



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:49 am GMT

PDB ID : 3MVQ  
Title : Bovine Glutamate dehydrogenase complexed with zinc  
Authors : Smith, T.J.; Li, M.  
Deposited on : 2010-05-04  
Resolution : 2.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

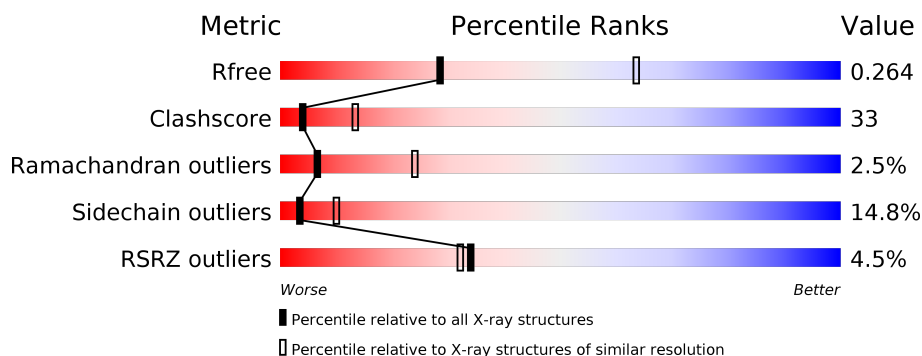
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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))
$R_{free}$	100719	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	501	<div> <div>4%</div> <div>48% 42% 8% ..</div> </div>
1	B	501	<div> <div>3%</div> <div>46% 44% 9% ..</div> </div>
1	C	501	<div> <div>7%</div> <div>45% 44% 9% .</div> </div>
1	D	501	<div> <div>4%</div> <div>49% 41% 8% .</div> </div>
1	E	501	<div> <div>4%</div> <div>46% 44% 9% .</div> </div>
1	F	501	<div> <div>4%</div> <div>45% 45% 10% .</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
2	GLU	C	502	-	-	X	-

## 2 Entry composition [i](#)

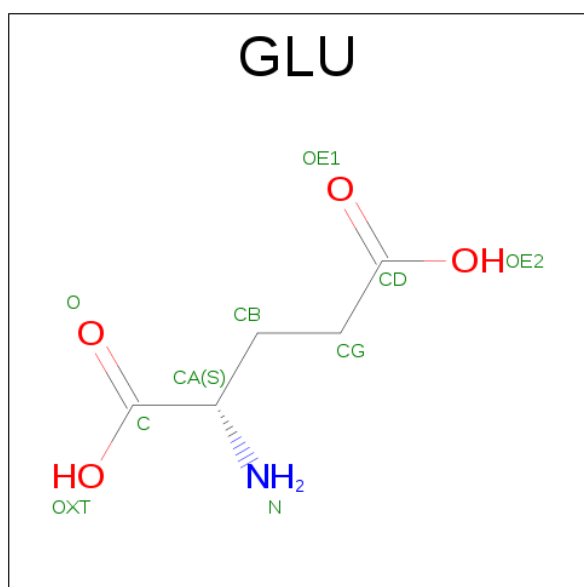
There are 5 unique types of molecules in this entry. The entry contains 23874 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase 1, mitochondrial.

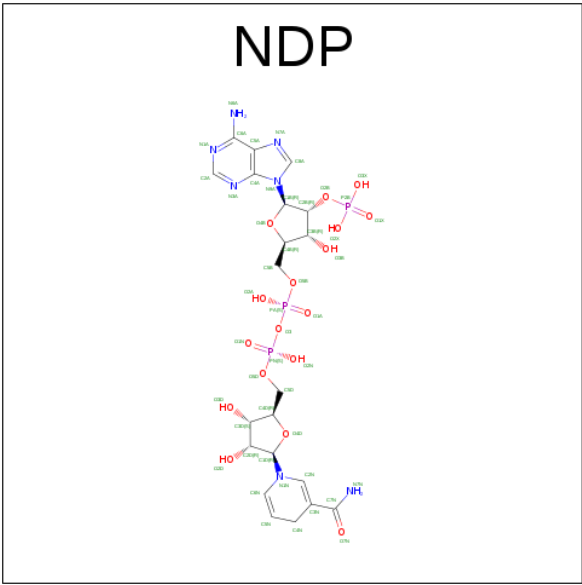
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	B	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	C	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	D	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	E	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	F	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



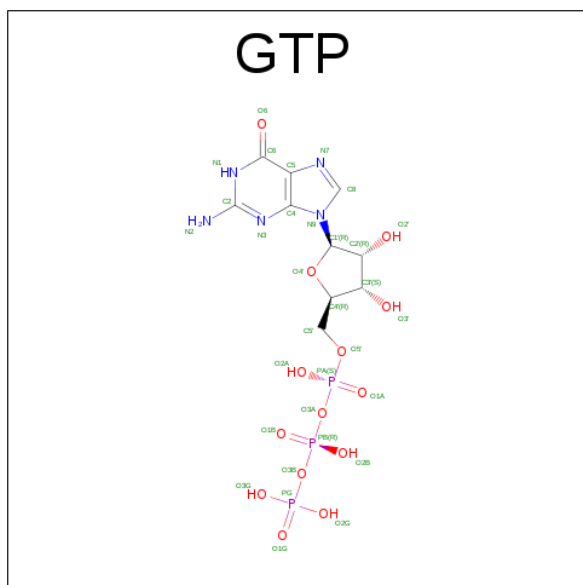
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Zn	0	0
			2	2		
5	E	2	Total	Zn	0	0
			2	2		

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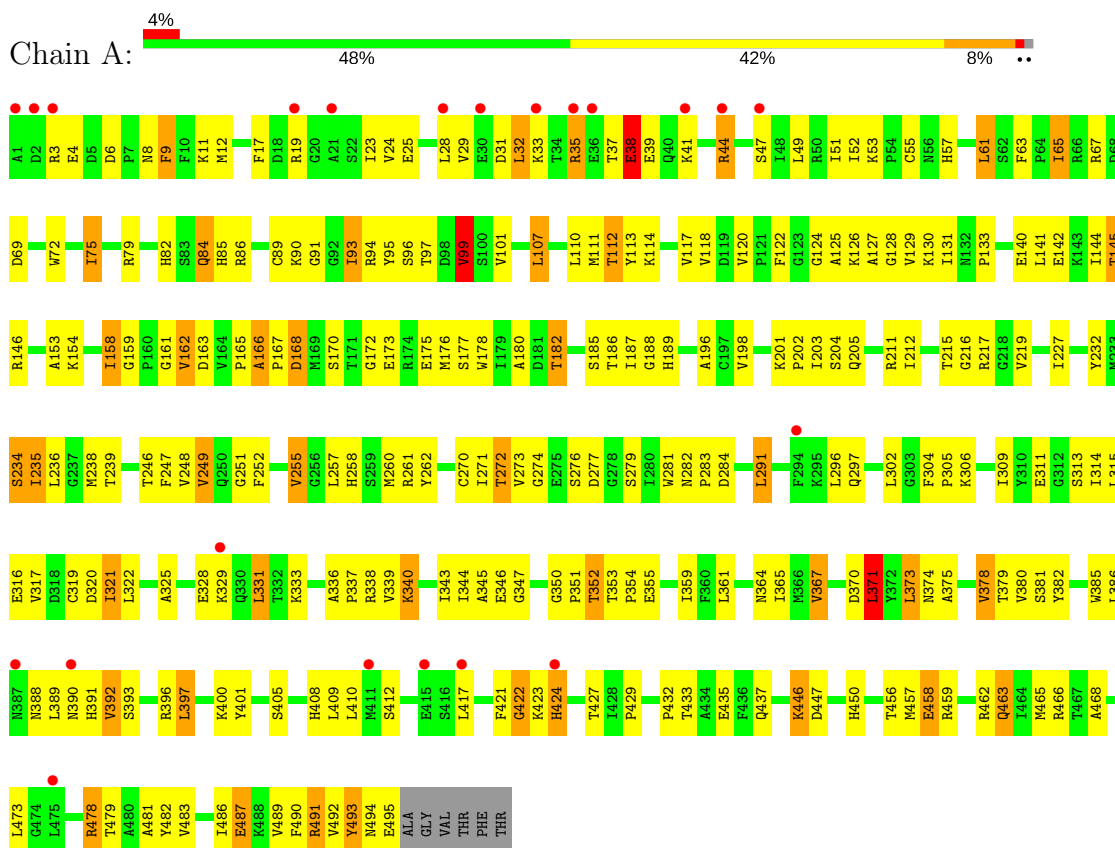
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	C	3	Total 3	Zn 3	0	0
5	A	2	Total 2	Zn 2	0	0
5	F	1	Total 1	Zn 1	0	0

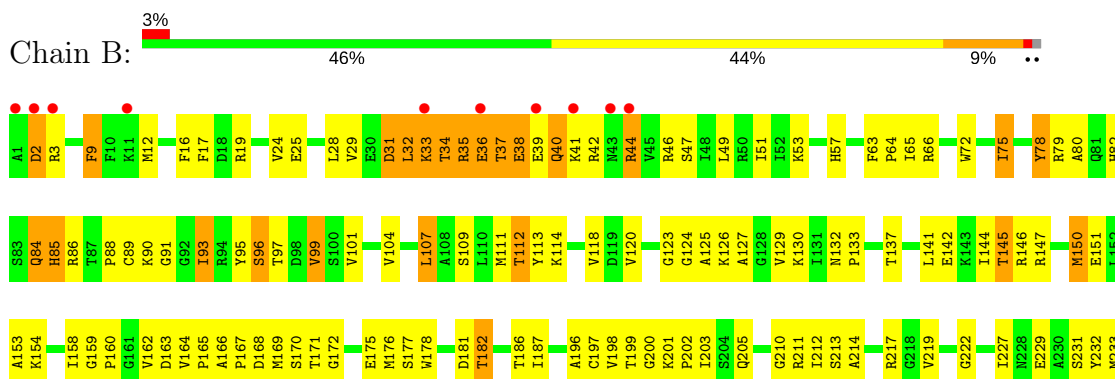
### 3 Residue-property plots

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

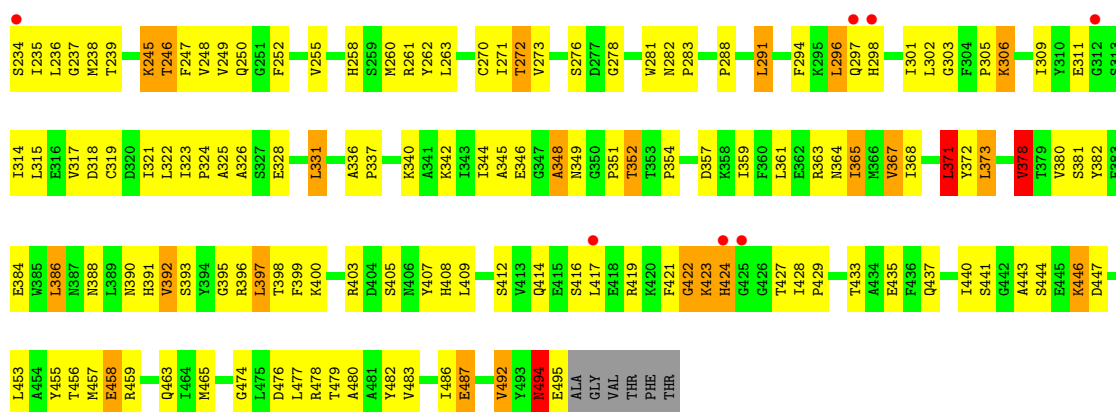
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



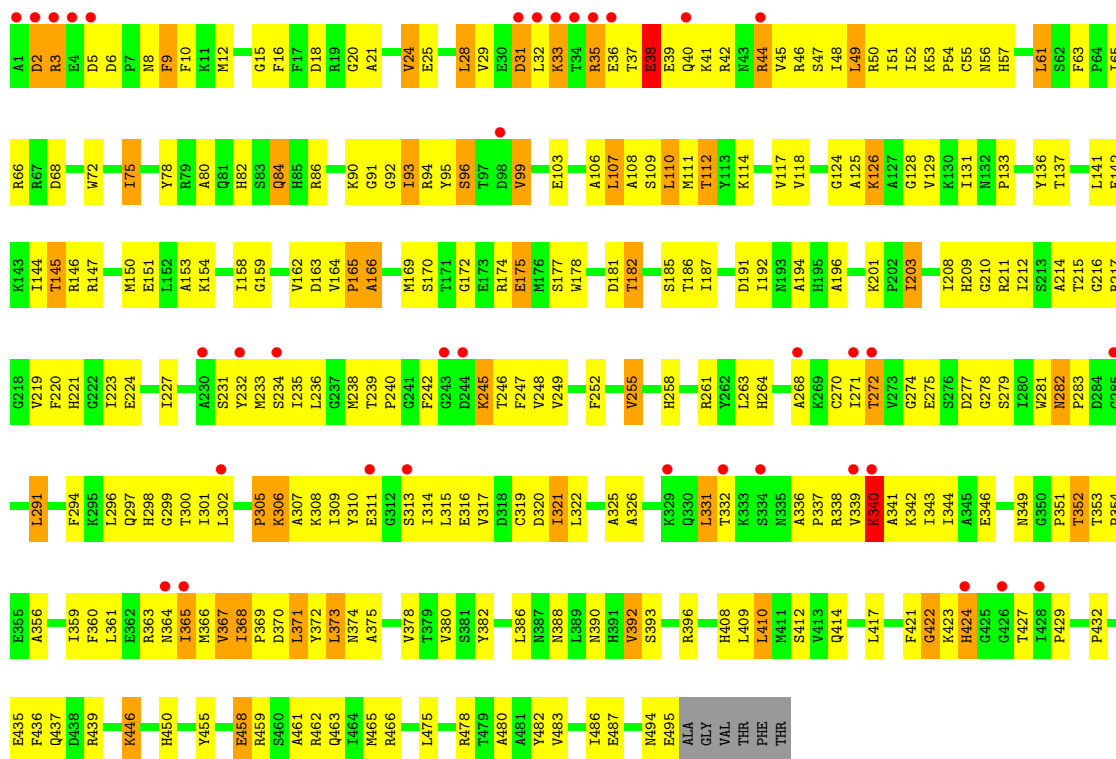
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



