3	2.21	0.41
1:C:260:ARG:HH11	1:C:314:LEU:HD11	1.86	0.41
2:E:167:ILE:HG23	2:E:254:PHE:CD2	2.56	0.41
6:K:33:LEU:O	6:K:37:VAL:HG22	2.21	0.41
1:B:85:LYS:HG2	1:B:86:GLU:N	2.36	0.41
1:C:32:ARG:HA	1:C:88:GLU:O	2.21	0.41
2:F:440:SER:O	2:F:444:VAL:HG23	2.21	0.41
1:B:385:LEU:HD22	1:B:447:ILE:HD12	2.02	0.41
1:C:270:TYR:O	1:C:328:VAL:HG23	2.20	0.41
2:F:106:ARG:HH21	2:F:209:LEU:HB3	1.85	0.41
1:A:50:GLN:HG2	2:E:71:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:GLN:HG2	1:A:166:ARG:N	2.36	0.41
6:O:52:ILE:O	6:O:55:PHE:HB3	2.21	0.41
6:P:52:ILE:O	6:P:55:PHE:HB3	2.21	0.41
1:A:185:ILE:HG12	1:A:203:CYS:SG	2.60	0.41
2:F:35:ASN:O	2:F:49:GLU:HA	2.21	0.41
1:A:26:ASN:O	1:A:27:LEU:HB3	2.21	0.41
1:B:166:ARG:HD2	1:B:308:LEU:HB3	2.02	0.41
1:A:332:GLN:HB3	2:D:318:THR:HB	2.03	0.41
2:E:289:MET:HG2	2:E:324:THR:HG22	2.02	0.41
2:D:277:SER:OG	2:D:278:ALA:N	2.55	0.41
6:O:4:VAL:HG23	6:P:6:ALA:HA	2.03	0.40
2:E:187:VAL:HG22	2:E:232:VAL:HB	2.02	0.40
2:F:95:ILE:HA	2:F:217:LEU:O	2.21	0.40
2:E:150:GLY:HA2	2:E:304:VAL:O	2.20	0.40
6:N:52:ILE:O	6:N:55:PHE:HB3	2.21	0.40
6:M:52:ILE:O	6:M:55:PHE:HB3	2.21	0.40
1:C:301:PHE:CE1	1:C:305:SER:HB3	2.56	0.40
1:A:52:GLU:OE1	2:E:68:GLU:HB2	2.21	0.40
1:B:105:LEU:N	1:B:105:LEU:HD12	2.35	0.40
2:D:338:GLY:O	2:D:342:LEU:HD13	2.22	0.40
2:F:300:LYS:HE3	2:F:300:LYS:HB2	1.90	0.40
3:G:77:ILE:HD13	3:G:110:ILE:HD12	2.03	0.40
2:F:97:ASN:HB2	2:F:103:ILE:CG2	2.51	0.40
2:D:254:PHE:HD1	2:D:307:VAL:HB	1.86	0.40
2:D:37:LEU:HB2	2:D:48:LEU:HB2	2.03	0.40
2:D:201:MET:CE	2:D:215:VAL:HG11	2.51	0.40
1:C:206:VAL:HG12	1:C:208:VAL:HG23	2.03	0.40
1:C:357:GLU:HG2	1:C:361:LYS:HE3	2.03	0.40
1:B:242:ALA:N	1:B:243:PRO:CD	2.85	0.40
1:B:99:VAL:HA	1:B:100:PRO:HD3	1.98	0.40
1:A:67:ASN:ND2	1:A:287:LEU:HB3	2.35	0.40
4:H:70:ILE:HD11	4:H:87:ALA:HB2	2.02	0.40
2:E:391:LEU:HB2	2:E:395:GLU:HG3	2.02	0.40
3:G:133:ILE:HG21	3:G:222:MET:CE	2.52	0.40
2:D:160:GLY:N	9:D:600:ADP:O3B	2.54	0.40
2:F:293:GLN:HE22	2:F:308:GLN:NE2	2.16	0.40
1:B:161:ILE:HD13	1:B:326:LEU:HD21	2.04	0.40
1:C:70:PRO:HA	2:D:72:ARG:NH2	2.36	0.40
3:G:184:ASN:O	3:G:188:ILE:HG13	2.20	0.40
2:E:348:VAL:O	2:E:350:PRO:HD3	2.21	0.40
1:A:192:ASN:OD1	1:A:200:LYS:HB3	2.22	0.40
1:B:170:ILE:HG23	1:B:353:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:396:LEU:O	1:B:399:TYR:HB3	2.21	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	483/510 (95%)	445 (92%)	34 (7%)	4 (1%)	27	81
1	B	483/510 (95%)	447 (92%)	35 (7%)	1 (0%)	56	94
1	C	483/510 (95%)	451 (93%)	32 (7%)	0	100	100
2	D	468/478 (98%)	443 (95%)	22 (5%)	3 (1%)	33	85
2	E	471/478 (98%)	436 (93%)	32 (7%)	3 (1%)	33	85
2	F	470/478 (98%)	438 (93%)	30 (6%)	2 (0%)	43	90
3	G	265/278 (95%)	246 (93%)	18 (7%)	1 (0%)	43	90
4	H	130/138 (94%)	115 (88%)	11 (8%)	4 (3%)	7	51
5	I	57/61 (93%)	48 (84%)	9 (16%)	0	100	100
6	J	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
6	K	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	L	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	M	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	N	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
6	O	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	P	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	Q	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	R	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	S	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	4050/4201 (96%)	3760 (93%)	272 (7%)	18 (0%)	43	90

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	72	ARG
2	D	279	VAL
2	E	32	ALA
2	E	279	VAL
2	F	279	VAL
4	H	93	LEU
1	A	348	THR
1	A	363	ILE
1	B	363	ILE
1	A	368	ASN
4	H	43	ALA
2	D	347	ALA
4	H	54	PRO
3	G	135	LYS
2	F	158	GLY
2	E	44	GLY
1	A	97	VAL
4	H	92	PRO

### 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	391/412 (95%)	390 (100%)	1 (0%)	96	99
1	B	390/412 (95%)	390 (100%)	0	100	100
1	C	391/412 (95%)	390 (100%)	1 (0%)	96	99
2	D	380/384 (99%)	379 (100%)	1 (0%)	96	99
2	E	382/384 (100%)	380 (100%)	2 (0%)	94	98
2	F	381/384 (99%)	381 (100%)	0	100	100
3	G	230/236 (98%)	230 (100%)	0	100	100
4	H	111/112 (99%)	110 (99%)	1 (1%)	87	97
5	I	25/48 (52%)	25 (100%)	0	100	100
6	J	56/56 (100%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	56/56 (100%)	56 (100%)	0	100	100
6	L	56/56 (100%)	56 (100%)	0	100	100
6	M	56/56 (100%)	56 (100%)	0	100	100
6	N	56/56 (100%)	56 (100%)	0	100	100
6	O	56/56 (100%)	56 (100%)	0	100	100
6	P	56/56 (100%)	56 (100%)	0	100	100
6	Q	56/56 (100%)	56 (100%)	0	100	100
6	R	56/56 (100%)	56 (100%)	0	100	100
6	S	56/56 (100%)	56 (100%)	0	100	100
All	All	3241/3344 (97%)	3235 (100%)	6 (0%)	96	99

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASP
1	C	166	ARG
2	D	315	ASP
2	E	120	ASP
2	E	316	ASP
4	H	32	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	72	GLN
1	A	149	GLN
1	A	245	GLN
1	A	262	ASN
1	A	351	GLN
1	A	368	ASN
1	A	381	GLN
1	B	26	ASN
1	B	28	ASN
1	B	48	ASN
1	B	174	GLN
1	B	192	ASN
1	B	217	GLN

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Mol	Chain	Res	Type
1	B	245	GLN
1	B	276	GLN
1	B	343	ASN
1	B	398	GLN
1	B	477	ASN
1	B	478	HIS
1	C	193	ASN
1	C	225	HIS
1	C	245	GLN
1	C	262	ASN
1	C	343	ASN
1	C	368	ASN
1	C	381	GLN
2	D	52	GLN
2	D	249	GLN
2	D	257	ASN
2	D	308	GLN
2	E	52	GLN
2	E	118	HIS
2	E	127	GLN
2	E	168	GLN
2	E	208	ASN
2	E	308	GLN
2	F	35	ASN
2	F	52	GLN
2	F	118	HIS
2	F	178	HIS
2	F	195	ASN
2	F	257	ASN
2	F	293	GLN
3	G	49	GLN
3	G	59	ASN
3	G	117	GLN
3	G	125	ASN
3	G	204	ASN
3	G	224	GLN
3	G	243	ASN
3	G	260	GLN
4	H	78	GLN
4	H	82	GLN
4	H	111	ASN
6	K	40	ASN

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Mol	Chain	Res	Type
6	L	40	ASN
6	M	40	ASN
6	N	40	ASN
6	O	40	ASN
6	P	40	ASN
6	Q	40	ASN
6	R	40	ASN
6	S	40	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ATP	A	600	8	33,33,33	0.99	2 (6%)	52,52,52	1.82	9 (17%)
7	ATP	B	600	8	33,33,33	1.05	2 (6%)	52,52,52	1.91	10 (19%)
7	ATP	C	600	8	33,33,33	1.04	2 (6%)	52,52,52	1.86	10 (19%)
9	ADP	D	600	8	29,29,29	1.06	2 (6%)	45,45,45	1.91	9 (20%)
9	ADP	F	600	8	29,29,29	1.06	2 (6%)	45,45,45	1.93	11 (24%)