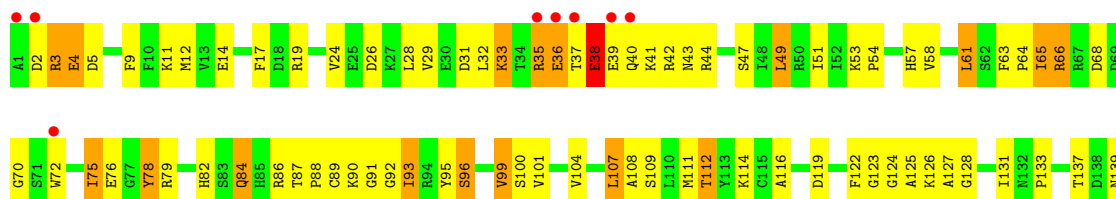


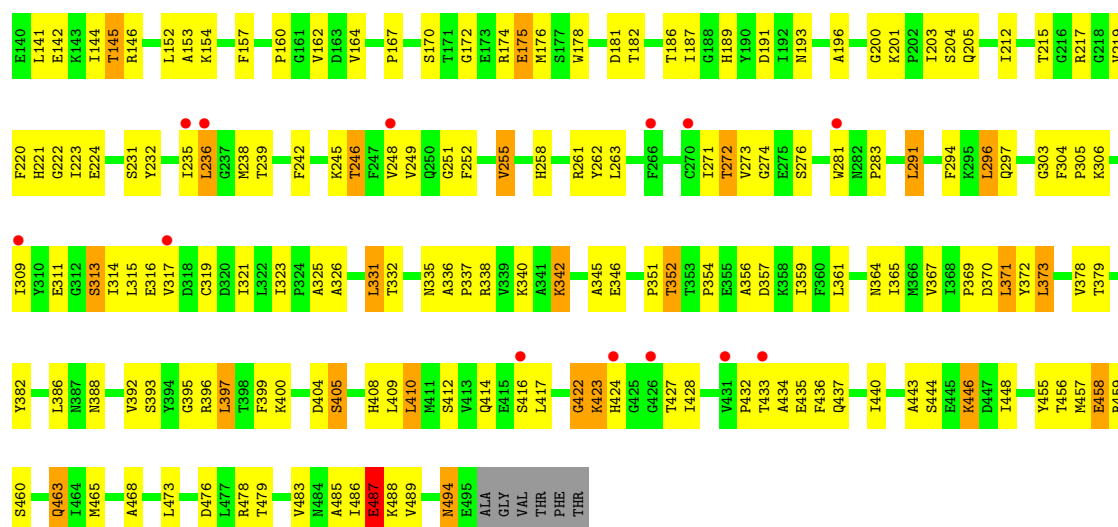


● Molecule 1: Glutamate dehydrogenase 1, mitochondrial

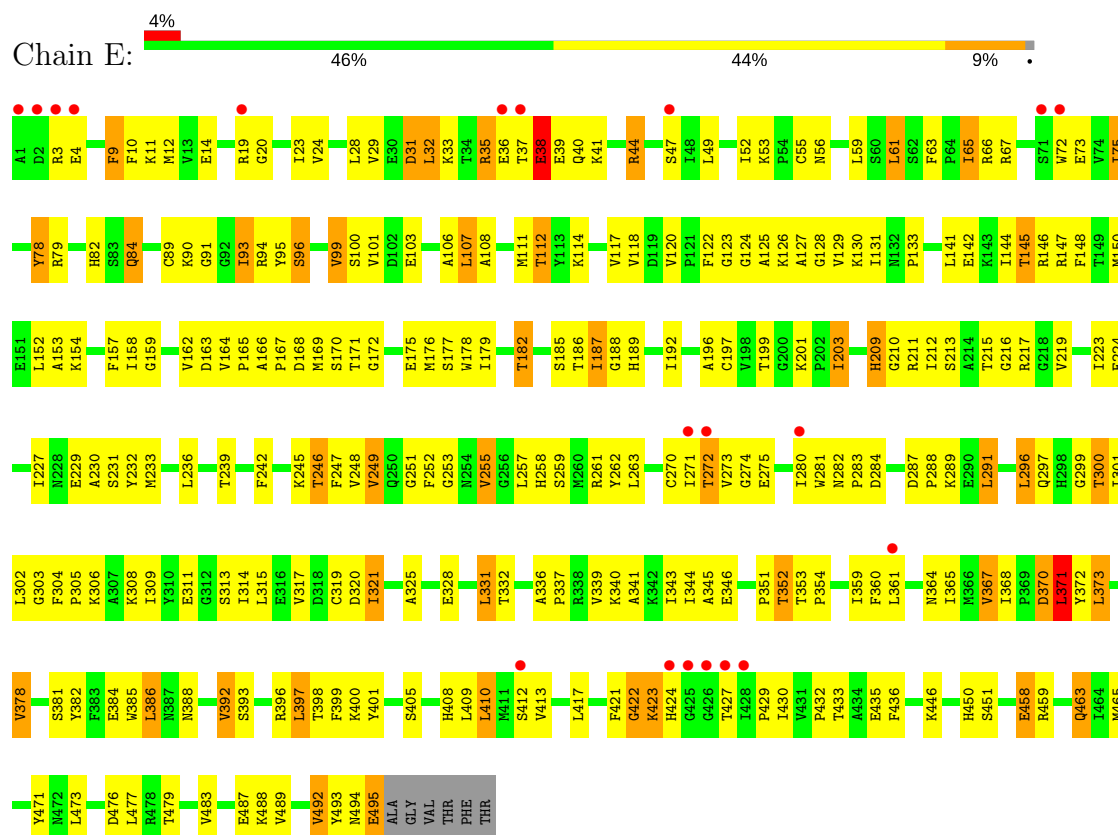


● Molecule 1: Glutamate dehydrogenase 1, mitochondrial

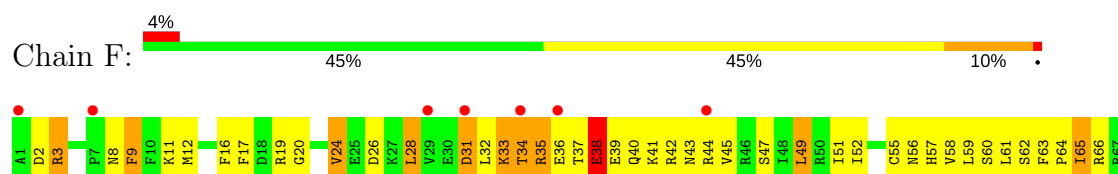




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



D68	K143	V219	E311	V378	Y455
W72	I144	I227	G312	T379	T456
I75	T145		S313	V380	M457
E76	R146		I314	S381	E458
G77	R147	A230	L315	Y382	R459
Y78	F148	S231	E316	F383	S460
R79	T149	Y232	V317	E384	A461
	M150	W233	D318	W385	R462
H82	E151	S234	C319	L386	M465
S83	L152	L235	D320	N387	N466
O84	A153		I321	N388	
H85		T239	L322	V392	L476
R86	I158		A325	S393	
	G159	F242		Y394	R478
C89	V162	G243	E328	G395	T479
K90	D163	D244	L331	R396	A480
G91	V164	K245		L397	A481
G92	P165	T246	A345	T398	Y482
I93	A166	F247	A346	F399	V483
R94	P167	V248	A347	K400	
Y95		V249	R337	Y401	L486
S96	S170		R338	E402	E487
T97	T171	F252	V339	R403	
D98	G172		K340		B491
Y99	E173	V255	A341	H408	
S100	R174	G256	K342	L409	M494
V101	E175	H258	L343	L410	E495
D102	M176		I344	M411	A496
E103	S177	R261	A346	S412	C497
	W178	Y262	C347		V498
L107	D181	L263	A348	S416	T499
A108	T182	H264	N349	L417	F500
S109			G350	E418	T501
L110	T186	C270	P351	R419	
M111	I187	T271	T352	K420	
T112	G188	T272	T353	F421	
Y113	H189	V273	P354	G422	
K114				K423	
	A196		D357	H424	
V117	C197	L280	K358	G425	
V118	V198	W281	I359	G426	
	T199	N282	F360	T427	
G123	G200	P283	L361	T428	
G124	K201	I286	E362	P429	
A125	P202	D287	R363	T430	
K126	I203	N288	N364	V431	
A127	S204	P288	I365	P432	
G128	Q205		M366	T433	
V129		L291	V367	A434	
K130	G210	F294	I368	E435	
I131	R211	K295	P369	F436	
N132	I212	L296	D370	Q437	
P133	S213	Q297	L371	D438	
	A214	H298	Y372	R439	
T137	T215		L373		
	G216	F304	N374	K446	
L141	R217	P305	A375	D447	
E142	G218	K306		I448	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.11Å 98.76Å 165.64Å 90.00° 101.55° 90.00°	Depositor
Resolution (Å)	45.88 – 2.94 47.44 – 2.94	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.88-2.94) 93.0 (47.44-2.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, $R_{free}$	0.223 , 0.262 0.203 , 0.264	Depositor DCC
$R_{free}$ test set	3821 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, NDP, ZN

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	0.46	0/3962	0.65	0/5348
1	B	0.46	0/3962	0.64	1/5348 (0.0%)
1	C	0.46	0/3962	0.63	0/5348
1	D	0.48	0/3962	0.63	0/5348
1	E	0.47	0/3962	0.63	0/5348
1	F	0.48	0/4005	0.65	0/5406
All	All	0.47	0/23815	0.64	1/32146 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3880	0	3843	281	0
1	B	3880	0	3843	278	0
1	C	3880	0	3843	292	0
1	D	3880	0	3843	237	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3880	0	3843	274	0
1	F	3922	0	3883	282	0
2	A	10	0	5	3	0
2	B	10	0	5	3	0
2	C	10	0	5	5	0
2	D	10	0	5	1	0
2	E	10	0	5	3	0
2	F	10	0	5	2	0
3	A	48	0	26	4	0
3	B	48	0	26	7	0
3	C	48	0	26	5	0
3	D	48	0	26	3	0
3	E	48	0	26	5	0
3	F	48	0	26	5	0
4	A	32	0	12	1	0
4	B	32	0	12	0	0
4	C	32	0	12	1	0
4	D	32	0	12	0	0
4	E	32	0	12	1	0
4	F	32	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	23874	0	23356	1557	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 33.