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
7	ATP	A	600	8	-	0/22/38/38	0/1/3/3
7	ATP	B	600	8	-	0/22/38/38	0/1/3/3
7	ATP	C	600	8	-	0/22/38/38	0/1/3/3
9	ADP	D	600	8	-	0/16/32/32	0/1/3/3
9	ADP	F	600	8	-	0/16/32/32	0/1/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	600	ADP	C5-C4	3.18	1.47	1.40
7	B	600	ATP	C5-C4	3.11	1.47	1.40
7	A	600	ATP	C5-C4	3.09	1.47	1.40
7	C	600	ATP	C5-C4	3.07	1.47	1.40
9	F	600	ADP	C4-N9	-2.99	1.33	1.37
9	F	600	ADP	C5-C4	2.97	1.47	1.40
7	C	600	ATP	C4-N9	-2.80	1.33	1.37
7	B	600	ATP	C4-N9	-2.55	1.34	1.37
9	D	600	ADP	C4-N9	-2.49	1.34	1.37
7	A	600	ATP	C4-N9	-2.49	1.34	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	600	ADP	N3-C2-N1	-6.25	123.49	128.71
7	B	600	ATP	N3-C2-N1	-6.02	123.67	128.71
9	D	600	ADP	N3-C2-N1	-5.98	123.71	128.71
7	C	600	ATP	N3-C2-N1	-5.97	123.72	128.71
7	A	600	ATP	N3-C4-N9	5.86	136.02	125.43
7	A	600	ATP	N3-C2-N1	-5.56	124.06	128.71
7	B	600	ATP	O4'-C1'-N9	5.43	113.49	108.44
7	C	600	ATP	N3-C4-N9	5.41	135.19	125.43
7	B	600	ATP	N3-C4-N9	5.28	134.97	125.43
9	D	600	ADP	N3-C4-N9	5.22	134.85	125.43
7	C	600	ATP	PB-O3B-PG	-4.86	117.42	131.68
9	F	600	ADP	N3-C4-N9	4.84	134.18	125.43
7	A	600	ATP	PA-O3A-PB	-4.12	119.61	131.68
9	D	600	ADP	O4'-C1'-N9	3.87	112.04	108.44
7	B	600	ATP	PA-O3A-PB	-3.87	120.33	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	600	ATP	PB-O3B-PG	-3.75	120.68	131.68
9	D	600	ADP	C4-C5-N7	-3.75	106.31	109.52
9	F	600	ADP	C3'-C2'-C1'	3.60	106.55	100.91
9	F	600	ADP	O4'-C1'-N9	3.53	111.72	108.44
9	F	600	ADP	C4-C5-N7	-3.47	106.55	109.52
7	A	600	ATP	C5-C4-N3	-3.38	118.34	125.70
9	D	600	ADP	C5-C4-N3	-3.33	118.46	125.70
7	C	600	ATP	PA-O3A-PB	-3.31	121.97	131.68
7	B	600	ATP	C4-C5-N7	-3.28	106.72	109.52
7	B	600	ATP	PB-O3B-PG	-3.24	122.19	131.68
7	B	600	ATP	C5-C4-N3	-3.20	118.73	125.70
7	C	600	ATP	C5-C4-N3	-3.19	118.76	125.70
9	D	600	ADP	C3'-C2'-C1'	3.17	105.87	100.91
7	C	600	ATP	C4-C5-N7	-3.10	106.86	109.52
7	C	600	ATP	O4'-C1'-N9	3.02	111.25	108.44
9	F	600	ADP	C2'-C1'-N9	-2.99	105.58	113.27
9	F	600	ADP	C5-C4-N3	-2.88	119.42	125.70
7	B	600	ATP	C3'-C2'-C1'	2.80	105.29	100.91
9	D	600	ADP	PA-O3A-PB	-2.75	123.62	131.68
9	F	600	ADP	PA-O3A-PB	-2.62	123.99	131.68
7	C	600	ATP	C3'-C2'-C1'	2.59	104.96	100.91
7	A	600	ATP	C3'-C2'-C1'	2.59	104.95	100.91
9	D	600	ADP	C2'-C1'-N9	-2.56	106.69	113.27
9	F	600	ADP	C8-N9-C4	2.53	108.83	106.90
9	D	600	ADP	C2-N3-C4	2.50	121.12	114.01
7	C	600	ATP	C8-N9-C4	2.40	108.73	106.90
7	B	600	ATP	C2-N3-C4	2.40	120.83	114.01
9	F	600	ADP	C2-N3-C4	2.33	120.65	114.01
7	C	600	ATP	C2-N3-C4	2.31	120.59	114.01
7	A	600	ATP	C2-N3-C4	2.31	120.59	114.01
7	A	600	ATP	C4-C5-N7	-2.31	107.54	109.52
9	F	600	ADP	C1'-N9-C4	-2.12	122.97	126.64
7	A	600	ATP	O4'-C1'-N9	-2.05	106.53	108.44
7	B	600	ATP	C8-N9-C4	2.03	108.45	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	485/510 (95%)	0.02	0 100 100	73, 73, 107, 107	0
1	B	485/510 (95%)	0.13	2 (0%) 90 68	111, 111, 149, 149	0
1	C	485/510 (95%)	0.03	1 (0%) 93 78	64, 64, 103, 130	0
2	D	470/478 (98%)	0.01	0 100 100	75, 75, 94, 94	0
2	E	473/478 (98%)	0.14	7 (1%) 70 33	95, 110, 157, 157	0
2	F	472/478 (98%)	0.06	0 100 100	89, 89, 102, 102	0
3	G	269/278 (96%)	0.11	0 100 100	92, 124, 132, 132	0
4	H	132/138 (95%)	0.23	0 100 100	106, 121, 170, 170	0
5	I	59/61 (96%)	-0.01	1 (1%) 67 31	126, 148, 148, 148	0
6	J	76/76 (100%)	0.44	1 (1%) 74 37	119, 119, 140, 140	0
6	K	76/76 (100%)	0.48	1 (1%) 74 37	131, 131, 132, 132	0
6	L	76/76 (100%)	0.34	0 100 100	122, 122, 137, 137	0
6	M	76/76 (100%)	0.44	3 (3%) 37 15	130, 130, 147, 147	0
6	N	76/76 (100%)	0.44	1 (1%) 74 37	148, 148, 168, 168	0
6	O	76/76 (100%)	0.59	4 (5%) 25 10	166, 166, 172, 172	0
6	P	76/76 (100%)	0.68	5 (6%) 18 8	169, 169, 182, 182	0
6	Q	76/76 (100%)	0.68	9 (11%) 5 3	157, 157, 169, 169	0
6	R	76/76 (100%)	0.54	4 (5%) 25 10	139, 139, 164, 164	0
6	S	76/76 (100%)	0.40	1 (1%) 74 37	128, 128, 141, 141	0
All	All	4090/4201 (97%)	0.15	40 (0%) 79 44	64, 107, 168, 182	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	Q	1	MET	5.6