All (1557) 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:F:93:ILE:HD11	1:F:95:TYR:CE1	1.78	1.18
1:C:38:GLU:HG2	1:C:39:GLU:N	1.58	1.13
1:D:392:VAL:HG11	1:D:397:LEU:HD11	1.27	1.12
1:F:38:GLU:HG2	1:F:39:GLU:H	1.00	1.09
1:E:38:GLU:HG2	1:E:39:GLU:H	0.96	1.09
1:B:82:HIS:HD2	1:B:112:THR:HG21	1.18	1.08
1:D:38:GLU:HG2	1:D:39:GLU:N	1.68	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLU:HG3	1:B:39:GLU:H	1.15	1.07
1:A:38:GLU:HG2	1:A:39:GLU:H	0.96	1.06
1:B:82:HIS:CD2	1:B:112:THR:HG21	1.91	1.05
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.19	1.05
1:C:93:ILE:HD11	1:C:95:TYR:CE1	1.92	1.04
1:D:38:GLU:HG2	1:D:39:GLU:H	0.92	1.04
1:C:38:GLU:HG2	1:C:39:GLU:H	0.91	1.03
1:A:478:ARG:HG3	1:A:478:ARG:HH11	1.18	1.02
1:B:37:THR:O	1:B:38:GLU:HG2	1.59	1.02
1:E:38:GLU:HG2	1:E:39:GLU:N	1.71	1.01
1:A:38:GLU:HG2	1:A:39:GLU:N	1.63	1.01
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.22	1.01
1:D:82:HIS:CD2	1:D:112:THR:HG21	1.96	1.00
1:A:107:LEU:HB3	1:A:126:LYS:HG2	1.41	1.00
1:F:82:HIS:CD2	1:F:112:THR:HG21	1.97	1.00
1:D:153:ALA:HB1	1:D:187:ILE:HG13	1.39	1.00
1:F:346:GLU:OE1	1:F:352:THR:HG23	1.61	0.99
1:E:107:LEU:HB3	1:E:126:LYS:HG2	1.44	0.99
1:F:38:GLU:HG2	1:F:39:GLU:N	1.74	0.98
1:A:112:THR:HG22	1:A:124:GLY:CA	1.93	0.98
1:A:141:LEU:O	1:A:145:THR:HG23	1.64	0.97
1:E:141:LEU:O	1:E:145:THR:HG23	1.64	0.97
1:B:93:ILE:HD11	1:B:95:TYR:CE1	2.01	0.95
1:D:35:ARG:HD3	1:D:35:ARG:H	1.29	0.95
1:C:337:PRO:HD3	1:C:359:ILE:HD13	1.47	0.95
1:D:93:ILE:HD11	1:D:95:TYR:CE1	2.02	0.95
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.02	0.94
1:B:35:ARG:H	1:B:35:ARG:HD3	1.32	0.94
1:E:112:THR:HG22	1:E:124:GLY:H	1.32	0.94
1:C:3:ARG:H	1:C:3:ARG:HD3	1.33	0.93
1:A:93:ILE:HD11	1:A:95:TYR:HE1	1.31	0.92
1:E:35:ARG:HD3	1:E:35:ARG:H	1.34	0.92
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.49	0.92
1:A:107:LEU:HG	1:A:126:LYS:HE3	1.49	0.92
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.34	0.91
1:C:112:THR:HG22	1:C:124:GLY:H	1.34	0.91
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.05	0.91
1:D:346:GLU:OE1	1:D:352:THR:HG23	1.69	0.91
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.35	0.91
1:A:457:MET:HA	1:A:457:MET:HE2	1.53	0.90
1:C:35:ARG:HD3	1:C:35:ARG:H	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LEU:HD21	1:C:417:LEU:HD13	1.53	0.90
2:B:502:GLU:HA	3:B:552:NDP:H41N	1.53	0.90
1:C:93:ILE:HD11	1:C:95:TYR:HE1	1.33	0.90
1:A:47:SER:HB3	1:D:72:TRP:HB2	1.54	0.88
1:C:112:THR:HG22	1:C:124:GLY:N	1.89	0.88
1:D:408:HIS:HB3	1:F:436:PHE:HB2	1.56	0.87
1:F:141:LEU:O	1:F:145:THR:HG23	1.74	0.87
1:D:38:GLU:CG	1:D:39:GLU:H	1.83	0.87
1:F:35:ARG:H	1:F:35:ARG:HD3	1.40	0.86
1:B:91:GLY:HA3	1:B:125:ALA:O	1.75	0.85
1:E:201:LYS:NZ	1:E:388:ASN:HD21	1.74	0.85
1:E:93:ILE:HD11	1:E:95:TYR:CE1	2.11	0.85
1:B:72:TRP:HB2	1:E:47:SER:HB3	1.58	0.85
1:A:478:ARG:HG3	1:A:478:ARG:NH1	1.90	0.85
1:C:112:THR:HG22	1:C:124:GLY:CA	2.06	0.85
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.25	0.85
1:A:112:THR:HG22	1:A:124:GLY:N	1.91	0.85
1:F:107:LEU:HB3	1:F:126:LYS:HG2	1.58	0.85
1:A:93:ILE:HD11	1:A:95:TYR:CE1	2.11	0.84
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.12	0.84
1:E:38:GLU:CG	1:E:39:GLU:H	1.86	0.84
1:E:112:THR:HG22	1:E:124:GLY:N	1.92	0.84
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.58	0.84
1:A:146:ARG:HE	1:A:182:THR:HG22	1.43	0.84
1:F:32:LEU:HD13	1:F:494:ASN:HD21	1.43	0.84
1:F:38:GLU:CG	1:F:39:GLU:H	1.89	0.83
1:A:112:THR:HG22	1:A:124:GLY:H	1.44	0.83
1:B:38:GLU:HG3	1:B:39:GLU:N	1.93	0.83
1:A:345:ALA:HB1	1:A:373:LEU:HD11	1.59	0.83
1:A:248:VAL:HB	1:A:272:THR:HG23	1.62	0.82
1:C:315:LEU:HD13	1:C:331:LEU:CD1	2.10	0.82
1:A:35:ARG:H	1:A:35:ARG:HD3	1.45	0.82
1:C:248:VAL:HG23	1:C:272:THR:O	1.80	0.82
1:D:346:GLU:HG2	1:D:351:PRO:HG2	1.60	0.82
1:E:153:ALA:HB1	1:E:187:ILE:HG13	1.62	0.81
1:C:38:GLU:CG	1:C:39:GLU:N	2.43	0.81
1:B:219:VAL:HG22	1:B:373:LEU:HD22	1.62	0.81
1:A:118:VAL:HG23	1:A:120:VAL:HG23	1.62	0.81
1:A:142:GLU:O	1:A:146:ARG:HG3	1.81	0.81
1:B:47:SER:HB3	1:E:72:TRP:HB2	1.62	0.80
1:B:248:VAL:HG12	1:B:319:CYS:SG	2.22	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.30	0.80
1:C:271:ILE:HD12	1:C:272:THR:HG22	1.64	0.79
1:D:271:ILE:HD12	1:D:272:THR:HG22	1.63	0.79
1:E:458:GLU:HG3	1:E:459:ARG:N	1.98	0.79
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.65	0.79
1:F:458:GLU:HG3	1:F:459:ARG:N	1.98	0.79
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.17	0.79
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.00	0.79
1:D:93:ILE:HD11	1:D:95:TYR:HE1	1.43	0.79
1:D:19:ARG:HG2	1:D:479:THR:HG21	1.63	0.78
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.27	0.78
1:C:279:SER:OG	1:C:314:ILE:HB	1.83	0.78
1:A:38:GLU:CG	1:A:39:GLU:N	2.45	0.78
1:E:337:PRO:HD3	1:E:359:ILE:HD13	1.64	0.78
1:A:346:GLU:OE1	1:A:352:THR:HG23	1.83	0.78
1:B:112:THR:HG22	1:B:124:GLY:CA	2.14	0.78
1:B:82:HIS:CD2	1:B:112:THR:CG2	2.67	0.78
1:D:82:HIS:CD2	1:D:112:THR:CG2	2.67	0.77
1:F:336:ALA:N	1:F:337:PRO:HD2	1.98	0.77
1:A:248:VAL:HG12	1:A:319:CYS:SG	2.24	0.77
1:D:178:TRP:HE1	1:F:498:VAL:CG2	1.96	0.77
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.49	0.77
1:B:201:LYS:NZ	1:B:388:ASN:HD21	1.82	0.77
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.32	0.77
1:B:107:LEU:HG	1:B:126:LYS:HE3	1.66	0.77
1:E:90:LYS:HD3	1:E:122:PHE:CE1	2.18	0.77
1:F:93:ILE:CD1	1:F:95:TYR:CE1	2.66	0.77
1:F:432:PRO:HB2	1:F:437:GLN:HG2	1.65	0.77
1:A:90:LYS:HD3	1:A:122:PHE:CE1	2.19	0.77
1:C:141:LEU:O	1:C:145:THR:HG23	1.84	0.77
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.19	0.77
1:B:93:ILE:HD11	1:B:95:TYR:HE1	1.50	0.76
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.65	0.76
1:C:178:TRP:O	1:C:182:THR:HG23	1.86	0.76
1:F:38:GLU:CG	1:F:39:GLU:N	2.46	0.76
1:F:497:GLY:O	1:F:498:VAL:HG13	1.86	0.76
1:C:219:VAL:HA	1:C:373:LEU:HD22	1.67	0.76
1:A:12:MET:HG3	1:A:354:PRO:HD3	1.68	0.76
1:C:65:ILE:HG13	1:C:144:ILE:HG12	1.68	0.76
1:F:201:LYS:NZ	1:F:388:ASN:HD21	1.83	0.76
1:B:112:THR:HG22	1:B:124:GLY:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.68	0.75
1:A:219:VAL:HA	1:A:373:LEU:CD2	2.16	0.75
1:C:32:LEU:HD13	1:C:494:ASN:ND2	2.00	0.75
1:F:93:ILE:HD11	1:F:95:TYR:HE1	1.46	0.75
1:B:336:ALA:N	1:B:337:PRO:HD2	2.02	0.75
1:C:38:GLU:CG	1:C:39:GLU:H	1.85	0.75
1:A:217:ARG:HB2	1:A:262:TYR:CE1	2.21	0.75
1:E:38:GLU:CG	1:E:39:GLU:N	2.45	0.75
1:E:417:LEU:HD13	1:F:417:LEU:HD21	1.67	0.74
1:A:353:THR:HB	1:A:354:PRO:HD2	1.68	0.74
1:F:112:THR:HG22	1:F:124:GLY:CA	2.17	0.74
1:F:20:GLY:O	1:F:24:VAL:HG22	1.87	0.74
1:A:201:LYS:NZ	1:A:388:ASN:HD21	1.84	0.74
1:F:82:HIS:CD2	1:F:112:THR:CG2	2.69	0.74
1:A:91:GLY:HA3	1:A:125:ALA:O	1.87	0.74
1:A:25:GLU:O	1:A:29:VAL:HG23	1.88	0.74
1:B:346:GLU:OE1	1:B:352:THR:HG23	1.88	0.74
1:F:99:VAL:HA	1:F:103:GLU:OE2	1.88	0.74
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.22	0.74
1:B:255:VAL:HG22	1:B:325:ALA:HB1	1.68	0.73
1:F:248:VAL:HG12	1:F:319:CYS:SG	2.28	0.73
1:F:196:ALA:HA	1:F:388:ASN:HD22	1.52	0.73
1:B:112:THR:HG22	1:B:124:GLY:N	2.04	0.73
1:C:32:LEU:HD13	1:C:494:ASN:HD22	1.51	0.73
1:C:48:ILE:O	1:C:52:ILE:HG13	1.89	0.73
1:F:346:GLU:HG2	1:F:351:PRO:HG2	1.69	0.73
1:A:19:ARG:HG2	1:A:479:THR:HG21	1.71	0.73
1:D:201:LYS:NZ	1:D:388:ASN:HD21	1.87	0.73
1:D:443:ALA:HB2	1:E:401:TYR:CD2	2.24	0.73
1:C:210:GLY:O	1:C:214:ALA:HB2	1.89	0.73
1:E:409:LEU:HD13	1:F:409:LEU:HD11	1.70	0.73
1:D:392:VAL:HG11	1:D:397:LEU:CD1	2.14	0.72
1:E:246:THR:HG22	1:E:320:ASP:H	1.54	0.72
1:E:19:ARG:HG2	1:E:479:THR:HG21	1.71	0.72
1:E:82:HIS:HD2	1:E:112:THR:HG21	1.52	0.72
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.24	0.72
1:A:166:ALA:HB1	1:A:167:PRO:CD	2.18	0.72
1:A:255:VAL:HG22	1:A:325:ALA:HB1	1.70	0.72
1:A:408:HIS:NE2	1:B:435:GLU:HG2	2.03	0.72
1:F:372:TYR:OH	1:F:461:ALA:HB2	1.88	0.72
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PHE:CZ	1:B:270:CYS:HB2	2.22	0.72
1:C:82:HIS:CD2	1:C:112:THR:CG2	2.73	0.72
1:C:126:LYS:HZ3	2:C:502:GLU:N	1.87	0.72
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.35	0.72
1:A:329:LYS:HG2	1:A:353:THR:HG22	1.72	0.72
1:E:271:ILE:HD12	1:E:272:THR:CG2	2.20	0.72
1:F:392:VAL:HG11	1:F:397:LEU:HD11	1.71	0.72
1:C:146:ARG:HE	1:C:182:THR:HG22	1.54	0.72
1:D:96:SER:O	1:D:99:VAL:HG13	1.90	0.72
1:F:427:THR:O	1:F:429:PRO:HD3	1.90	0.72
1:C:326:ALA:HB1	3:C:552:NDP:C8A	2.20	0.72
1:C:247:PHE:CZ	1:C:270:CYS:HB2	2.25	0.71
1:C:281:TRP:O	1:C:307:ALA:HB1	1.90	0.71
1:E:91:GLY:HA3	1:E:125:ALA:O	1.90	0.71
1:C:35:ARG:CD	1:C:35:ARG:H	2.03	0.71
1:F:374:ASN:HB2	3:F:552:NDP:H5N	1.72	0.71
1:E:175:GLU:O	1:E:179:ILE:HG13	1.91	0.71
1:C:346:GLU:HG2	1:C:351:PRO:HG2	1.73	0.71
1:B:417:LEU:HD21	1:C:417:LEU:CD1	2.21	0.71
1:B:38:GLU:HG3	1:B:40:GLN:H	1.56	0.71
1:C:112:THR:CG2	1:C:124:GLY:H	2.03	0.71
1:C:337:PRO:HD3	1:C:359:ILE:CD1	2.20	0.71
1:A:178:TRP:O	1:A:182:THR:HG23	1.90	0.70
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.25	0.70
1:A:315:LEU:HD13	1:A:331:LEU:HD13	1.72	0.70
1:F:252:PHE:CE2	1:F:291:LEU:HD13	2.26	0.70
1:A:219:VAL:HA	1:A:373:LEU:HD22	1.72	0.70
1:C:214:ALA:HB1	1:C:380:VAL:HG21	1.72	0.70
1:C:146:ARG:NH2	1:C:181:ASP:OD2	2.24	0.70
1:D:457:MET:HA	1:D:457:MET:CE	2.21	0.70
1:F:65:ILE:HG13	1:F:144:ILE:CG1	2.21	0.70
1:B:344:ILE:HB	1:B:367:VAL:HG12	1.72	0.70
1:C:72:TRP:HB2	1:F:47:SER:HB3	1.73	0.70
1:E:24:VAL:HG11	1:E:483:VAL:HG13	1.73	0.70
1:B:219:VAL:HA	1:B:373:LEU:CD2	2.22	0.69
1:E:172:GLY:H	1:E:175:GLU:HG2	1.57	0.69
1:E:32:LEU:HD13	1:E:494:ASN:HD21	1.57	0.69
1:F:56:ASN:HD22	1:F:84:GLN:NE2	1.89	0.69
1:A:417:LEU:HD13	1:C:417:LEU:HD21	1.73	0.69
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.36	0.69
1:F:107:LEU:HG	1:F:126:LYS:HE3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ASP:HB2	1:C:374:ASN:HD21	1.57	0.69
1:A:409:LEU:HD13	1:C:409:LEU:HD11	1.75	0.69
1:D:38:GLU:CG	1:D:39:GLU:N	2.43	0.69
1:F:496:ALA:C	1:F:498:VAL:H	1.95	0.69
1:B:213:SER:HB2	1:B:258:HIS:CD2	2.27	0.69
1:D:303:GLY:H	1:D:309:ILE:HD11	1.58	0.69
1:E:271:ILE:HD12	1:E:272:THR:HG23	1.74	0.69
1:E:321:ILE:HG23	1:E:343:ILE:HB	1.73	0.69
1:D:141:LEU:O	1:D:145:THR:HG23	1.93	0.69
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.27	0.69
1:C:346:GLU:OE1	1:C:352:THR:HG23	1.92	0.69
1:B:271:ILE:HD11	1:B:319:CYS:HB3	1.73	0.69
1:D:379:THR:O	1:D:382:TYR:HB3	1.92	0.69
1:D:248:VAL:HG23	1:D:272:THR:O	1.93	0.69
1:E:117:VAL:HG21	1:E:371:LEU:HD22	1.75	0.69
1:B:400:LYS:HB2	1:C:455:TYR:HB2	1.75	0.69
1:A:272:THR:HG21	1:A:317:VAL:HG11	1.75	0.68
1:A:344:ILE:HB	1:A:367:VAL:HG12	1.75	0.68
1:C:432:PRO:HB2	1:C:437:GLN:HG2	1.75	0.68
1:B:232:TYR:HE2	1:B:465:MET:HG2	1.58	0.68
1:C:231:SER:O	1:C:235:ILE:HD13	1.93	0.68
1:C:126:LYS:NZ	2:C:502:GLU:N	2.41	0.68
1:F:422:GLY:C	1:F:423:LYS:HD2	2.14	0.68
1:A:114:LYS:HA	1:A:371:LEU:HD23	1.73	0.68
1:A:257:LEU:O	1:A:257:LEU:HD12	1.92	0.68
1:C:107:LEU:HB3	1:C:126:LYS:HG2	1.74	0.68
1:B:147:ARG:O	1:B:151:GLU:HG2	1.94	0.68
1:E:495:GLU:OE1	1:F:204:SER:HB3	1.93	0.68
1:A:117:VAL:HG21	1:A:371:LEU:HD22	1.76	0.68
1:B:9:PHE:HD2	1:B:9:PHE:O	1.77	0.68
1:F:396:ARG:HD2	1:F:396:ARG:O	1.92	0.68
1:B:35:ARG:CD	1:B:35:ARG:H	2.01	0.68
1:C:246:THR:OG1	1:C:271:ILE:HG12	1.94	0.68
1:C:336:ALA:N	1:C:337:PRO:HD2	2.09	0.68
1:C:322:LEU:HB3	1:C:344:ILE:CD1	2.23	0.68
1:D:139:ASN:OD1	1:F:501:THR:HG21	1.92	0.68
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.75	0.68
1:A:79:ARG:HD2	1:A:127:ALA:HB2	1.76	0.68
1:B:427:THR:O	1:B:429:PRO:HD3	1.94	0.68
1:C:366:MET:HG3	1:C:475:LEU:HD22	1.76	0.68
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:TYR:HB3	1:D:133:PRO:HG3	1.76	0.68
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.24	0.68
1:A:112:THR:CG2	1:A:124:GLY:H	2.06	0.67
1:E:107:LEU:HG	1:E:126:LYS:HE3	1.76	0.67
1:B:65:ILE:HG13	1:B:144:ILE:HG12	1.76	0.67
1:F:91:GLY:HA3	1:F:125:ALA:O	1.95	0.67
1:A:6:ASP:OD1	1:A:329:LYS:HD2	1.95	0.67
1:B:196:ALA:HA	1:B:388:ASN:HD22	1.60	0.67
1:A:271:ILE:HD12	1:A:272:THR:HG22	1.77	0.67
1:A:57:HIS:CE1	1:A:84:GLN:HE22	2.13	0.67
1:B:392:VAL:HG11	1:B:397:LEU:HD11	1.75	0.67
1:C:75:ILE:C	1:C:75:ILE:HD13	2.14	0.67
1:C:232:TYR:HE2	1:C:465:MET:HG2	1.60	0.67
1:C:458:GLU:HG3	1:C:459:ARG:N	2.09	0.67
1:E:259:SER:O	1:E:263:LEU:HD12	1.94	0.67
1:A:159:GLY:HA3	1:A:162:VAL:HG13	1.77	0.67
1:C:158:ILE:HG12	1:C:159:GLY:N	2.10	0.66
1:C:99:VAL:HA	1:C:103:GLU:OE2	1.95	0.66
1:D:32:LEU:HD13	1:D:494:ASN:OD1	1.95	0.66
1:B:303:GLY:N	1:B:309:ILE:HD11	2.10	0.66
1:C:462:ARG:HG3	1:C:466:ARG:HH22	1.60	0.66
1:F:338:ARG:HG3	1:F:338:ARG:O	1.95	0.66
1:A:392:VAL:HG11	1:A:397:LEU:HD11	1.77	0.66
1:A:82:HIS:CD2	1:A:112:THR:CG2	2.76	0.66
1:A:146:ARG:HE	1:A:182:THR:CG2	2.09	0.66
1:A:146:ARG:NE	1:A:182:THR:HG22	2.10	0.66
1:A:390:ASN:O	1:A:392:VAL:HG23	1.96	0.66
1:E:353:THR:HB	1:E:354:PRO:HD2	1.76	0.66
1:F:478:ARG:HH11	1:F:478:ARG:HG3	1.59	0.66
1:E:75:ILE:HD13	1:E:75:ILE:C	2.16	0.66
1:E:146:ARG:HA	1:E:182:THR:HG21	1.77	0.66
1:E:37:THR:HG22	1:E:41:LYS:HE3	1.76	0.66
1:E:53:LYS:O	1:E:82:HIS:HE1	1.79	0.66
1:D:116:ALA:O	1:D:488:LYS:HD2	1.95	0.65
1:F:141:LEU:O	1:F:145:THR:CG2	2.44	0.65
1:E:10:PHE:HA	1:E:106:ALA:HB2	1.77	0.65
1:A:90:LYS:HD3	1:A:122:PHE:CD1	2.32	0.65
1:E:427:THR:O	1:E:429:PRO:HD3	1.97	0.65
1:F:252:PHE:CZ	1:F:291:LEU:HD13	2.31	0.65
1:A:117:VAL:CG2	1:A:371:LEU:HD22	2.27	0.65
1:C:146:ARG:NE	1:C:182:THR:HG22	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ILE:HD11	1:E:345:ALA:CB	2.26	0.65
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.78	0.65
1:D:435:GLU:HG2	1:E:408:HIS:CE1	2.31	0.65
1:A:427:THR:O	1:A:429:PRO:HD3	1.96	0.65
1:C:248:VAL:HB	1:C:272:THR:HG23	1.78	0.65
1:E:52:ILE:HG12	1:E:493:TYR:CE1	2.32	0.65
1:D:409:LEU:HD11	1:F:409:LEU:HD13	1.78	0.65
1:B:133:PRO:HG2	1:B:170:SER:HB3	1.79	0.65
1:B:273:VAL:HG21	1:B:291:LEU:HD12	1.79	0.65
1:C:219:VAL:HA	1:C:373:LEU:CD2	2.27	0.65
1:D:112:THR:HG22	1:D:124:GLY:CA	2.26	0.65
1:D:219:VAL:HA	1:D:373:LEU:CD2	2.27	0.65
1:D:433:THR:HG23	1:E:412:SER:HA	1.78	0.65
1:A:19:ARG:CG	1:A:479:THR:HG21	2.27	0.64
1:D:255:VAL:HG22	1:D:325:ALA:HB1	1.79	0.64
1:B:271:ILE:CG2	1:B:283:PRO:HA	2.28	0.64
1:B:263:LEU:CD1	1:B:323:ILE:HD11	2.28	0.64
1:B:315:LEU:HD13	1:B:331:LEU:HD13	1.79	0.64
1:F:65:ILE:HG13	1:F:144:ILE:HG13	1.79	0.64
1:B:47:SER:O	1:B:51:ILE:HG13	1.96	0.64
1:C:55:CYS:O	1:F:62:SER:HB2	1.97	0.64
1:E:413:VAL:HG12	1:E:430:ILE:HG13	1.78	0.64
1:F:353:THR:HB	1:F:354:PRO:HD2	1.78	0.64
1:C:3:ARG:HD3	1:C:3:ARG:N	2.11	0.64
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.77	0.64
1:E:211:ARG:HD2	1:E:211:ARG:O	1.97	0.64
1:A:435:GLU:HG2	1:C:408:HIS:NE2	2.13	0.64
1:B:112:THR:CG2	1:B:124:GLY:H	2.11	0.64
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.45	0.64
1:B:114:LYS:HA	1:B:371:LEU:CD2	2.28	0.64
1:C:322:LEU:HB3	1:C:344:ILE:HD13	1.80	0.64
1:D:175:GLU:HA	1:D:178:TRP:CE3	2.33	0.64
1:E:75:ILE:O	1:E:75:ILE:HD13	1.97	0.64
1:B:37:THR:O	1:B:38:GLU:CG	2.41	0.64
1:B:32:LEU:HD13	1:B:494:ASN:HD21	1.62	0.64
1:D:53:LYS:O	1:D:82:HIS:HE1	1.80	0.64
1:C:332:THR:HG22	1:C:353:THR:CG2	2.28	0.64
1:C:261:ARG:NH2	4:C:503:GTP:C8	2.66	0.63
1:F:95:TYR:OH	1:F:145:THR:HB	1.97	0.63
1:A:272:THR:CG2	1:A:317:VAL:HG11	2.29	0.63
1:C:277:ASP:O	1:C:302:LEU:HD11	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:ALA:HA	1:E:388:ASN:HD22	1.63	0.63
1:E:346:GLU:HG2	1:E:351:PRO:HG2	1.79	0.63
1:B:210:GLY:O	1:B:214:ALA:HB2	1.98	0.63
1:E:32:LEU:CD1	1:E:494:ASN:HD21	2.10	0.63
1:E:435:GLU:HG2	1:F:408:HIS:NE2	2.13	0.63
1:A:232:TYR:HE2	1:A:465:MET:HG2	1.63	0.63
1:E:258:HIS:HD2	1:E:261:ARG:NH1	1.95	0.63
1:C:315:LEU:HD13	1:C:331:LEU:HD12	1.79	0.63
1:C:223:ILE:HD12	1:C:263:LEU:HD11	1.81	0.63
1:D:37:THR:HG22	1:D:41:LYS:HE3	1.80	0.63
1:E:248:VAL:HG12	1:E:319:CYS:SG	2.38	0.63
1:B:255:VAL:CG2	1:B:325:ALA:HB1	2.27	0.63
1:B:303:GLY:H	1:B:309:ILE:HD11	1.63	0.63
1:E:232:TYR:O	1:E:236:LEU:HB2	1.99	0.63
1:E:112:THR:HG22	1:E:124:GLY:CA	2.27	0.63
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.46	0.62
1:C:93:ILE:HG13	1:C:93:ILE:O	1.99	0.62
1:E:272:THR:HG22	1:E:281:TRP:HD1	1.64	0.62
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.29	0.62
1:F:153:ALA:HB1	1:F:187:ILE:HG13	1.80	0.62
1:A:346:GLU:HG2	1:A:351:PRO:HG2	1.80	0.62
1:B:446:LYS:HZ3	1:B:446:LYS:HB2	1.63	0.62
1:A:417:LEU:CD1	1:C:417:LEU:HD21	2.29	0.62
1:B:271:ILE:HG22	1:B:283:PRO:HA	1.81	0.62
1:B:315:LEU:HD13	1:B:331:LEU:CD1	2.29	0.62
1:F:153:ALA:HA	1:F:158:ILE:HG22	1.81	0.62
1:C:9:PHE:CE1	1:C:107:LEU:HD13	2.34	0.62
1:E:368:ILE:HB	1:E:373:LEU:HD12	1.81	0.62
1:C:3:ARG:H	1:C:3:ARG:CD	2.10	0.62
1:E:63:PHE:CD1	1:E:147:ARG:HG3	2.35	0.62
1:C:271:ILE:HD12	1:C:272:THR:CG2	2.28	0.62
1:D:248:VAL:HB	1:D:272:THR:HG23	1.81	0.62
1:E:91:GLY:O	1:E:165:PRO:HA	2.00	0.62
1:B:271:ILE:HD12	1:B:272:THR:CG2	2.29	0.62
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.29	0.62
1:D:107:LEU:HG	1:D:126:LYS:HE3	1.81	0.62
1:F:201:LYS:HZ1	1:F:388:ASN:HD21	1.48	0.62
1:F:271:ILE:HD12	1:F:272:THR:CG2	2.30	0.62
1:A:202:PRO:HB2	1:A:205:GLN:HG3	1.81	0.62
1:F:247:PHE:CZ	1:F:270:CYS:HB2	2.35	0.62
1:A:95:TYR:HB3	1:A:133:PRO:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:GLU:HG3	1:D:459:ARG:N	2.16	0.61
1:D:219:VAL:HA	1:D:373:LEU:HD22	1.83	0.61
1:F:146:ARG:HA	1:F:182:THR:HG21	1.82	0.61
1:B:214:ALA:HB1	1:B:380:VAL:HG21	1.83	0.61
1:D:172:GLY:H	1:D:175:GLU:HG2	1.64	0.61
1:D:336:ALA:N	1:D:337:PRO:HD2	2.15	0.61
1:E:217:ARG:HB2	1:E:262:TYR:CE1	2.35	0.61
1:D:35:ARG:H	1:D:35:ARG:CD	2.02	0.61
1:D:485:ALA:O	1:D:489:VAL:HG23	2.01	0.61
1:D:47:SER:O	1:D:51:ILE:HG13	2.01	0.61
1:F:255:VAL:HG22	1:F:325:ALA:HB1	1.81	0.61
1:C:92:GLY:O	1:C:126:LYS:HD3	2.00	0.61
1:C:117:VAL:HG21	1:C:371:LEU:HD22	1.83	0.61
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.31	0.61
1:F:457:MET:HA	1:F:457:MET:HE2	1.83	0.61
1:A:336:ALA:N	1:A:337:PRO:HD2	2.15	0.61
1:C:201:LYS:HZ1	1:C:388:ASN:HD21	1.49	0.61
1:F:148:PHE:CE2	1:F:152:LEU:HD11	2.35	0.61
1:F:315:LEU:HD13	1:F:331:LEU:CD1	2.30	0.61
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.30	0.61
1:B:57:HIS:HD2	1:E:61:LEU:HD12	1.66	0.61
1:A:153:ALA:HB1	1:A:187:ILE:HG13	1.81	0.60
1:A:392:VAL:HG22	1:B:386:LEU:HD11	1.83	0.60
1:A:91:GLY:O	1:A:165:PRO:HA	2.01	0.60
1:B:126:LYS:HG3	1:B:127:ALA:N	2.16	0.60
1:E:201:LYS:NZ	1:E:388:ASN:ND2	2.48	0.60
1:E:117:VAL:CG2	1:E:371:LEU:HD22	2.30	0.60
1:C:217:ARG:CZ	1:C:450:HIS:CD2	2.85	0.60
1:D:167:PRO:HD3	1:D:200:GLY:HA3	1.83	0.60
1:B:164:VAL:HG13	1:B:198:VAL:HA	1.83	0.60
1:C:20:GLY:O	1:C:24:VAL:HG22	2.01	0.60
1:D:395:GLY:HA3	1:D:399:PHE:CZ	2.37	0.60
1:D:92:GLY:O	1:D:126:LYS:HD3	2.02	0.60
1:A:313:SER:HB3	1:A:316:GLU:HG3	1.81	0.60
1:A:52:ILE:HD13	1:A:489:VAL:HG12	1.84	0.60
1:F:325:ALA:HA	1:F:348:ALA:HB2	1.83	0.60
1:A:446:LYS:HG3	1:A:447:ASP:H	1.67	0.60
1:F:37:THR:O	1:F:38:GLU:HB3	2.01	0.60
1:B:408:HIS:HB3	1:C:436:PHE:HB2	1.83	0.60
1:C:47:SER:HB3	1:F:72:TRP:HB2	1.82	0.60
1:D:231:SER:O	1:D:235:ILE:HD13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:HB1	1:B:187:ILE:HG13	1.83	0.60
1:C:211:ARG:O	1:C:211:ARG:HD2	2.00	0.60
1:D:417:LEU:HD21	1:F:417:LEU:HD13	1.83	0.60
1:B:150:MET:O	1:B:154:LYS:HG3	2.01	0.60
1:B:457:MET:HA	1:B:457:MET:CE	2.31	0.60
1:D:263:LEU:CD1	1:D:323:ILE:HD11	2.32	0.60
1:A:166:ALA:HB1	1:A:167:PRO:HD3	1.81	0.60
1:C:57:HIS:HD2	1:F:61:LEU:HD12	1.67	0.60
1:C:427:THR:O	1:C:429:PRO:HD3	2.02	0.60
1:F:219:VAL:HA	1:F:373:LEU:HD22	1.82	0.60
1:F:82:HIS:CG	1:F:109:SER:HA	2.37	0.60
1:F:8:ASN:OD1	1:F:11:LYS:HG3	2.02	0.60
1:B:146:ARG:HG2	1:B:182:THR:HG21	1.82	0.59
1:B:64:PRO:O	1:B:65:ILE:HD13	2.02	0.59
1:C:24:VAL:HG13	1:C:483:VAL:HG22	1.83	0.59
1:C:315:LEU:HD13	1:C:331:LEU:HD13	1.83	0.59
1:E:203:ILE:HD11	1:E:209:HIS:HA	1.83	0.59
1:E:336:ALA:N	1:E:337:PRO:HD2	2.15	0.59
1:F:199:THR:HG22	1:F:384:GLU:HG2	1.82	0.59
1:F:369:PRO:HG3	1:F:478:ARG:HA	1.82	0.59
1:B:95:TYR:OH	1:B:145:THR:HG22	2.02	0.59
1:D:369:PRO:HG3	1:D:478:ARG:HA	1.84	0.59
1:D:114:LYS:HZ2	2:D:502:GLU:N	2.00	0.59
1:A:24:VAL:HG11	1:A:483:VAL:HG13	1.82	0.59
1:B:390:ASN:O	1:B:392:VAL:HG23	2.01	0.59
1:E:229:GLU:HG3	1:E:231:SER:HB3	1.84	0.59
1:E:219:VAL:HA	1:E:373:LEU:HD22	1.84	0.59
1:A:247:PHE:CZ	1:A:270:CYS:HB2	2.38	0.59
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.84	0.59
1:B:96:SER:O	1:B:99:VAL:CG1	2.50	0.59
1:C:245:LYS:HD2	1:C:245:LYS:N	2.17	0.59
1:C:271:ILE:CG2	1:C:283:PRO:HA	2.31	0.59
1:A:63:PHE:CZ	1:A:75:ILE:CD1	2.85	0.59
1:B:24:VAL:HG11	1:B:483:VAL:HG13	1.84	0.59
1:D:457:MET:HE2	1:D:457:MET:HA	1.83	0.59
1:A:446:LYS:HG3	1:A:447:ASP:N	2.17	0.59
1:C:281:TRP:O	1:C:282:ASN:HB2	2.03	0.59
1:C:271:ILE:HG22	1:C:283:PRO:HA	1.85	0.59
1:E:227:ILE:HD11	1:E:245:LYS:HG2	1.85	0.59
1:F:9:PHE:CE1	1:F:107:LEU:HD13	2.38	0.59
1:F:112:THR:HG22	1:F:124:GLY:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HD11	1:A:319:CYS:HB3	1.83	0.59
1:D:223:ILE:HD11	1:D:345:ALA:CB	2.32	0.59
1:A:8:ASN:OD1	1:A:11:LYS:HG3	2.02	0.59
1:C:298:HIS:O	1:C:300:THR:N	2.36	0.59
1:E:422:GLY:C	1:E:423:LYS:HD2	2.23	0.59
1:B:408:HIS:ND1	1:C:439:ARG:HD2	2.18	0.59
1:D:397:LEU:O	1:F:448:ILE:HD12	2.02	0.59
1:E:315:LEU:HD13	1:E:331:LEU:HD13	1.84	0.59
1:A:417:LEU:HD21	1:B:417:LEU:CD1	2.33	0.58
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.85	0.58
1:C:18:ASP:O	1:C:21:ALA:HB3	2.03	0.58
1:C:246:THR:O	1:C:320:ASP:HB2	2.03	0.58
1:A:433:THR:HG23	1:C:412:SER:OG	2.03	0.58
1:C:63:PHE:CZ	1:C:75:ILE:CD1	2.86	0.58
1:D:414:GLN:HG3	1:D:428:ILE:O	2.03	0.58
1:D:96:SER:O	1:D:99:VAL:CG1	2.51	0.58
1:A:490:PHE:O	1:A:491:ARG:CB	2.51	0.58
1:B:271:ILE:HD12	1:B:272:THR:HG23	1.86	0.58
1:C:321:ILE:HG23	1:C:343:ILE:HB	1.84	0.58
1:D:422:GLY:C	1:D:423:LYS:HD2	2.23	0.58
1:F:322:LEU:HB3	1:F:344:ILE:HD12	1.86	0.58
1:A:422:GLY:C	1:A:423:LYS:HD2	2.24	0.58
1:C:258:HIS:HD2	1:C:261:ARG:NH1	2.01	0.58
1:D:95:TYR:OH	1:D:145:THR:HB	2.03	0.58
1:E:118:VAL:HG23	1:E:120:VAL:HG23	1.84	0.58
1:F:32:LEU:HD13	1:F:494:ASN:ND2	2.15	0.58
1:A:257:LEU:HD12	1:A:257:LEU:C	2.24	0.58
1:C:68:ASP:OD1	1:C:137:THR:HG21	2.03	0.58
1:C:421:PHE:N	1:C:421:PHE:CD2	2.69	0.58
1:F:108:ALA:O	1:F:111:MET:HB2	2.03	0.58
1:F:172:GLY:H	1:F:175:GLU:HG2	1.69	0.58
1:D:152:LEU:HD22	1:D:157:PHE:HB3	1.85	0.58
1:E:95:TYR:OH	1:E:145:THR:HG22	2.04	0.58
1:E:150:MET:O	1:E:154:LYS:HG3	2.04	0.58
1:F:107:LEU:CB	1:F:126:LYS:HG2	2.32	0.58
1:F:65:ILE:HG13	1:F:144:ILE:HG12	1.86	0.58
1:A:85:HIS:CD2	1:A:86:ARG:HG2	2.38	0.58
1:E:246:THR:CG2	1:E:320:ASP:H	2.15	0.58
1:A:271:ILE:HD12	1:A:272:THR:CG2	2.34	0.58
1:D:271:ILE:HD12	1:D:272:THR:CG2	2.33	0.58
1:D:342:LYS:N	1:D:342:LYS:HD3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:PRO:HB3	1:E:436:PHE:CD2	2.36	0.58
1:A:131:ILE:O	1:A:133:PRO:HD3	2.04	0.57
1:E:95:TYR:HB3	1:E:133:PRO:HG3	1.85	0.57
1:A:154:LYS:HD3	1:E:185:SER:O	2.04	0.57
1:C:332:THR:HG22	1:C:353:THR:HG21	1.86	0.57
1:E:291:LEU:HD21	1:E:301:ILE:HG22	1.84	0.57
1:A:232:TYR:CE2	1:A:465:MET:HG2	2.38	0.57
1:C:215:THR:O	1:C:219:VAL:HG23	2.04	0.57
1:D:412:SER:OG	1:F:433:THR:HG23	2.04	0.57
1:F:35:ARG:H	1:F:35:ARG:CD	2.10	0.57
1:C:339:VAL:O	1:C:340:LYS:HB2	2.05	0.57
1:F:90:LYS:HE3	1:F:381:SER:HB3	1.87	0.57
1:B:17:PHE:CE1	1:B:486:ILE:HG12	2.40	0.57
1:B:111:MET:HE1	2:B:502:GLU:HG3	1.87	0.57
1:D:336:ALA:HB2	1:D:356:ALA:HB1	1.86	0.57
1:E:23:ILE:HG22	1:E:471:TYR:CD1	2.40	0.57
1:E:463:GLN:OE1	1:E:488:LYS:NZ	2.35	0.57
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.40	0.57
1:B:250:GLN:NE2	1:B:315:LEU:HD21	2.20	0.57
1:C:63:PHE:CZ	1:C:75:ILE:HD12	2.40	0.57
1:D:248:VAL:HG12	1:D:319:CYS:SG	2.45	0.57
1:E:308:LYS:HG3	1:E:309:ILE:O	2.05	0.57
1:F:368:ILE:HB	1:F:373:LEU:HD12	1.85	0.57
1:C:196:ALA:HA	1:C:388:ASN:HD22	1.70	0.57
1:D:89:CYS:HA	1:D:123:GLY:O	2.05	0.57
1:E:427:THR:HG23	1:E:427:THR:O	2.04	0.57
1:B:146:ARG:HE	1:B:182:THR:HG22	1.69	0.57
1:B:326:ALA:O	3:B:552:NDP:H4D	2.05	0.57
1:D:370:ASP:OD1	1:D:371:LEU:N	2.34	0.57
1:E:196:ALA:HB2	1:E:388:ASN:HB2	1.87	0.57
1:B:38:GLU:CG	1:B:39:GLU:N	2.61	0.56
1:C:37:THR:HG22	1:C:41:LYS:HE3	1.85	0.56
1:D:63:PHE:CZ	1:D:75:ILE:CD1	2.87	0.56
1:C:310:TYR:CZ	1:C:317:VAL:HG22	2.40	0.56
1:E:96:SER:O	1:E:99:VAL:CG1	2.53	0.56
1:B:233:MET:HA	1:B:233:MET:HE2	1.86	0.56
1:D:107:LEU:HB3	1:D:126:LYS:HG2	1.86	0.56
1:D:64:PRO:O	1:D:65:ILE:HD13	2.05	0.56
1:F:258:HIS:HD2	1:F:261:ARG:NH1	1.97	0.56
1:F:346:GLU:HG2	1:F:351:PRO:CG	2.35	0.56
1:F:59:LEU:O	1:F:78:TYR:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:HA	1:A:371:LEU:CD2	2.35	0.56
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.87	0.56
1:E:29:VAL:HG13	1:E:41:LYS:HB3	1.87	0.56
1:F:93:ILE:CD1	1:F:95:TYR:HE1	2.11	0.56
1:B:260:MET:HE1	1:B:288:PRO:HA	1.86	0.56
1:C:370:ASP:HB2	1:C:374:ASN:ND2	2.20	0.56
1:E:89:CYS:HA	1:E:123:GLY:O	2.05	0.56
1:F:227:ILE:HD11	1:F:245:LYS:HG2	1.86	0.56
1:F:382:TYR:O	1:F:386:LEU:HD22	2.05	0.56
1:F:24:VAL:HG13	1:F:483:VAL:HG13	1.88	0.56
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.87	0.56
1:C:146:ARG:HE	1:C:182:THR:CG2	2.18	0.56
1:E:20:GLY:O	1:E:24:VAL:HG22	2.06	0.56
1:B:482:TYR:O	1:B:486:ILE:HD12	2.05	0.56
1:E:274:GLY:O	1:E:275:GLU:HG2	2.05	0.56
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.88	0.56
1:C:466:ARG:HB2	1:C:466:ARG:NH1	2.20	0.56
1:E:75:ILE:HD11	1:E:129:VAL:HG13	1.87	0.56
1:A:107:LEU:CG	1:A:126:LYS:HE3	2.30	0.56
1:A:432:PRO:HB2	1:A:437:GLN:HG2	1.87	0.56
1:C:371:LEU:HD12	1:C:482:TYR:CE1	2.41	0.56
1:E:272:THR:OG1	1:E:314:ILE:HD11	2.04	0.56
1:A:37:THR:HG22	1:A:41:LYS:HE3	1.87	0.56
1:F:271:ILE:C	1:F:272:THR:HG22	2.26	0.56
1:D:205:GLN:NE2	1:F:496:ALA:HB2	2.20	0.56
1:F:63:PHE:CZ	1:F:75:ILE:CD1	2.89	0.56
1:A:370:ASP:OD1	1:A:371:LEU:N	2.29	0.56
1:B:38:GLU:H	1:B:41:LYS:HD2	1.71	0.56
1:D:3:ARG:HD2	1:D:4:GLU:N	2.20	0.56
1:E:23:ILE:CG2	1:E:471:TYR:CD1	2.89	0.56
1:A:458:GLU:HG3	1:A:459:ARG:N	2.21	0.55
1:B:222:GLY:HA2	1:B:372:TYR:OH	2.06	0.55
1:B:42:ARG:O	1:B:46:ARG:HG3	2.06	0.55
1:B:381:SER:O	1:B:384:GLU:HB3	2.06	0.55
1:E:99:VAL:HG13	1:E:130:LYS:HA	1.88	0.55
1:A:196:ALA:HB2	1:A:388:ASN:HB2	1.88	0.55
1:A:211:ARG:HH22	3:A:552:NDP:H72N	1.53	0.55
1:D:17:PHE:CE1	1:D:486:ILE:HG12	2.42	0.55
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.88	0.55
1:E:175:GLU:H	1:E:175:GLU:CD	2.10	0.55
1:E:90:LYS:HD3	1:E:122:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:MET:HA	1:F:150:MET:HE3	1.88	0.55
1:F:374:ASN:HB2	3:F:552:NDP:C5N	2.36	0.55
1:F:201:LYS:HZ2	1:F:388:ASN:HD21	1.52	0.55
1:F:457:MET:HA	1:F:457:MET:CE	2.37	0.55
1:F:84:GLN:C	1:F:86:ARG:H	2.08	0.55
1:A:23:ILE:HD12	1:A:473:LEU:HD21	1.88	0.55
1:A:345:ALA:HB1	1:A:373:LEU:CD1	2.33	0.55
1:B:201:LYS:HZ2	1:B:388:ASN:HD21	1.53	0.55
1:D:459:ARG:O	1:D:463:GLN:HG2	2.06	0.55
1:F:211:ARG:HH22	3:F:552:NDP:H72N	1.55	0.55
1:A:113:TYR:C	1:A:371:LEU:HD21	2.27	0.55
1:B:409:LEU:HD11	1:C:409:LEU:HD13	1.87	0.55
1:F:496:ALA:HB3	1:F:498:VAL:O	2.05	0.55
1:F:75:ILE:HG12	1:F:76:GLU:N	2.20	0.55
1:C:368:ILE:HB	1:C:373:LEU:HD12	1.88	0.55
1:C:39:GLU:C	1:C:41:LYS:H	2.09	0.55
1:D:167:PRO:CD	1:D:200:GLY:HA3	2.37	0.55
1:F:201:LYS:HZ2	1:F:388:ASN:ND2	2.04	0.55
1:F:495:GLU:O	1:F:497:GLY:N	2.37	0.55
1:A:281:TRP:CZ2	1:A:283:PRO:CG	2.90	0.55
1:A:427:THR:O	1:A:427:THR:HG23	2.06	0.55
1:D:315:LEU:HD13	1:D:331:LEU:HD13	1.88	0.55
1:D:443:ALA:HB2	1:E:401:TYR:CE2	2.42	0.55
1:E:495:GLU:OE1	1:F:204:SER:CB	2.55	0.55
1:C:203:ILE:HD11	1:C:209:HIS:HA	1.89	0.55
1:E:79:ARG:NH2	1:E:163:ASP:OD2	2.39	0.55
1:E:489:VAL:O	1:E:492:VAL:HG13	2.07	0.55
1:B:96:SER:O	1:B:99:VAL:HG13	2.06	0.55
1:D:186:THR:O	1:D:189:HIS:ND1	2.30	0.55
1:D:248:VAL:CG2	1:D:272:THR:HG23	2.37	0.55
1:D:346:GLU:HG2	1:D:351:PRO:CG	2.34	0.55
1:E:246:THR:CG2	1:E:319:CYS:HA	2.37	0.55
1:F:142:GLU:O	1:F:146:ARG:HG3	2.07	0.55
1:B:177:SER:HB2	1:B:202:PRO:HG2	1.89	0.55
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.37	0.55
1:C:47:SER:O	1:C:51:ILE:HG13	2.07	0.55
1:E:94:ARG:HB2	1:E:168:ASP:OD1	2.07	0.55
1:F:95:TYR:HB3	1:F:133:PRO:HG3	1.88	0.55
1:A:232:TYR:O	1:A:236:LEU:HB2	2.07	0.54
1:B:141:LEU:O	1:B:145:THR:HG23	2.07	0.54
1:D:314:ILE:HG23	1:D:315:LEU:N	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:PHE:CZ	1:E:75:ILE:HD12	2.42	0.54
1:F:478:ARG:NH1	1:F:478:ARG:HG3	2.22	0.54
1:A:154:LYS:HD2	1:E:189:HIS:HB3	1.88	0.54
1:B:273:VAL:HG21	1:B:291:LEU:CD1	2.35	0.54
1:B:444:SER:O	1:B:447:ASP:HB2	2.07	0.54
1:B:90:LYS:HD2	1:B:164:VAL:O	2.06	0.54
1:F:131:ILE:O	1:F:133:PRO:HD3	2.07	0.54
1:C:24:VAL:HB	1:C:28:LEU:HD22	1.90	0.54
1:D:146:ARG:NH2	1:D:181:ASP:OD2	2.40	0.54
1:E:166:ALA:HB1	1:E:167:PRO:HD2	1.88	0.54
1:F:174:ARG:O	1:F:177:SER:HB3	2.08	0.54
1:F:146:ARG:NH2	1:F:181:ASP:OD2	2.40	0.54
1:F:271:ILE:HD12	1:F:272:THR:HG22	1.90	0.54
1:F:294:PHE:CE2	1:F:298:HIS:ND1	2.75	0.54
1:B:248:VAL:HG23	1:B:272:THR:OG1	2.08	0.54
1:B:408:HIS:CE1	1:C:435:GLU:HG2	2.43	0.54
1:F:84:GLN:C	1:F:86:ARG:N	2.61	0.54
1:B:378:VAL:HA	1:B:381:SER:HB2	1.87	0.54
1:C:37:THR:O	1:C:38:GLU:HB3	2.08	0.54
1:F:178:TRP:O	1:F:182:THR:HG22	2.07	0.54
1:A:112:THR:CG2	1:A:124:GLY:HA3	2.30	0.54
1:A:172:GLY:H	1:A:175:GLU:HG2	1.72	0.54
1:A:19:ARG:HG2	1:A:479:THR:CG2	2.37	0.54
1:C:344:ILE:HB	1:C:367:VAL:CG1	2.38	0.54
1:D:201:LYS:HZ1	1:D:388:ASN:HD21	1.55	0.54
1:F:219:VAL:HA	1:F:373:LEU:CD2	2.38	0.54
1:F:32:LEU:CD1	1:F:494:ASN:HD21	2.19	0.54
1:A:490:PHE:O	1:A:491:ARG:HB3	2.07	0.54
1:B:95:TYR:HB3	1:B:133:PRO:HG3	1.89	0.54
1:C:90:LYS:HD2	1:C:164:VAL:HB	1.89	0.54
1:E:90:LYS:HD2	1:E:164:VAL:HB	1.90	0.54
1:F:210:GLY:O	1:F:214:ALA:HB2	2.08	0.54
1:A:344:ILE:HB	1:A:367:VAL:CG1	2.38	0.54
1:B:89:CYS:HA	1:B:123:GLY:O	2.08	0.54
1:C:63:PHE:CE1	1:C:75:ILE:HD12	2.42	0.54
1:D:108:ALA:O	1:D:111:MET:HB2	2.08	0.54
1:B:19:ARG:HG2	1:B:479:THR:HG21	1.90	0.54
1:C:108:ALA:O	1:C:111:MET:HB2	2.08	0.54
1:C:158:ILE:HG12	1:C:159:GLY:H	1.72	0.54
1:C:308:LYS:HG3	1:C:309:ILE:O	2.07	0.54
1:E:346:GLU:OE1	1:E:352:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LYS:HA	1:E:371:LEU:HD23	1.89	0.54
1:F:427:THR:HG23	1:F:427:THR:O	2.08	0.54
1:A:400:LYS:HB2	1:B:455:TYR:HB2	1.89	0.53
1:C:114:LYS:HA	1:C:371:LEU:HD23	1.89	0.53
1:F:112:THR:HG22	1:F:124:GLY:H	1.71	0.53
1:F:2:ASP:O	1:F:3:ARG:HB2	2.07	0.53
1:B:272:THR:HG21	1:B:317:VAL:HG21	1.90	0.53
1:C:186:THR:OG1	1:C:187:ILE:N	2.36	0.53
1:C:21:ALA:HA	1:C:486:ILE:HD13	1.90	0.53
1:D:303:GLY:N	1:D:309:ILE:HD11	2.22	0.53
1:D:326:ALA:O	3:D:552:NDP:H4D	2.08	0.53
1:D:201:LYS:HZ2	1:D:388:ASN:HD21	1.56	0.53
1:F:68:ASP:OD1	1:F:137:THR:HG21	2.09	0.53
1:B:146:ARG:NE	1:B:182:THR:HG22	2.24	0.53
1:B:368:ILE:HB	1:B:373:LEU:HD12	1.90	0.53
1:E:32:LEU:HD13	1:E:494:ASN:ND2	2.22	0.53
1:A:107:LEU:HB3	1:A:126:LYS:CG	2.28	0.53
1:C:117:VAL:CG2	1:C:371:LEU:HD22	2.38	0.53
1:D:2:ASP:CG	1:D:3:ARG:N	2.61	0.53
1:E:39:GLU:C	1:E:41:LYS:H	2.10	0.53
1:F:232:TYR:CE2	1:F:465:MET:HG2	2.43	0.53
1:F:47:SER:O	1:F:51:ILE:HG13	2.09	0.53
1:B:172:GLY:H	1:B:175:GLU:HG2	1.73	0.53
1:C:44:ARG:HH22	1:C:494:ASN:HB2	1.73	0.53
1:D:26:ASP:HA	1:D:42:ARG:NH2	2.24	0.53
1:B:446:LYS:NZ	1:B:446:LYS:HB2	2.24	0.53
1:D:314:ILE:HA	1:D:317:VAL:HG23	1.90	0.53
1:D:432:PRO:HB2	1:D:437:GLN:HG2	1.89	0.53
1:D:19:ARG:HG2	1:D:479:THR:CG2	2.37	0.53
1:D:53:LYS:O	1:D:82:HIS:CE1	2.62	0.53
1:A:248:VAL:CB	1:A:272:THR:HG23	2.37	0.53
1:B:82:HIS:HD2	1:B:112:THR:CG2	2.03	0.53
1:C:374:ASN:HB2	3:C:552:NDP:C5N	2.39	0.53
1:C:114:LYS:NZ	2:C:502:GLU:O	2.42	0.53
1:D:222:GLY:HA2	1:D:372:TYR:OH	2.08	0.53
1:D:346:GLU:CG	1:D:351:PRO:HG2	2.37	0.53
1:E:255:VAL:HG22	1:E:325:ALA:HB1	1.90	0.53
1:D:24:VAL:HG11	1:D:483:VAL:HG13	1.90	0.53
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.91	0.53
1:B:166:ALA:HA	1:B:199:THR:O	2.08	0.53
1:F:114:LYS:HA	1:F:371:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ILE:C	1:D:272:THR:HG22	2.28	0.53
1:D:314:ILE:CG2	1:D:315:LEU:N	2.71	0.53
1:D:19:ARG:CG	1:D:479:THR:HG21	2.38	0.53
1:E:201:LYS:HZ2	1:E:388:ASN:ND2	2.07	0.53
1:A:328:GLU:HB2	1:A:350:GLY:O	2.09	0.52
1:A:489:VAL:HG12	1:A:490:PHE:N	2.24	0.52
1:A:57:HIS:HE1	1:A:84:GLN:HE22	1.54	0.52
1:C:255:VAL:HG22	1:C:325:ALA:HB1	1.91	0.52
1:E:246:THR:O	1:E:320:ASP:HB2	2.09	0.52
1:D:417:LEU:HD21	1:F:417:LEU:CD1	2.39	0.52
1:E:432:PRO:HA	1:F:412:SER:HB3	1.91	0.52
1:A:17:PHE:CE2	1:A:53:LYS:HG3	2.44	0.52
1:B:422:GLY:C	1:B:423:LYS:HD2	2.30	0.52
1:B:85:HIS:HD2	1:B:492:VAL:HG21	1.73	0.52
1:E:378:VAL:HA	1:E:381:SER:HB2	1.91	0.52
1:A:67:ARG:HD2	1:A:140:GLU:OE1	2.10	0.52
1:B:171:THR:HB	1:B:175:GLU:HG3	1.91	0.52
1:E:199:THR:HA	1:E:384:GLU:OE1	2.09	0.52
2:E:502:GLU:HA	3:E:552:NDP:H41N	1.92	0.52
1:B:346:GLU:HG2	1:B:351:PRO:HG2	1.90	0.52
1:D:75:ILE:HG12	1:D:76:GLU:N	2.24	0.52
1:E:346:GLU:HG2	1:E:351:PRO:CG	2.40	0.52
1:A:55:CYS:HA	1:A:82:HIS:HA	1.91	0.52
1:B:38:GLU:HG2	1:B:40:GLN:HG2	1.91	0.52
1:B:227:ILE:HD11	1:B:245:LYS:HG2	1.92	0.52
1:E:252:PHE:CZ	1:E:257:LEU:HD13	2.44	0.52
1:E:291:LEU:CD2	1:E:301:ILE:HG22	2.40	0.52
1:A:371:LEU:HD12	1:A:482:TYR:CD1	2.44	0.52
1:B:478:ARG:HG3	1:B:478:ARG:HH11	1.75	0.52
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.91	0.52
1:E:59:LEU:O	1:E:78:TYR:HA	2.09	0.52
1:C:10:PHE:HA	1:C:106:ALA:HB2	1.90	0.52
1:C:220:PHE:CD2	1:C:221:HIS:N	2.78	0.52
1:C:217:ARG:NH2	1:C:450:HIS:CD2	2.78	0.52
1:C:462:ARG:NH1	1:C:465:MET:HE1	2.25	0.52
1:E:112:THR:CG2	1:E:124:GLY:H	2.12	0.52
1:E:417:LEU:CD1	1:F:417:LEU:HD21	2.40	0.52
1:B:346:GLU:HG2	1:B:351:PRO:CG	2.40	0.52
1:B:457:MET:HE1	1:B:457:MET:HA	1.92	0.52
1:A:277:ASP:O	1:A:302:LEU:HD11	2.09	0.51
1:B:107:LEU:HB3	1:B:126:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:CB	1:B:258:HIS:CD2	2.92	0.51
1:C:163:ASP:O	1:C:165:PRO:HD3	2.10	0.51
1:F:339:VAL:HG12	1:F:341:ALA:H	1.75	0.51
1:A:90:LYS:HE3	1:A:381:SER:HB3	1.92	0.51
1:B:248:VAL:O	1:B:248:VAL:HG13	2.10	0.51
1:B:446:LYS:HZ3	1:B:446:LYS:CB	2.24	0.51
1:C:236:LEU:HD21	1:C:343:ILE:HG12	1.92	0.51
1:E:103:GLU:O	1:E:107:LEU:HB2	2.10	0.51
1:E:245:LYS:HA	1:E:320:ASP:OD1	2.10	0.51
1:E:53:LYS:O	1:E:82:HIS:CE1	2.62	0.51
1:F:272:THR:OG1	1:F:273:VAL:N	2.42	0.51
1:F:321:ILE:HG23	1:F:343:ILE:HB	1.92	0.51
1:F:372:TYR:CZ	1:F:461:ALA:HB2	2.46	0.51
1:B:84:GLN:O	1:B:86:ARG:N	2.44	0.51
1:D:248:VAL:HG21	1:D:314:ILE:HG12	1.91	0.51
1:B:414:GLN:HG3	1:B:428:ILE:O	2.10	0.51
1:C:214:ALA:CB	1:C:380:VAL:HG21	2.39	0.51
1:B:107:LEU:CG	1:B:126:LYS:HE3	2.39	0.51
1:C:252:PHE:CZ	1:C:291:LEU:HD13	2.46	0.51
1:C:396:ARG:HD2	1:C:396:ARG:O	2.10	0.51
1:C:39:GLU:C	1:C:41:LYS:N	2.62	0.51
1:C:96:SER:O	1:C:99:VAL:CG1	2.59	0.51
1:F:37:THR:O	1:F:38:GLU:CB	2.58	0.51
1:E:345:ALA:HB1	1:E:373:LEU:CD1	2.41	0.51
1:B:146:ARG:CG	1:B:182:THR:HG21	2.40	0.51
1:C:94:ARG:O	1:C:128:GLY:HA2	2.11	0.51
1:C:374:ASN:HB2	3:C:552:NDP:H5N	1.91	0.51
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.93	0.51