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Mol	Chain	Res	Type	RSRZ
6	P	1	MET	4.9
6	M	1	MET	4.2
6	N	1	MET	4.0
2	E	435	LYS	4.0
6	Q	65	CYS	3.8
6	R	76	VAL	3.7
6	O	1	MET	3.5
6	M	74	PHE	2.9
6	O	26	ILE	2.9
6	R	52	ILE	2.9
6	Q	66	LEU	2.9
2	E	434	LEU	2.7
6	P	75	GLY	2.7
6	R	34	ILE	2.7
1	B	85	LYS	2.6
6	Q	61	THR	2.6
6	M	72	LEU	2.6
2	E	443	ALA	2.5
5	I	1	SER	2.5
2	E	89	ARG	2.5
6	P	33	LEU	2.4
6	P	9	TYR	2.4
2	E	441	PHE	2.4
6	Q	74	PHE	2.3
6	S	74	PHE	2.3
2	E	445	LEU	2.3
6	O	67	MET	2.3
6	J	2	GLN	2.3
6	P	76	VAL	2.3
2	E	442	LYS	2.2
1	B	438	LEU	2.2
6	K	76	VAL	2.2
6	Q	47	VAL	2.2
6	Q	73	LEU	2.1
6	O	28	ILE	2.1
6	R	33	LEU	2.1
6	Q	33	LEU	2.1
6	Q	76	VAL	2.1
1	C	495	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	ATP	C	600	31/31	0.23	0.33	71,71,71,71	0
7	ATP	B	600	31/31	0.20	-0.08	123,123,123,123	0
9	ADP	D	600	27/27	0.23	-0.12	71,71,71,71	0
7	ATP	A	600	31/31	0.22	-0.23	68,68,68,68	0
9	ADP	F	600	27/27	0.24	-0.39	114,114,114,114	0
8	MG	F	601	1/1	0.22	-0.85	114,114,114,114	0
8	MG	A	601	1/1	0.29	-	68,68,68,68	0
8	MG	B	601	1/1	0.18	-	123,123,123,123	0
8	MG	D	601	1/1	0.31	-	71,71,71,71	0
8	MG	C	601	1/1	0.23	-	71,71,71,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.