1:F:353:THR:HB	1:F:354:PRO:CD	2.39	0.51
1:E:435:GLU:HB3	1:F:408:HIS:CD2	2.45	0.51
1:A:142:GLU:OE2	1:A:146:ARG:NH1	2.44	0.51
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.46	0.51
1:C:248:VAL:HG22	1:C:249:VAL:N	2.25	0.51
1:C:359:ILE:O	1:C:363:ARG:HB2	2.11	0.51
1:E:392:VAL:HG11	1:E:397:LEU:HD11	1.92	0.51
1:F:232:TYR:HE2	1:F:465:MET:HG2	1.74	0.51
1:F:211:ARG:NH2	2:F:502:GLU:HG3	2.26	0.51
1:B:323:ILE:HG12	1:B:345:ALA:HB3	1.93	0.51
1:B:407:TYR:CZ	1:B:440:ILE:HD13	2.45	0.51
1:C:245:LYS:HA	1:C:320:ASP:OD1	2.11	0.51
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:LEU:HB3	1:E:476:ASP:HB3	1.92	0.51
1:A:196:ALA:HB2	1:A:388:ASN:CB	2.40	0.51
1:D:417:LEU:HD13	1:E:417:LEU:HD21	1.93	0.51
1:E:19:ARG:HG2	1:E:479:THR:CG2	2.41	0.51
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.93	0.51
1:F:214:ALA:HB1	1:F:380:VAL:HG21	1.92	0.51
1:B:337:PRO:HD3	1:B:359:ILE:CD1	2.41	0.50
1:C:95:TYR:OH	1:C:145:THR:HB	2.11	0.50
1:E:421:PHE:CD2	1:E:421:PHE:N	2.77	0.50
1:F:118:VAL:HG11	1:F:375:ALA:HB3	1.91	0.50
1:A:291:LEU:O	1:A:291:LEU:HD22	2.11	0.50
1:B:211:ARG:O	1:B:211:ARG:HD2	2.11	0.50
1:B:32:LEU:HD11	1:B:44:ARG:HH12	1.75	0.50
1:B:75:ILE:O	1:B:75:ILE:HD13	2.11	0.50
1:D:58:VAL:HG11	1:D:101:VAL:HG23	1.94	0.50
1:E:249:VAL:HG22	1:E:251:GLY:O	2.12	0.50
1:E:370:ASP:CG	1:E:371:LEU:H	2.13	0.50
1:F:214:ALA:CB	1:F:380:VAL:HG21	2.40	0.50
1:A:478:ARG:HH11	1:A:478:ARG:CG	2.03	0.50
1:A:69:ASP:C	1:A:69:ASP:OD2	2.50	0.50
1:C:2:ASP:O	1:C:6:ASP:HB2	2.12	0.50
1:C:349:ASN:ND2	2:C:502:GLU:OXT	2.37	0.50
1:E:166:ALA:HB1	1:E:167:PRO:CD	2.41	0.50
1:E:219:VAL:HA	1:E:373:LEU:CD2	2.41	0.50
1:E:111:MET:SD	2:E:502:GLU:OXT	2.69	0.50
1:F:416:SER:HA	1:F:419:ARG:NH1	2.26	0.50
1:B:483:VAL:O	1:B:487:GLU:HB2	2.10	0.50
1:C:165:PRO:O	1:C:166:ALA:HB2	2.10	0.50
1:C:232:TYR:CE2	1:C:465:MET:HG2	2.42	0.50
1:A:185:SER:O	1:E:154:LYS:HD3	2.11	0.50
1:E:217:ARG:HA	1:E:262:TYR:CD1	2.46	0.50
1:A:274:GLY:HA3	1:A:314:ILE:HD12	1.94	0.50
1:B:126:LYS:NZ	1:B:168:ASP:OD2	2.45	0.50
1:E:303:GLY:H	1:E:309:ILE:HD11	1.76	0.50
1:F:114:LYS:HA	1:F:371:LEU:CD2	2.41	0.50
1:E:492:VAL:O	1:F:205:GLN:NE2	2.44	0.50
1:A:483:VAL:O	1:A:487:GLU:HB2	2.12	0.50
1:B:336:ALA:N	1:B:337:PRO:CD	2.73	0.50
1:C:110:LEU:O	1:C:114:LYS:HB2	2.11	0.50
1:A:248:VAL:HG13	1:A:322:LEU:HD12	1.92	0.50
1:B:245:LYS:HD2	1:B:245:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ALA:HB3	1:B:359:ILE:HD12	1.94	0.50
1:B:75:ILE:HD11	1:B:129:VAL:HG13	1.93	0.50
1:C:421:PHE:O	1:C:422:GLY:C	2.50	0.50
1:D:460:SER:HA	1:D:463:GLN:CG	2.42	0.50
1:A:172:GLY:O	1:A:176:MET:HG2	2.10	0.50
1:E:10:PHE:CA	1:E:106:ALA:HB2	2.42	0.50
1:F:118:VAL:HG11	1:F:375:ALA:CB	2.42	0.50
1:A:339:VAL:O	1:A:340:LYS:HB2	2.12	0.50
1:D:409:LEU:HD13	1:E:409:LEU:HD11	1.93	0.50
1:F:163:ASP:O	1:F:165:PRO:HD3	2.12	0.50
1:A:111:MET:HE1	1:A:378:VAL:HG11	1.94	0.49
1:D:3:ARG:C	1:D:5:ASP:H	2.14	0.49
1:A:189:HIS:HE1	1:E:187:ILE:HD12	1.77	0.49
1:E:56:ASN:HD22	1:E:84:GLN:NE2	2.10	0.49
1:B:88:PRO:HG3	1:B:160:PRO:O	2.12	0.49
1:B:113:TYR:C	1:B:371:LEU:HD21	2.33	0.49
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.12	0.49
1:E:423:LYS:HD2	1:E:423:LYS:N	2.26	0.49
1:F:271:ILE:HD11	1:F:319:CYS:HB3	1.94	0.49
1:F:264:HIS:CD2	1:F:288:PRO:HD3	2.47	0.49
1:F:366:MET:HG3	1:F:475:LEU:HD22	1.94	0.49
1:A:446:LYS:O	1:A:447:ASP:C	2.50	0.49
1:B:91:GLY:O	1:B:165:PRO:HA	2.13	0.49
1:B:246:THR:CG2	1:B:319:CYS:HA	2.42	0.49
1:C:65:ILE:HG13	1:C:144:ILE:CG1	2.40	0.49
1:D:107:LEU:CB	1:D:126:LYS:HE3	2.43	0.49
1:F:84:GLN:O	1:F:86:ARG:N	2.45	0.49
1:A:321:ILE:HG23	1:A:343:ILE:CG2	2.42	0.49
1:A:412:SER:HA	1:B:433:THR:HG23	1.93	0.49
1:C:44:ARG:NH2	1:C:494:ASN:HB2	2.26	0.49
1:D:252:PHE:CZ	1:D:291:LEU:HD13	2.47	0.49
1:F:199:THR:HA	1:F:384:GLU:OE1	2.13	0.49
1:E:272:THR:HB	1:E:280:ILE:O	2.13	0.49
1:F:271:ILE:O	1:F:272:THR:HG22	2.13	0.49
1:F:495:GLU:C	1:F:497:GLY:H	2.16	0.49
1:B:199:THR:HA	1:B:384:GLU:OE1	2.11	0.49
1:D:427:THR:O	1:D:427:THR:HG23	2.12	0.49
1:E:433:THR:HG23	1:F:412:SER:OG	2.13	0.49
1:B:163:ASP:OD2	1:B:163:ASP:C	2.51	0.49
1:C:316:GLU:CD	1:C:338:ARG:HD2	2.32	0.49
1:D:272:THR:HG21	1:D:317:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:SER:HB2	3:D:552:NDP:O2X	2.13	0.49
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.94	0.49
1:F:19:ARG:HG2	1:F:479:THR:HG21	1.95	0.49
1:A:95:TYR:OH	1:A:145:THR:HG22	2.13	0.49
1:B:258:HIS:HD2	1:B:261:ARG:NH1	2.11	0.49
1:B:263:LEU:HD11	1:B:323:ILE:HD11	1.94	0.49
1:B:112:THR:CB	1:B:124:GLY:H	2.26	0.49
1:C:214:ALA:HB1	1:C:380:VAL:CG2	2.42	0.49
1:D:423:LYS:HD2	1:D:423:LYS:N	2.27	0.49
1:F:202:PRO:HD2	1:F:205:GLN:HB2	1.94	0.49
1:F:17:PHE:CE1	1:F:486:ILE:HG12	2.48	0.49
1:A:337:PRO:HD3	1:A:359:ILE:HD13	1.95	0.49
1:B:399:PHE:HA	1:B:441:SER:O	2.13	0.49
1:C:223:ILE:CD1	1:C:263:LEU:HD11	2.43	0.49
1:D:215:THR:O	1:D:219:VAL:HG23	2.13	0.49
1:E:427:THR:O	1:E:429:PRO:CD	2.60	0.49
1:E:67:ARG:NE	1:E:73:GLU:OE1	2.46	0.49
1:D:142:GLU:OE1	1:F:498:VAL:HG21	2.12	0.49
1:F:92:GLY:O	1:F:126:LYS:HD3	2.12	0.49
1:A:211:ARG:HD3	1:A:380:VAL:HG12	1.94	0.48
1:D:178:TRP:HE1	1:F:498:VAL:HG21	1.78	0.48
1:D:5:ASP:OD2	1:D:332:THR:HB	2.13	0.48
1:D:95:TYR:HB3	1:D:133:PRO:CG	2.41	0.48
1:E:258:HIS:CD2	1:E:261:ARG:NH1	2.73	0.48
1:E:35:ARG:CD	1:E:35:ARG:H	2.08	0.48
1:E:55:CYS:HA	1:E:82:HIS:HA	1.95	0.48
1:F:374:ASN:CB	3:F:552:NDP:H5N	2.43	0.48
1:A:408:HIS:CD2	1:B:435:GLU:HB3	2.48	0.48
1:A:456:THR:OG1	1:C:396:ARG:NH2	2.45	0.48
1:E:271:ILE:HD12	1:E:272:THR:HG22	1.92	0.48
1:F:75:ILE:HD11	1:F:129:VAL:HG13	1.95	0.48
1:B:363:ARG:NH1	1:B:365:ILE:HD11	2.29	0.48
1:D:468:ALA:HA	1:D:473:LEU:HD12	1.94	0.48
1:A:353:THR:HB	1:A:354:PRO:CD	2.42	0.48
1:B:324:PRO:HD2	1:B:345:ALA:O	2.13	0.48
1:C:494:ASN:OD1	1:C:495:GLU:N	2.46	0.48
1:D:232:TYR:CE2	1:D:465:MET:HG2	2.48	0.48
1:F:12:MET:CE	1:F:16:PHE:HE1	2.25	0.48
1:F:186:THR:OG1	1:F:187:ILE:N	2.44	0.48
1:F:35:ARG:O	1:F:37:THR:HG23	2.14	0.48
1:A:493:TYR:O	1:A:494:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:HD2	1:A:9:PHE:O	1.96	0.48
1:B:198:VAL:HG22	1:B:199:THR:N	2.28	0.48
1:B:219:VAL:HA	1:B:373:LEU:HD23	1.95	0.48
1:B:278:GLY:HA3	1:B:302:LEU:HD21	1.96	0.48
1:C:341:ALA:O	1:C:365:ILE:HG23	2.14	0.48
1:D:178:TRP:HE1	1:F:498:VAL:HG22	1.78	0.48
1:B:317:VAL:CG1	1:B:318:ASP:N	2.77	0.48
1:E:93:ILE:HD11	1:E:95:TYR:HE1	1.70	0.48
1:A:186:THR:O	1:A:189:HIS:ND1	2.46	0.48
1:B:414:GLN:OE1	1:B:429:PRO:HA	2.14	0.48
1:B:97:THR:HG23	1:B:132:ASN:HB2	1.95	0.48
1:C:248:VAL:CG2	1:C:249:VAL:N	2.76	0.48
1:E:325:ALA:O	3:E:552:NDP:H51N	2.14	0.48
1:E:315:LEU:HD13	1:E:331:LEU:CD1	2.44	0.48
1:A:371:LEU:HD12	1:A:482:TYR:CE1	2.49	0.48
1:A:75:ILE:HD11	1:A:129:VAL:HG13	1.96	0.48
1:B:167:PRO:HD3	1:B:200:GLY:HA3	1.96	0.48
1:B:84:GLN:C	1:B:86:ARG:N	2.67	0.48
1:C:131:ILE:O	1:C:133:PRO:HD3	2.14	0.48
1:C:41:LYS:O	1:C:45:VAL:HG23	2.13	0.48
1:D:174:ARG:HD2	1:D:178:TRP:CH2	2.49	0.48
1:E:186:THR:OG1	1:E:187:ILE:N	2.47	0.48
1:E:275:GLU:HG3	1:E:301:ILE:CD1	2.44	0.48
1:E:339:VAL:HG11	1:E:344:ILE:HD11	1.95	0.48
1:E:37:THR:O	1:E:38:GLU:HB3	2.14	0.48
1:E:82:HIS:CD2	1:E:112:THR:CG2	2.92	0.48
1:A:186:THR:OG1	1:A:187:ILE:N	2.47	0.48
1:B:342:LYS:HD3	1:B:342:LYS:N	2.29	0.48
1:C:278:GLY:HA3	1:C:302:LEU:HD21	1.96	0.48
1:D:248:VAL:HG21	1:D:314:ILE:CG1	2.44	0.48
1:D:408:HIS:CE1	1:F:435:GLU:HG2	2.49	0.48
1:E:93:ILE:HB	1:E:127:ALA:HB3	1.95	0.48
1:D:160:PRO:O	1:E:192:ILE:HD12	2.14	0.48
1:E:291:LEU:O	1:E:291:LEU:HD22	2.14	0.48
1:E:382:TYR:OH	1:F:392:VAL:HG13	2.14	0.48
1:F:272:THR:HG21	1:F:317:VAL:HG21	1.96	0.48
1:A:468:ALA:HA	1:A:473:LEU:HD12	1.96	0.48
1:A:9:PHE:CE1	1:A:328:GLU:HG3	2.49	0.48
1:B:75:ILE:C	1:B:75:ILE:HD13	2.33	0.48
1:E:247:PHE:CZ	1:E:270:CYS:HB2	2.48	0.48
1:E:398:THR:O	1:E:399:PHE:C	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:THR:O	1:F:189:HIS:ND1	2.47	0.48
1:F:165:PRO:HD2	1:F:197:CYS:O	2.14	0.48
1:B:35:ARG:O	1:B:37:THR:N	2.46	0.47
1:D:236:LEU:HA	1:D:236:LEU:HD12	1.67	0.47
1:D:396:ARG:O	1:D:396:ARG:HD2	2.13	0.47
1:D:88:PRO:HD2	1:D:122:PHE:CE2	2.49	0.47
1:E:282:ASN:C	1:E:282:ASN:OD1	2.52	0.47
1:D:99:VAL:HG21	1:D:128:GLY:C	2.34	0.47
1:A:61:LEU:HD12	1:D:57:HIS:HD2	1.79	0.47
1:A:47:SER:CB	1:D:72:TRP:HB2	2.36	0.47
1:A:99:VAL:HG22	1:A:99:VAL:O	2.13	0.47
1:B:232:TYR:CE2	1:B:465:MET:HG2	2.43	0.47
1:C:147:ARG:O	1:C:151:GLU:HG2	2.14	0.47
1:C:339:VAL:HG12	1:C:341:ALA:H	1.79	0.47
1:C:339:VAL:HG21	1:C:360:PHE:CZ	2.49	0.47
1:F:126:LYS:NZ	2:F:502:GLU:N	2.62	0.47
1:B:294:PHE:CE2	1:B:298:HIS:ND1	2.76	0.47
1:C:462:ARG:NH1	1:C:465:MET:CE	2.77	0.47
1:F:345:ALA:HB1	1:F:373:LEU:CD1	2.45	0.47
1:C:61:LEU:HD12	1:F:57:HIS:HD2	1.78	0.47
1:A:173:GLU:OE2	1:A:202:PRO:HA	2.14	0.47
1:B:82:HIS:N	1:B:124:GLY:O	2.47	0.47
1:B:2:ASP:HB3	1:B:3:ARG:H	1.51	0.47
1:B:458:GLU:HG3	1:B:459:ARG:N	2.29	0.47
1:C:174:ARG:O	1:C:177:SER:HB3	2.14	0.47
1:D:263:LEU:HD11	1:D:323:ILE:HD11	1.97	0.47
1:E:175:GLU:HA	1:E:178:TRP:CE3	2.49	0.47
1:F:336:ALA:N	1:F:337:PRO:CD	2.75	0.47
1:F:378:VAL:HA	1:F:381:SER:HB2	1.96	0.47
1:F:56:ASN:HD22	1:F:84:GLN:HE21	1.60	0.47
1:A:96:SER:O	1:A:130:LYS:HA	2.15	0.47
1:C:153:ALA:HB1	1:C:187:ILE:HG13	1.96	0.47
1:C:363:ARG:NH1	1:C:365:ILE:HD11	2.30	0.47
1:D:107:LEU:CG	1:D:126:LYS:HE3	2.45	0.47
1:D:53:LYS:N	1:D:54:PRO:HD2	2.30	0.47
1:E:63:PHE:CZ	1:E:75:ILE:CD1	2.98	0.47
1:A:79:ARG:CD	1:A:127:ALA:HB2	2.43	0.47
1:E:152:LEU:O	1:E:153:ALA:C	2.53	0.47
1:A:409:LEU:C	1:A:409:LEU:HD23	2.35	0.47
1:B:141:LEU:HA	1:B:141:LEU:HD23	1.70	0.47
1:C:271:ILE:H	1:C:271:ILE:HG13	1.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:ILE:HG12	1:E:159:GLY:N	2.30	0.47
1:E:271:ILE:O	1:E:272:THR:HG22	2.15	0.47
1:F:49:LEU:HA	1:F:49:LEU:HD12	1.64	0.47
1:B:291:LEU:HD21	1:B:301:ILE:HG22	1.97	0.47
1:B:421:PHE:N	1:B:421:PHE:CD2	2.81	0.47
1:C:211:ARG:HA	1:C:380:VAL:HG11	1.96	0.47
1:C:414:GLN:OE1	1:C:429:PRO:HA	2.15	0.47
1:F:171:THR:HB	1:F:175:GLU:HG3	1.96	0.47
1:F:448:ILE:HD13	1:F:448:ILE:HA	1.72	0.47
1:A:118:VAL:HG23	1:A:120:VAL:CG2	2.41	0.47
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.97	0.47
1:B:248:VAL:HG13	1:B:322:LEU:HD12	1.96	0.47
1:C:344:ILE:HB	1:C:367:VAL:HG12	1.97	0.47
1:E:339:VAL:HG21	1:E:360:PHE:CE1	2.50	0.47
1:E:19:ARG:CG	1:E:479:THR:HG21	2.44	0.47
1:F:272:THR:OG1	1:F:314:ILE:HD11	2.15	0.47
1:A:163:ASP:C	1:A:163:ASP:OD2	2.53	0.47
1:A:304:PHE:CD1	1:A:305:PRO:HD2	2.50	0.47
1:A:433:THR:HG23	1:C:412:SER:HA	1.97	0.47
1:B:99:VAL:HG22	1:B:99:VAL:O	2.13	0.47
1:B:9:PHE:O	1:B:9:PHE:CD2	2.63	0.47
1:C:313:SER:HB3	1:C:316:GLU:HG3	1.96	0.47
1:C:246:THR:CG2	1:C:319:CYS:HA	2.45	0.47
1:D:248:VAL:CG2	1:D:314:ILE:HD11	2.45	0.47
1:D:314:ILE:HG23	1:D:315:LEU:HD23	1.97	0.47
1:F:271:ILE:HD12	1:F:272:THR:HG23	1.97	0.47
1:A:37:THR:HG22	1:A:41:LYS:CE	2.46	0.46
1:A:72:TRP:HB2	1:D:47:SER:HB3	1.97	0.46
1:B:371:LEU:HD12	1:B:482:TYR:CE1	2.49	0.46
1:C:196:ALA:HA	1:C:388:ASN:ND2	2.28	0.46
1:C:478:ARG:HG2	1:C:482:TYR:CE1	2.50	0.46
1:D:82:HIS:CG	1:D:109:SER:HA	2.50	0.46
1:D:112:THR:HG22	1:D:124:GLY:N	2.30	0.46
1:F:153:ALA:HA	1:F:158:ILE:CG2	2.45	0.46
1:F:322:LEU:HB3	1:F:344:ILE:CD1	2.45	0.46
1:A:114:LYS:NZ	2:A:502:GLU:OXT	2.42	0.46
1:A:51:ILE:O	1:A:51:ILE:HG22	2.14	0.46
1:A:408:HIS:CE1	1:B:435:GLU:HG2	2.49	0.46
1:C:332:THR:HG22	1:C:353:THR:HG23	1.95	0.46
1:C:5:ASP:HB3	1:C:332:THR:HB	1.97	0.46
1:C:96:SER:O	1:C:99:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ALA:HA	1:D:388:ASN:HD22	1.81	0.46
1:D:313:SER:HB3	1:D:316:GLU:HG3	1.98	0.46
1:E:242:PHE:CE1	1:E:263:LEU:HD23	2.51	0.46
1:E:103:GLU:OE1	1:E:328:GLU:OE1	2.33	0.46
1:F:341:ALA:O	1:F:365:ILE:HG23	2.14	0.46
1:A:201:LYS:NZ	1:A:388:ASN:ND2	2.59	0.46
1:A:236:LEU:HA	1:A:236:LEU:HD12	1.62	0.46
1:C:172:GLY:H	1:C:175:GLU:HG2	1.80	0.46
1:C:33:LYS:HE3	1:C:33:LYS:HB2	1.82	0.46
1:E:142:GLU:O	1:E:146:ARG:HG3	2.14	0.46
1:E:232:TYR:HE2	1:E:465:MET:HG2	1.81	0.46
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.77	0.46
1:A:371:LEU:HD13	1:A:481:ALA:HB1	1.97	0.46
1:B:211:ARG:HH12	3:B:552:NDP:H72N	1.63	0.46
1:C:314:ILE:HG12	1:C:314:ILE:O	2.14	0.46
1:C:84:GLN:C	1:C:86:ARG:N	2.68	0.46
1:C:84:GLN:C	1:C:86:ARG:H	2.18	0.46
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.98	0.46
1:E:172:GLY:H	1:E:175:GLU:CG	2.27	0.46
1:F:89:CYS:HA	1:F:123:GLY:O	2.15	0.46
1:D:400:LYS:HB2	1:F:455:TYR:HB2	1.97	0.46
1:A:161:GLY:HA3	1:C:192:ILE:HA	1.97	0.46
1:B:118:VAL:HG23	1:B:120:VAL:HG23	1.96	0.46
1:B:328:GLU:HA	1:B:351:PRO:HA	1.96	0.46
1:C:141:LEU:O	1:C:145:THR:CG2	2.61	0.46
1:D:114:LYS:HA	1:D:371:LEU:CD2	2.46	0.46
1:F:28:LEU:O	1:F:31:ASP:HB2	2.15	0.46
1:A:79:ARG:CG	1:A:127:ALA:HB2	2.45	0.46
1:B:33:LYS:O	1:B:34:THR:C	2.54	0.46
1:C:315:LEU:HB3	1:C:331:LEU:HD11	1.96	0.46
1:C:332:THR:HA	1:C:356:ALA:HB2	1.96	0.46
1:D:246:THR:CG2	1:D:319:CYS:HA	2.46	0.46
1:F:94:ARG:O	1:F:128:GLY:HA2	2.16	0.46
1:F:248:VAL:HB	1:F:272:THR:HG23	1.97	0.46
1:A:85:HIS:CE1	1:A:489:VAL:HG22	2.51	0.46
1:B:233:MET:CE	1:B:233:MET:HA	2.45	0.46
1:B:213:SER:HA	1:B:258:HIS:CG	2.51	0.46
1:B:36:GLU:O	1:B:37:THR:O	2.34	0.46
1:B:403:ARG:O	1:B:407:TYR:CD1	2.69	0.46
1:B:459:ARG:O	1:B:463:GLN:HG2	2.16	0.46
1:C:409:LEU:C	1:C:409:LEU:HD23	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:GLU:C	1:E:41:LYS:N	2.68	0.46
1:F:281:TRP:O	1:F:282:ASN:HB2	2.16	0.46
1:A:271:ILE:C	1:A:272:THR:HG22	2.36	0.46
1:C:15:GLY:O	1:C:16:PHE:C	2.53	0.46
1:C:275:GLU:HG3	1:C:301:ILE:HD13	1.98	0.46
1:F:245:LYS:HD2	1:F:245:LYS:N	2.31	0.46
1:B:114:LYS:HA	1:B:371:LEU:HD23	1.96	0.46
1:C:281:TRP:CG	1:C:282:ASN:N	2.84	0.46
1:C:211:ARG:HD3	1:C:380:VAL:HG12	1.97	0.46
1:E:232:TYR:CE2	1:E:465:MET:HG2	2.50	0.46
1:B:342:LYS:O	1:B:365:ILE:HG22	2.15	0.46
1:B:53:LYS:O	1:B:82:HIS:HE1	1.99	0.46
1:E:94:ARG:O	1:E:128:GLY:HA2	2.16	0.46
1:B:477:LEU:O	1:B:480:ALA:HB3	2.16	0.45
1:C:187:ILE:HD13	1:C:187:ILE:N	2.31	0.45
1:D:141:LEU:O	1:D:145:THR:CG2	2.63	0.45
1:D:217:ARG:HA	1:D:262:TYR:CD1	2.51	0.45
1:E:131:ILE:HG13	1:E:131:ILE:O	2.16	0.45
1:E:40:GLN:HE21	1:E:40:GLN:HB3	1.60	0.45
1:F:112:THR:CG2	1:F:124:GLY:H	2.29	0.45
1:F:150:MET:HA	1:F:150:MET:CE	2.43	0.45
1:A:321:ILE:HG23	1:A:343:ILE:HB	1.98	0.45
1:A:57:HIS:HE1	1:A:84:GLN:NE2	2.14	0.45
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.98	0.45
1:E:332:THR:HG22	1:E:353:THR:CG2	2.46	0.45
1:E:96:SER:O	1:E:99:VAL:HG12	2.16	0.45
1:B:202:PRO:O	1:B:203:ILE:C	2.55	0.45
1:C:131:ILE:HB	1:C:136:TYR:CE2	2.51	0.45
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.15	0.45
1:D:186:THR:OG1	1:D:187:ILE:N	2.47	0.45
1:A:459:ARG:O	1:A:463:GLN:HG2	2.17	0.45
1:A:52:ILE:HD13	1:A:489:VAL:CG1	2.45	0.45
1:D:248:VAL:CB	1:D:272:THR:HG23	2.45	0.45
1:D:336:ALA:N	1:D:337:PRO:CD	2.78	0.45
1:E:165:PRO:HD2	1:E:197:CYS:O	2.16	0.45
1:E:65:ILE:HG13	1:E:144:ILE:HG12	1.98	0.45
1:F:178:TRP:O	1:F:182:THR:CG2	2.65	0.45
1:A:248:VAL:HG21	1:A:314:ILE:HG12	1.99	0.45
1:A:373:LEU:O	1:A:373:LEU:HD22	2.17	0.45
1:B:381:SER:O	1:B:384:GLU:N	2.49	0.45
1:B:416:SER:HA	1:B:419:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLY:O	1:C:219:VAL:HB	2.17	0.45
1:D:220:PHE:CE1	1:D:242:PHE:CE2	3.05	0.45
1:D:314:ILE:O	1:D:317:VAL:HG23	2.16	0.45
1:D:434:ALA:O	1:D:437:GLN:HB2	2.16	0.45
1:E:451:SER:HB2	1:F:400:LYS:HB3	1.97	0.45
1:F:247:PHE:HB2	1:F:321:ILE:O	2.16	0.45
1:F:347:GLY:O	1:F:374:ASN:HB3	2.16	0.45
1:A:258:HIS:HD2	1:A:261:ARG:NH1	2.11	0.45
2:A:502:GLU:HA	3:A:552:NDP:H41N	1.98	0.45
1:B:409:LEU:O	1:B:412:SER:HB2	2.16	0.45
1:B:80:ALA:O	1:B:125:ALA:HA	2.17	0.45
1:C:336:ALA:H	1:C:337:PRO:HD2	1.81	0.45
1:F:402:GLU:O	1:F:403:ARG:C	2.53	0.45
1:B:158:ILE:HG12	1:B:159:GLY:N	2.32	0.45
1:B:16:PHE:O	1:B:19:ARG:HB3	2.17	0.45
1:B:271:ILE:C	1:B:272:THR:HG22	2.36	0.45
1:B:409:LEU:C	1:B:409:LEU:HD23	2.37	0.45
1:B:19:ARG:HG2	1:B:479:THR:CG2	2.46	0.45
1:C:185:SER:O	1:D:154:LYS:HD3	2.16	0.45
1:D:371:LEU:HD23	1:D:371:LEU:HA	1.75	0.45
1:D:455:TYR:HB2	1:E:400:LYS:HB2	1.98	0.45
1:A:189:HIS:CE1	1:E:187:ILE:HD12	2.51	0.45
1:A:204:SER:OG	1:A:205:GLN:HG2	2.16	0.45
1:A:219:VAL:HA	1:A:373:LEU:HD21	1.94	0.45
1:A:424:HIS:ND1	1:A:424:HIS:N	2.65	0.45
1:A:417:LEU:HD21	1:B:417:LEU:HD11	1.98	0.45
1:D:79:ARG:CG	1:D:127:ALA:HB2	2.47	0.45
1:D:255:VAL:HG13	3:D:552:NDP:O2N	2.16	0.45
1:F:58:VAL:HG11	1:F:101:VAL:HG23	1.99	0.45
1:A:65:ILE:HG13	1:A:144:ILE:HG12	1.97	0.45
1:E:319:CYS:O	1:E:341:ALA:HA	2.17	0.45
1:A:282:ASN:OD1	1:A:284:ASP:HB2	2.17	0.45
1:A:126:LYS:NZ	2:A:502:GLU:N	2.65	0.45
1:A:409:LEU:CD1	1:C:409:LEU:HD11	2.46	0.45
1:E:117:VAL:HG11	1:E:372:TYR:HB2	1.99	0.45
1:F:82:HIS:CE1	1:F:109:SER:HB3	2.52	0.45
1:C:110:LEU:HD12	1:C:110:LEU:HA	1.63	0.44
1:C:462:ARG:HG3	1:C:466:ARG:NH2	2.29	0.44
1:D:249:VAL:HG22	1:D:251:GLY:O	2.16	0.44
1:D:273:VAL:HG12	1:D:274:GLY:N	2.32	0.44
1:D:296:LEU:HD22	1:D:296:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ILE:C	1:D:75:ILE:HD13	2.37	0.44
1:A:316:GLU:OE2	1:A:338:ARG:HD2	2.17	0.44
1:B:296:LEU:HD22	1:B:296:LEU:HA	1.79	0.44
1:B:317:VAL:HG12	1:B:318:ASP:N	2.32	0.44
1:B:196:ALA:HB2	1:B:388:ASN:HB3	1.98	0.44
1:C:12:MET:HE2	1:C:16:PHE:HE1	1.83	0.44
1:C:342:LYS:HD3	1:C:342:LYS:N	2.33	0.44
1:C:91:GLY:O	1:C:165:PRO:HA	2.17	0.44
1:F:421:PHE:O	1:F:422:GLY:C	2.55	0.44
1:F:446:LYS:CB	1:F:446:LYS:NZ	2.80	0.44
1:D:272:THR:CG2	1:D:317:VAL:HG11	2.47	0.44
1:A:309:ILE:HD12	1:A:309:ILE:N	2.33	0.44
1:A:39:GLU:C	1:A:41:LYS:H	2.18	0.44
1:B:234:SER:O	1:B:237:GLY:N	2.50	0.44
1:B:169:MET:CG	3:B:552:NDP:H3D	2.48	0.44
1:C:367:VAL:O	1:C:369:PRO:HD3	2.16	0.44
1:C:446:LYS:CB	1:C:446:LYS:NZ	2.80	0.44
1:D:408:HIS:ND1	1:F:439:ARG:HD2	2.33	0.44
1:D:444:SER:OG	1:D:446:LYS:HG3	2.17	0.44
1:E:59:LEU:HB2	1:E:157:PHE:CZ	2.52	0.44
1:F:167:PRO:HD3	1:F:200:GLY:HA3	2.00	0.44
1:F:246:THR:O	1:F:320:ASP:HB2	2.16	0.44
1:F:353:THR:O	1:F:357:ASP:HB2	2.17	0.44
1:F:214:ALA:HB1	1:F:380:VAL:CG2	2.48	0.44
1:C:72:TRP:HB3	1:F:51:ILE:HD11	2.00	0.44
1:B:99:VAL:HG13	1:B:130:LYS:HA	1.99	0.44
1:B:202:PRO:HB2	1:B:205:GLN:HG3	1.99	0.44
1:B:63:PHE:CZ	1:B:75:ILE:CD1	3.00	0.44
1:B:9:PHE:C	1:B:9:PHE:CD2	2.90	0.44
1:D:152:LEU:HD22	1:D:157:PHE:CB	2.46	0.44
1:D:337:PRO:HD3	1:D:359:ILE:HD13	1.99	0.44
1:A:161:GLY:CA	1:C:192:ILE:HG13	2.48	0.44
1:B:217:ARG:HA	1:B:262:TYR:CD1	2.53	0.44
1:C:242:PHE:CE1	1:C:263:LEU:CD2	3.00	0.44
1:C:424:HIS:N	1:C:424:HIS:ND1	2.66	0.44
1:C:463:GLN:HB3	1:C:463:GLN:HE21	1.60	0.44
1:C:480:ALA:O	1:C:483:VAL:HB	2.17	0.44
1:D:316:GLU:OE2	1:D:338:ARG:HD2	2.16	0.44
1:E:90:LYS:HB2	1:E:122:PHE:CG	2.53	0.44
1:E:95:TYR:HB3	1:E:133:PRO:CG	2.47	0.44
1:F:93:ILE:O	1:F:93:ILE:HG13	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:SER:HB3	1:A:316:GLU:CG	2.47	0.44
1:B:25:GLU:O	1:B:29:VAL:HG23	2.18	0.44
1:E:282:ASN:OD1	1:E:284:ASP:N	2.51	0.44
1:F:82:HIS:ND1	1:F:109:SER:HB3	2.33	0.44
1:F:272:THR:HB	1:F:280:ILE:O	2.17	0.44
1:F:340:LYS:HE2	1:F:340:LYS:HB2	1.73	0.44
1:C:46:ARG:O	1:C:50:ARG:HB2	2.17	0.44
1:D:456:THR:HG22	1:D:457:MET:HE3	2.00	0.44
1:F:12:MET:HE2	1:F:16:PHE:HE1	1.82	0.44
1:F:457:MET:CA	1:F:457:MET:HE2	2.46	0.44
1:C:298:HIS:C	1:C:300:THR:H	2.21	0.44
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.83	0.44
1:F:26:ASP:HA	1:F:42:ARG:NH2	2.33	0.44
1:A:188:GLY:O	1:A:189:HIS:C	2.54	0.43
1:A:95:TYR:OH	1:A:145:THR:HB	2.18	0.43
1:B:231:SER:O	1:B:235:ILE:HD13	2.18	0.43
1:B:344:ILE:HB	1:B:367:VAL:CG1	2.45	0.43
1:C:10:PHE:CA	1:C:106:ALA:HB2	2.48	0.43
1:D:93:ILE:HA	1:D:127:ALA:O	2.18	0.43
1:D:68:ASP:OD1	1:D:137:THR:HG21	2.18	0.43
1:D:242:PHE:O	1:D:245:LYS:HB2	2.18	0.43
1:D:33:LYS:HE3	1:D:33:LYS:HB2	1.81	0.43
1:D:37:THR:HG22	1:D:41:LYS:CE	2.47	0.43
1:F:236:LEU:HD12	1:F:236:LEU:HA	1.84	0.43
1:A:178:TRP:O	1:A:182:THR:CG2	2.64	0.43
1:A:274:GLY:HA2	1:A:279:SER:HA	2.00	0.43
1:B:31:ASP:O	1:B:32:LEU:C	2.56	0.43
1:C:326:ALA:O	3:C:552:NDP:H4D	2.18	0.43
1:D:37:THR:O	1:D:40:GLN:HG2	2.17	0.43
1:E:108:ALA:O	1:E:111:MET:HB2	2.19	0.43
1:E:99:VAL:HG21	1:E:128:GLY:C	2.38	0.43
1:E:148:PHE:CE2	1:E:152:LEU:HD11	2.52	0.43
1:F:142:GLU:O	1:F:143:LYS:C	2.55	0.43
1:A:159:GLY:CA	1:A:162:VAL:HG13	2.44	0.43
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.81	0.43
1:B:348:ALA:HB3	1:B:351:PRO:HB3	2.01	0.43
1:C:37:THR:O	1:C:38:GLU:CB	2.66	0.43
1:D:17:PHE:HZ	1:D:49:LEU:HD12	1.83	0.43
1:D:272:THR:HG21	1:D:317:VAL:HG11	2.00	0.43
1:F:395:GLY:O	1:F:397:LEU:N	2.51	0.43
1:B:79:ARG:HG3	1:B:127:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:VAL:HG13	1:B:322:LEU:CD1	2.48	0.43
1:B:331:LEU:HA	1:B:331:LEU:HD12	1.77	0.43
1:C:95:TYR:HB3	1:C:133:PRO:HG3	1.99	0.43
1:D:448:ILE:HA	1:D:448:ILE:HD13	1.81	0.43
1:F:423:LYS:N	1:F:423:LYS:HD2	2.33	0.43
1:A:462:ARG:NH1	1:A:465:MET:HE1	2.34	0.43
1:B:165:PRO:C	1:B:198:VAL:HG23	2.39	0.43
1:B:187:ILE:HD12	1:F:189:HIS:HE1	1.83	0.43
1:B:371:LEU:HA	1:B:371:LEU:HD23	1.66	0.43
1:B:373:LEU:O	1:B:373:LEU:HD23	2.18	0.43
1:C:245:LYS:CD	1:C:245:LYS:N	2.81	0.43
1:C:264:HIS:HA	1:C:268:ALA:O	2.19	0.43
1:C:169:MET:CG	3:C:552:NDP:H3D	2.49	0.43
1:C:75:ILE:HD13	1:C:75:ILE:O	2.18	0.43
1:E:11:LYS:HA	1:E:14:GLU:HB2	2.01	0.43
1:F:146:ARG:CB	1:F:182:THR:HG21	2.48	0.43
1:F:230:ALA:O	1:F:231:SER:C	2.55	0.43
1:F:424:HIS:N	1:F:424:HIS:ND1	2.65	0.43
1:A:180:ALA:HB2	1:A:198:VAL:CG1	2.49	0.43
1:A:255:VAL:HG13	3:A:552:NDP:O2N	2.19	0.43
1:A:450:HIS:CE1	4:A:503:GTP:O1B	2.72	0.43
1:A:84:GLN:C	1:A:86:ARG:N	2.72	0.43
1:A:99:VAL:HG21	1:A:128:GLY:C	2.39	0.43
1:B:29:VAL:HG13	1:B:41:LYS:HB3	2.00	0.43
1:E:188:GLY:O	1:E:189:HIS:C	2.57	0.43
1:E:299:GLY:O	1:E:300:THR:HB	2.18	0.43
2:B:502:GLU:CA	3:B:552:NDP:H41N	2.38	0.43
1:C:118:VAL:HG11	1:C:375:ALA:HB3	2.00	0.43
1:C:410:LEU:HD12	1:C:410:LEU:HA	1.75	0.43
1:D:36:GLU:HB3	1:D:40:GLN:OE1	2.18	0.43
1:D:37:THR:O	1:D:38:GLU:CB	2.67	0.43
1:E:172:GLY:O	1:E:176:MET:HG2	2.19	0.43
1:E:248:VAL:HG23	1:E:272:THR:OG1	2.18	0.43
1:F:49:LEU:HD12	1:F:52:ILE:HD12	2.00	0.43
1:A:85:HIS:HB2	1:A:492:VAL:HG11	2.00	0.43
1:A:9:PHE:CD1	1:A:328:GLU:HG3	2.54	0.43
1:B:107:LEU:CB	1:B:126:LYS:HE3	2.48	0.43
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.76	0.43
1:C:126:LYS:HB2	1:C:126:LYS:HE2	1.85	0.43
1:C:56:ASN:HD22	1:C:84:GLN:NE2	2.16	0.43
1:D:11:LYS:HA	1:D:14:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LYS:HA	1:D:371:LEU:HD23	2.00	0.43
1:E:450:HIS:CE1	4:E:503:GTP:O1B	2.72	0.43
1:A:459:ARG:O	1:A:462:ARG:HB3	2.19	0.43
1:B:78:TYR:O	1:B:127:ALA:HA	2.18	0.43
1:B:282:ASN:C	1:B:282:ASN:OD1	2.57	0.43
1:B:371:LEU:HD12	1:B:482:TYR:CD1	2.54	0.43
1:C:446:LYS:HB2	1:C:446:LYS:HZ2	1.84	0.43
1:C:29:VAL:HG22	1:C:45:VAL:HG21	2.00	0.43
1:D:242:PHE:CE1	1:D:263:LEU:CD2	3.02	0.43
1:E:248:VAL:CG1	1:E:319:CYS:SG	3.06	0.43
1:E:477:LEU:HA	1:E:477:LEU:HD23	1.75	0.43
1:A:257:LEU:O	1:A:260:MET:HB3	2.18	0.43
1:B:391:HIS:O	1:C:382:TYR:OH	2.28	0.43
1:D:410:LEU:HA	1:D:410:LEU:HD12	1.64	0.43
1:E:215:THR:HG23	1:E:216:GLY:N	2.34	0.43
1:E:273:VAL:HG12	1:E:274:GLY:N	2.34	0.43
1:E:246:THR:HG23	1:E:319:CYS:HA	2.01	0.43
1:E:44:ARG:HH12	1:E:494:ASN:ND2	2.17	0.43
1:F:65:ILE:CG1	1:F:144:ILE:HG12	2.48	0.43
1:F:462:ARG:NH1	1:F:465:MET:CE	2.82	0.43
1:F:496:ALA:C	1:F:498:VAL:N	2.66	0.43
1:A:126:LYS:NZ	1:A:168:ASP:OD2	2.48	0.42
1:A:177:SER:HB2	1:A:202:PRO:HG2	2.01	0.42
1:A:347:GLY:O	1:A:374:ASN:HB3	2.19	0.42
1:A:37:THR:O	1:A:38:GLU:HB3	2.18	0.42
1:B:146:ARG:NH2	1:B:181:ASP:OD2	2.52	0.42
1:B:146:ARG:CB	1:B:182:THR:HG21	2.48	0.42
1:C:150:MET:O	1:C:154:LYS:HG3	2.19	0.42
1:C:191:ASP:HB3	1:C:194:ALA:HB2	2.00	0.42
1:C:390:ASN:O	1:C:392:VAL:HG23	2.19	0.42
1:D:95:TYR:OH	1:D:145:THR:CB	2.67	0.42
1:F:337:PRO:O	1:F:363:ARG:NE	2.52	0.42
1:F:361:LEU:HD22	1:F:361:LEU:HA	1.77	0.42
1:F:55:CYS:HA	1:F:82:HIS:HA	2.00	0.42
1:A:249:VAL:HG22	1:A:251:GLY:O	2.19	0.42
1:A:273:VAL:HG21	1:A:291:LEU:HD12	2.01	0.42
1:A:196:ALA:HA	1:A:388:ASN:HD22	1.85	0.42
1:B:175:GLU:HA	1:B:178:TRP:CE3	2.53	0.42
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.53	0.42
1:B:476:ASP:OD2	1:B:479:THR:HG23	2.18	0.42
1:C:82:HIS:CG	1:C:109:SER:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ASN:C	1:D:337:PRO:HD2	2.40	0.42
1:D:79:ARG:HA	1:D:127:ALA:HA	2.01	0.42
1:E:171:THR:HB	1:E:175:GLU:HG3	2.01	0.42
1:E:224:GLU:HB2	1:E:242:PHE:HE2	1.84	0.42
1:D:443:ALA:N	1:E:401:TYR:CE2	2.87	0.42
1:F:31:ASP:O	1:F:32:LEU:C	2.57	0.42
1:A:118:VAL:HG11	1:A:375:ALA:HB3	2.00	0.42
1:A:215:THR:HG23	1:A:216:GLY:H	1.85	0.42
1:A:234:SER:O	1:A:235:ILE:C	2.57	0.42
1:A:336:ALA:N	1:A:337:PRO:CD	2.82	0.42
1:A:37:THR:O	1:A:38:GLU:CB	2.68	0.42
1:A:389:LEU:O	1:A:391:HIS:ND1	2.52	0.42
1:A:95:TYR:OH	1:A:145:THR:CG2	2.68	0.42
1:B:160:PRO:HD3	1:B:197:CYS:HB3	2.01	0.42
1:B:271:ILE:HD12	1:B:272:THR:HG22	2.00	0.42
1:B:252:PHE:CZ	1:B:291:LEU:HD13	2.55	0.42
1:B:395:GLY:HA3	1:B:399:PHE:CZ	2.54	0.42
1:E:331:LEU:HA	1:E:331:LEU:HD12	1.76	0.42
1:A:313:SER:C	1:A:315:LEU:N	2.73	0.42
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.78	0.42
1:E:196:ALA:HB1	1:E:385:TRP:CD1	2.54	0.42
1:E:233:MET:HA	1:E:233:MET:HE2	2.02	0.42
1:F:242:PHE:CE1	1:F:263:LEU:CD2	3.03	0.42
1:F:39:GLU:C	1:F:41:LYS:H	2.23	0.42
1:F:421:PHE:N	1:F:421:PHE:CD2	2.87	0.42
1:A:215:THR:HG23	1:A:216:GLY:N	2.35	0.42
1:A:489:VAL:C	1:A:490:PHE:O	2.57	0.42
1:A:96:SER:O	1:A:99:VAL:CG1	2.67	0.42
1:B:142:GLU:OE2	1:B:146:ARG:NH1	2.53	0.42
1:D:131:ILE:O	1:D:131:ILE:HG13	2.17	0.42
1:D:291:LEU:O	1:D:294:PHE:N	2.52	0.42
1:E:272:THR:HG21	1:E:317:VAL:HG21	2.01	0.42
1:E:303:GLY:N	1:E:309:ILE:HD11	2.33	0.42
1:F:328:GLU:HB2	1:F:350:GLY:O	2.19	0.42
1:A:409:LEU:O	1:A:409:LEU:HD23	2.19	0.42
1:B:118:VAL:HB	1:B:456:THR:CG2	2.50	0.42
1:B:477:LEU:HA	1:B:477:LEU:HD23	1.86	0.42
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.73	0.42
1:D:29:VAL:HG13	1:D:41:LYS:HB3	2.02	0.42
1:D:91:GLY:HA3	1:D:125:ALA:O	2.19	0.42
1:E:272:THR:CG2	1:E:281:TRP:HD1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:ALA:HB2	1:E:388:ASN:CB	2.48	0.42
1:E:38:GLU:HG3	1:E:39:GLU:HG2	2.00	0.42
1:F:234:SER:O	1:F:235:ILE:C	2.56	0.42
1:F:40:GLN:HB3	1:F:40:GLN:HE21	1.59	0.42
1:F:498:VAL:HB	1:F:499:THR:H	1.69	0.42
1:A:378:VAL:HA	1:A:381:SER:HB2	2.02	0.42
1:A:93:ILE:HG13	1:A:94:ARG:N	2.27	0.42
1:C:248:VAL:CG2	1:C:314:ILE:HD11	2.49	0.42
1:E:370:ASP:OD1	1:E:371:LEU:N	2.47	0.42
1:E:37:THR:O	1:E:38:GLU:CB	2.67	0.42
1:F:215:THR:HB	3:F:552:NDP:H42N	2.01	0.42
1:F:117:VAL:HG21	1:F:371:LEU:HD22	2.02	0.42
1:A:107:LEU:HA	1:A:107:LEU:HD12	1.73	0.42
1:A:75:ILE:HD11	1:A:129:VAL:CG1	2.49	0.42
1:C:51:ILE:HG23	1:F:64:PRO:HB3	2.02	0.42
1:D:221:HIS:O	1:D:224:GLU:HB3	2.20	0.42
1:E:275:GLU:HG3	1:E:301:ILE:HD11	2.02	0.42
1:E:344:ILE:HB	1:E:367:VAL:HG12	2.02	0.42
1:A:370:ASP:HB2	1:A:374:ASN:HD21	1.84	0.42
1:C:208:ILE:HG22	1:C:211:ARG:HB2	2.02	0.42
1:C:305:PRO:O	1:C:307:ALA:N	2.51	0.42
1:C:446:LYS:HB2	1:C:446:LYS:NZ	2.35	0.42
1:C:53:LYS:N	1:C:54:PRO:CD	2.83	0.42
1:D:142:GLU:OE2	1:D:146:ARG:NH1	2.53	0.42
1:D:476:ASP:OD2	1:D:479:THR:HG23	2.20	0.42
1:E:100:SER:O	1:E:101:VAL:C	2.59	0.42
1:F:337:PRO:HD3	1:F:359:ILE:HD13	2.01	0.42
1:F:33:LYS:O	1:F:34:THR:C	2.58	0.42
1:A:462:ARG:NH1	1:A:465:MET:CE	2.83	0.42
1:B:227:ILE:HG23	1:B:227:ILE:O	2.20	0.42
1:B:229:GLU:HG3	1:B:231:SER:HB3	2.01	0.42
1:D:271:ILE:HD11	1:D:319:CYS:HB3	2.01	0.42
1:D:409:LEU:HD23	1:D:409:LEU:O	2.20	0.42
1:D:84:GLN:C	1:D:86:ARG:N	2.73	0.42
1:E:281:TRP:O	1:E:282:ASN:HB2	2.19	0.42
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.01	0.42
1:F:313:SER:HB3	1:F:316:GLU:CD	2.40	0.42
1:A:211:ARG:HA	1:A:380:VAL:HG11	2.01	0.41
1:C:25:GLU:OE2	1:C:42:ARG:NH1	2.53	0.41
1:C:31:ASP:O	1:C:32:LEU:C	2.58	0.41
1:C:90:LYS:HD2	1:C:164:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:MET:HG3	1:E:354:PRO:HD3	2.02	0.41
1:E:253:GLY:HA3	3:E:552:NDP:O5B	2.20	0.41
1:E:213:SER:CB	1:E:258:HIS:CD2	3.03	0.41
1:F:281:TRP:CZ2	1:F:283:PRO:CG	3.00	0.41
1:A:201:LYS:HZ1	1:A:388:ASN:ND2	2.09	0.41
1:B:82:HIS:CG	1:B:109:SER:HA	2.55	0.41
1:B:252:PHE:CE2	1:B:291:LEU:HD13	2.54	0.41
1:B:382:TYR:CE1	1:B:386:LEU:HD22	2.55	0.41
1:C:353:THR:HB	1:C:354:PRO:HD2	2.01	0.41
1:D:65:ILE:HG13	1:D:144:ILE:HG13	2.02	0.41
1:D:248:VAL:CG2	1:D:314:ILE:HG12	2.50	0.41
1:D:79:ARG:HB2	1:D:127:ALA:HB2	2.03	0.41
1:E:169:MET:O	1:E:170:SER:HB2	2.20	0.41
1:A:379:THR:O	1:A:382:TYR:HB3	2.20	0.41
1:A:435:GLU:HG2	1:C:408:HIS:CE1	2.55	0.41
1:B:416:SER:O	1:B:419:ARG:HB3	2.20	0.41
1:C:142:GLU:OE2	1:C:146:ARG:NH1	2.53	0.41
1:C:63:PHE:CD1	1:C:147:ARG:HG3	2.55	0.41
1:C:227:ILE:HA	1:C:233:MET:SD	2.60	0.41
1:C:224:GLU:HB2	1:C:242:PHE:CE2	2.54	0.41
1:C:274:GLY:HA2	1:C:279:SER:HA	2.01	0.41
1:C:436:PHE:CG	1:C:436:PHE:O	2.74	0.41
1:E:224:GLU:HB2	1:E:242:PHE:CE2	2.54	0.41
1:F:368:ILE:HB	1:F:373:LEU:CD1	2.50	0.41
1:F:79:ARG:HG3	1:F:127:ALA:HB2	2.01	0.41
1:A:272:THR:HG21	1:A:317:VAL:HG21	2.02	0.41
1:A:63:PHE:CZ	1:A:75:ILE:HD12	2.56	0.41
1:B:38:GLU:CG	1:B:39:GLU:H	1.92	0.41
1:C:309:ILE:N	1:C:309:ILE:HD12	2.35	0.41
1:C:65:ILE:HA	1:C:65:ILE:HD13	1.68	0.41
1:C:75:ILE:HD11	1:C:129:VAL:HG13	2.02	0.41
1:D:100:SER:O	1:D:101:VAL:C	2.59	0.41
1:A:57:HIS:HD2	1:D:61:LEU:HD12	1.85	0.41
1:E:9:PHE:HD2	1:E:9:PHE:O	2.04	0.41
1:F:487:GLU:OE2	1:F:491:ARG:NH1	2.53	0.41
1:A:189:HIS:CE1	1:E:187:ILE:CD1	3.03	0.41
1:B:453:LEU:HD12	1:B:453:LEU:O	2.20	0.41
1:B:349:ASN:ND2	3:B:552:NDP:O2D	2.46	0.41
1:E:10:PHE:HD2	1:E:106:ALA:HA	1.86	0.41
1:F:35:ARG:O	1:F:37:THR:N	2.54	0.41
1:A:246:THR:HG22	1:A:320:ASP:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:TRP:O	1:B:282:ASN:HB2	2.20	0.41
1:B:303:GLY:H	1:B:309:ILE:CD1	2.31	0.41
1:C:316:GLU:OE1	1:C:338:ARG:HD2	2.20	0.41
1:C:338:ARG:O	1:C:338:ARG:HG3	2.20	0.41
1:D:78:TYR:CD1	1:D:78:TYR:N	2.88	0.41
1:D:87:THR:HB	1:D:88:PRO:HA	2.02	0.41
1:F:201:LYS:NZ	1:F:388:ASN:ND2	2.57	0.41
1:F:28:LEU:HD12	1:F:28:LEU:HA	1.77	0.41
1:F:337:PRO:O	1:F:363:ARG:CZ	2.68	0.41
1:A:175:GLU:HA	1:A:178:TRP:CE3	2.55	0.41
1:A:276:SER:OG	3:A:552:NDP:P2B	2.79	0.41
1:A:333:LYS:HD2	1:A:355:GLU:HG2	2.03	0.41
1:B:236:LEU:HD12	1:B:236:LEU:HA	1.85	0.41
1:B:84:GLN:HE21	1:B:84:GLN:HB2	1.69	0.41
1:C:291:LEU:HA	1:C:291:LEU:HD23	1.89	0.41
1:C:344:ILE:HB	1:C:367:VAL:HG13	2.01	0.41
1:C:29:VAL:CG2	1:C:45:VAL:HG21	2.50	0.41
1:E:65:ILE:HD13	1:E:65:ILE:HA	1.63	0.41
1:F:146:ARG:CA	1:F:182:THR:HG21	2.49	0.41
1:E:386:LEU:HD21	1:F:392:VAL:HG13	2.01	0.41
1:A:63:PHE:CE1	1:A:75:ILE:HD12	2.56	0.41
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.55	0.41
1:B:346:GLU:HB2	1:B:368:ILE:O	2.19	0.41
1:B:35:ARG:HD3	1:B:35:ARG:N	2.14	0.41
1:E:162:VAL:O	1:E:163:ASP:HB2	2.21	0.41
1:F:374:ASN:OD1	1:F:374:ASN:C	2.59	0.41
1:F:39:GLU:C	1:F:41:LYS:N	2.72	0.41
1:A:111:MET:CA	1:A:111:MET:HE3	2.50	0.41
1:A:346:GLU:HG2	1:A:351:PRO:CG	2.50	0.41
1:A:65:ILE:HA	1:A:65:ILE:HD13	1.62	0.41
1:C:281:TRP:O	1:C:282:ASN:CB	2.67	0.41
1:D:90:LYS:HD2	1:D:164:VAL:HB	2.03	0.41
1:D:167:PRO:HG3	1:D:176:MET:CG	2.50	0.41
1:D:191:ASP:C	1:D:193:ASN:H	2.23	0.41
1:D:460:SER:HA	1:D:463:GLN:HG2	2.03	0.41
1:E:224:GLU:HA	1:E:227:ILE:HG22	2.03	0.41
1:E:95:TYR:CD1	1:E:129:VAL:HB	2.56	0.41
1:A:158:ILE:HA	1:A:163:ASP:O	2.20	0.41
1:A:37:THR:HG22	1:A:41:LYS:NZ	2.35	0.41
1:B:314:ILE:HA	1:B:317:VAL:HG23	2.02	0.41
1:B:398:THR:O	1:B:399:PHE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PHE:CE2	1:B:53:LYS:CG	3.03	0.41
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.89	0.41
1:C:196:ALA:HB2	1:C:388:ASN:CB	2.51	0.41
1:C:339:VAL:HG21	1:C:360:PHE:CE1	2.55	0.41
1:D:119:ASP:O	1:E:396:ARG:NH1	2.53	0.41
1:D:486:ILE:O	1:D:487:GLU:C	2.58	0.41
1:E:107:LEU:HD12	1:E:107:LEU:HA	1.88	0.41
1:E:90:LYS:HB2	1:E:122:PHE:CD1	2.56	0.41
1:F:159:GLY:HA3	1:F:162:VAL:HG13	2.03	0.41
1:F:257:LEU:HD12	1:F:257:LEU:O	2.21	0.41
1:F:371:LEU:HA	1:F:371:LEU:HD23	1.81	0.41
1:A:153:ALA:HA	1:A:158:ILE:HG22	2.03	0.41
1:A:32:LEU:HD11	1:A:44:ARG:NH1	2.36	0.41
1:B:90:LYS:HE2	1:B:164:VAL:HG12	2.03	0.41
1:D:79:ARG:CB	1:D:127:ALA:HB2	2.51	0.41
1:D:175:GLU:HA	1:D:178:TRP:HE3	1.82	0.41
1:D:416:SER:CB	1:F:430:ILE:HA	2.50	0.41
1:E:289:LYS:HD2	1:E:289:LYS:HA	1.83	0.41
1:E:430:ILE:HA	1:F:416:SER:HB3	2.03	0.41
2:E:502:GLU:HA	3:E:552:NDP:C4N	2.51	0.41
1:F:462:ARG:HG3	1:F:466:ARG:HH22	1.86	0.41
1:F:96:SER:OG	1:F:98:ASP:HB2	2.21	0.41
1:A:53:LYS:O	1:A:82:HIS:HE1	2.03	0.40
1:B:276:SER:HB2	3:B:552:NDP:O2X	2.21	0.40
1:C:232:TYR:O	1:C:236:LEU:HB2	2.21	0.40
1:C:45:VAL:HG12	1:C:49:LEU:HD23	2.01	0.40
1:C:82:HIS:HD2	1:C:112:THR:CG2	2.04	0.40
1:E:229:GLU:O	1:E:230:ALA:C	2.60	0.40
1:E:31:ASP:O	1:E:32:LEU:C	2.59	0.40
1:F:201:LYS:HB2	1:F:201:LYS:HE2	1.85	0.40
1:F:65:ILE:HD13	1:F:65:ILE:HA	1.64	0.40
1:A:196:ALA:HB1	1:A:385:TRP:CD1	2.56	0.40
1:A:409:LEU:O	1:A:412:SER:HB2	2.21	0.40
1:A:421:PHE:CD2	1:A:421:PHE:N	2.86	0.40
1:C:234:SER:O	1:C:235:ILE:C	2.60	0.40
1:C:5:ASP:OD2	1:C:332:THR:HB	2.20	0.40
1:C:8:ASN:O	1:C:9:PHE:C	2.60	0.40
1:E:176:MET:O	1:E:177:SER:C	2.58	0.40
1:E:213:SER:HB2	1:E:258:HIS:CD2	2.56	0.40
1:F:286:ILE:HG23	1:F:304:PHE:HE2	1.87	0.40
1:F:113:TYR:C	1:F:371:LEU:HD21	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:ARG:O	1:F:45:VAL:HB	2.21	0.40
1:A:457:MET:CE	1:A:457:MET:HA	2.38	0.40
1:A:96:SER:OG	1:A:97:THR:N	2.54	0.40
1:B:32:LEU:HD11	1:B:44:ARG:NH1	2.37	0.40
1:B:424:HIS:ND1	1:B:424:HIS:N	2.69	0.40
1:C:294:PHE:CE1	1:C:300:THR:O	2.74	0.40
1:C:427:THR:HG23	1:C:427:THR:O	2.21	0.40
1:D:66:ARG:CZ	1:D:70:GLY:O	2.69	0.40
1:F:370:ASP:HB2	1:F:374:ASN:ND2	2.36	0.40
1:F:371:LEU:HD13	1:F:481:ALA:HB1	2.03	0.40
1:A:466:ARG:NH1	1:A:466:ARG:HB2	2.37	0.40
1:B:291:LEU:CD2	1:B:301:ILE:HG22	2.51	0.40
1:D:167:PRO:HG3	1:D:176:MET:HG2	2.03	0.40
1:D:2:ASP:OD1	1:D:5:ASP:O	2.39	0.40
1:D:417:LEU:HB3	1:D:428:ILE:HD13	2.03	0.40
1:E:175:GLU:N	1:E:175:GLU:CD	2.74	0.40
1:E:331:LEU:HG	1:E:360:PHE:HZ	1.86	0.40
1:E:255:VAL:HG11	3:E:552:NDP:O4D	2.21	0.40
1:F:271:ILE:C	1:F:272:THR:CG2	2.90	0.40
1:A:118:VAL:HG11	1:A:375:ALA:CB	2.52	0.40
1:A:216:GLY:HA2	1:A:219:VAL:HB	2.03	0.40
1:A:423:LYS:HD2	1:A:423:LYS:N	2.36	0.40
1:B:186:THR:OG1	1:B:187:ILE:N	2.53	0.40
1:C:211:ARG:NH2	2:C:502:GLU:HG2	2.36	0.40
1:C:80:ALA:O	1:C:125:ALA:HA	2.22	0.40
1:D:304:PHE:HA	1:D:305:PRO:HD2	1.94	0.40
1:D:436:PHE:O	1:D:440:ILE:HB	2.22	0.40
1:E:24:VAL:HG13	1:E:483:VAL:HG22	2.03	0.40
1:E:273:VAL:HG21	1:E:291:LEU:HD12	2.02	0.40
1:E:296:LEU:HA	1:E:296:LEU:HD22	1.70	0.40
1:E:301:ILE:HG13	1:E:302:LEU:N	2.37	0.40
1:F:107:LEU:HA	1:F:107:LEU:HD12	1.72	0.40
1:F:172:GLY:H	1:F:175:GLU:CG	2.34	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	493/501 (98%)	428 (87%)	52 (10%)	13 (3%)	6	23
1	B	493/501 (98%)	429 (87%)	49 (10%)	15 (3%)	5	19
1	C	493/501 (98%)	424 (86%)	55 (11%)	14 (3%)	6	21
1	D	493/501 (98%)	427 (87%)	57 (12%)	9 (2%)	10	33
1	E	493/501 (98%)	427 (87%)	56 (11%)	10 (2%)	9	30
1	F	499/501 (100%)	424 (85%)	62 (12%)	13 (3%)	6	23
All	All	2964/3006 (99%)	2559 (86%)	331 (11%)	74 (2%)	6	24

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	371	LEU
1	B	34	THR
1	B	37	THR
1	B	38	GLU
1	C	38	GLU
1	C	282	ASN
1	D	4	GLU
1	D	38	GLU
1	D	404	ASP
1	E	38	GLU
1	E	371	LEU
1	F	38	GLU
1	F	496	ALA
1	F	498	VAL
1	A	234	SER
1	A	422	GLY
1	B	85	HIS
1	B	306	LYS
1	B	422	GLY

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Mol	Chain	Res	Type
1	C	36	GLU
1	C	299	GLY
1	C	306	LYS
1	C	422	GLY
1	D	405	SER
1	D	422	GLY
1	E	370	ASP
1	E	422	GLY
1	F	3	ARG
1	F	36	GLU
1	F	396	ARG
1	F	422	GLY
1	A	235	ILE
1	A	396	ARG
1	A	491	ARG
1	B	348	ALA
1	D	204	SER
1	E	31	ASP
1	E	36	GLU
1	A	31	ASP
1	A	32	LEU
1	B	31	ASP
1	B	474	GLY
1	C	2	ASP
1	C	31	ASP
1	E	32	LEU
1	E	209	HIS
1	F	34	THR
1	F	231	SER
1	F	371	LEU
1	A	493	TYR
1	B	396	ARG
1	B	494	ASN
1	C	126	LYS
1	C	166	ALA
1	C	340	LYS
1	D	36	GLU
1	E	187	ILE
1	E	210	GLY
1	F	31	ASP
1	F	500	PHE
1	A	168	ASP

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Mol	Chain	Res	Type
1	B	32	LEU
1	B	36	GLU
1	B	305	PRO
1	B	371	LEU
1	C	305	PRO
1	D	487	GLU
1	A	99	VAL
1	A	166	ALA
1	C	165	PRO
1	F	165	PRO
1	C	240	PRO
1	D	203	ILE

### 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	416/420 (99%)	356 (86%)	60 (14%)	4	10
1	B	416/420 (99%)	353 (85%)	63 (15%)	3	9
1	C	416/420 (99%)	358 (86%)	58 (14%)	4	12
1	D	416/420 (99%)	352 (85%)	64 (15%)	3	9
1	E	416/420 (99%)	355 (85%)	61 (15%)	3	10
1	F	420/420 (100%)	356 (85%)	64 (15%)	3	9
All	All	2500/2520 (99%)	2130 (85%)	370 (15%)	3	10

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	9	PHE
1	A	28	LEU
1	A	33	LYS
1	A	35	ARG

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Mol	Chain	Res	Type
1	A	38	GLU
1	A	44	ARG
1	A	49	LEU
1	A	61	LEU
1	A	65	ILE
1	A	75	ILE
1	A	84	GLN
1	A	93	ILE
1	A	99	VAL
1	A	101	VAL
1	A	107	LEU
1	A	110	LEU
1	A	112	THR
1	A	145	THR
1	A	158	ILE
1	A	162	VAL
1	A	182	THR
1	A	203	ILE
1	A	212	ILE
1	A	227	ILE
1	A	238	MET
1	A	239	THR
1	A	249	VAL
1	A	255	VAL
1	A	272	THR
1	A	291	LEU
1	A	296	LEU
1	A	297	GLN
1	A	306	LYS
1	A	311	GLU
1	A	321	ILE
1	A	331	LEU
1	A	340	LYS
1	A	352	THR
1	A	361	LEU
1	A	364	ASN
1	A	365	ILE
1	A	367	VAL
1	A	371	LEU
1	A	373	LEU
1	A	378	VAL
1	A	386	LEU

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Mol	Chain	Res	Type
1	A	392	VAL
1	A	393	SER
1	A	397	LEU
1	A	405	SER
1	A	410	LEU
1	A	424	HIS
1	A	446	LYS
1	A	458	GLU
1	A	463	GLN
1	A	478	ARG
1	A	487	GLU
1	A	495	GLU
1	B	2	ASP
1	B	9	PHE
1	B	28	LEU
1	B	33	LYS
1	B	35	ARG
1	B	40	GLN
1	B	44	ARG
1	B	49	LEU
1	B	66	ARG
1	B	75	ILE
1	B	78	TYR
1	B	84	GLN
1	B	93	ILE
1	B	96	SER
1	B	99	VAL
1	B	101	VAL
1	B	104	VAL
1	B	107	LEU
1	B	112	THR
1	B	137	THR
1	B	145	THR
1	B	150	MET
1	B	162	VAL
1	B	176	MET
1	B	182	THR
1	B	212	ILE
1	B	238	MET
1	B	239	THR
1	B	245	LYS
1	B	246	THR

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Mol	Chain	Res	Type
1	B	249	VAL
1	B	272	THR
1	B	291	LEU
1	B	296	LEU
1	B	297	GLN
1	B	306	LYS
1	B	311	GLU
1	B	321	ILE
1	B	331	LEU
1	B	340	LYS
1	B	352	THR
1	B	357	ASP
1	B	361	LEU
1	B	364	ASN
1	B	365	ILE
1	B	367	VAL
1	B	371	LEU
1	B	373	LEU
1	B	378	VAL
1	B	386	LEU
1	B	392	VAL
1	B	393	SER
1	B	397	LEU
1	B	405	SER
1	B	423	LYS
1	B	424	HIS
1	B	437	GLN
1	B	446	LYS
1	B	458	GLU
1	B	487	GLU
1	B	492	VAL
1	B	494	ASN
1	B	495	GLU
1	C	3	ARG
1	C	9	PHE
1	C	24	VAL
1	C	28	LEU
1	C	33	LYS
1	C	35	ARG
1	C	38	GLU
1	C	40	GLN
1	C	44	ARG

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Mol	Chain	Res	Type
1	C	49	LEU
1	C	61	LEU
1	C	66	ARG
1	C	75	ILE
1	C	78	TYR
1	C	84	GLN
1	C	93	ILE
1	C	96	SER
1	C	99	VAL
1	C	107	LEU
1	C	110	LEU
1	C	112	THR
1	C	145	THR
1	C	162	VAL
1	C	175	GLU
1	C	182	THR
1	C	203	ILE
1	C	212	ILE
1	C	238	MET
1	C	239	THR
1	C	245	LYS
1	C	255	VAL
1	C	272	THR
1	C	291	LEU
1	C	296	LEU
1	C	297	GLN
1	C	306	LYS
1	C	311	GLU
1	C	321	ILE
1	C	331	LEU
1	C	340	LYS
1	C	352	THR
1	C	361	LEU
1	C	364	ASN
1	C	365	ILE
1	C	367	VAL
1	C	368	ILE
1	C	371	LEU
1	C	373	LEU
1	C	378	VAL
1	C	386	LEU
1	C	392	VAL

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Mol	Chain	Res	Type
1	C	393	SER
1	C	410	LEU
1	C	423	LYS
1	C	424	HIS
1	C	446	LYS
1	C	458	GLU
1	C	487	GLU
1	D	3	ARG
1	D	9	PHE
1	D	28	LEU
1	D	31	ASP
1	D	33	LYS
1	D	35	ARG
1	D	38	GLU
1	D	43	ASN
1	D	44	ARG
1	D	49	LEU
1	D	61	LEU
1	D	65	ILE
1	D	66	ARG
1	D	75	ILE
1	D	78	TYR
1	D	84	GLN
1	D	93	ILE
1	D	96	SER
1	D	99	VAL
1	D	104	VAL
1	D	107	LEU
1	D	112	THR
1	D	145	THR
1	D	162	VAL
1	D	175	GLU
1	D	182	THR
1	D	212	ILE
1	D	236	LEU
1	D	238	MET
1	D	239	THR
1	D	246	THR
1	D	255	VAL
1	D	272	THR
1	D	291	LEU
1	D	296	LEU

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Mol	Chain	Res	Type
1	D	297	GLN
1	D	306	LYS
1	D	311	GLU
1	D	313	SER
1	D	321	ILE
1	D	331	LEU
1	D	340	LYS
1	D	342	LYS
1	D	352	THR
1	D	357	ASP
1	D	361	LEU
1	D	364	ASN
1	D	365	ILE
1	D	367	VAL
1	D	371	LEU
1	D	373	LEU
1	D	378	VAL
1	D	386	LEU
1	D	393	SER
1	D	397	LEU
1	D	405	SER
1	D	410	LEU
1	D	423	LYS
1	D	424	HIS
1	D	446	LYS
1	D	458	GLU
1	D	463	GLN
1	D	487	GLU
1	D	494	ASN
1	E	3	ARG
1	E	4	GLU
1	E	9	PHE
1	E	28	LEU
1	E	33	LYS
1	E	35	ARG
1	E	38	GLU
1	E	44	ARG
1	E	49	LEU
1	E	61	LEU
1	E	65	ILE
1	E	66	ARG
1	E	75	ILE

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Mol	Chain	Res	Type
1	E	78	TYR
1	E	84	GLN
1	E	93	ILE
1	E	96	SER
1	E	99	VAL
1	E	107	LEU
1	E	112	THR
1	E	145	THR
1	E	182	THR
1	E	203	ILE
1	E	212	ILE
1	E	239	THR
1	E	246	THR
1	E	249	VAL
1	E	255	VAL
1	E	272	THR
1	E	291	LEU
1	E	296	LEU
1	E	297	GLN
1	E	300	THR
1	E	306	LYS
1	E	311	GLU
1	E	313	SER
1	E	321	ILE
1	E	331	LEU
1	E	340	LYS
1	E	352	THR
1	E	361	LEU
1	E	364	ASN
1	E	365	ILE
1	E	367	VAL
1	E	371	LEU
1	E	373	LEU
1	E	378	VAL
1	E	386	LEU
1	E	392	VAL
1	E	393	SER
1	E	397	LEU
1	E	405	SER
1	E	410	LEU
1	E	423	LYS
1	E	424	HIS

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Mol	Chain	Res	Type
1	E	446	LYS
1	E	458	GLU
1	E	463	GLN
1	E	487	GLU
1	E	492	VAL
1	E	495	GLU
1	F	9	PHE
1	F	24	VAL
1	F	28	LEU
1	F	33	LYS
1	F	35	ARG
1	F	38	GLU
1	F	43	ASN
1	F	44	ARG
1	F	49	LEU
1	F	60	SER
1	F	65	ILE
1	F	66	ARG
1	F	75	ILE
1	F	78	TYR
1	F	84	GLN
1	F	93	ILE
1	F	96	SER
1	F	101	VAL
1	F	107	LEU
1	F	112	THR
1	F	145	THR
1	F	162	VAL
1	F	182	THR
1	F	203	ILE
1	F	212	ILE
1	F	217	ARG
1	F	239	THR
1	F	244	ASP
1	F	245	LYS
1	F	249	VAL
1	F	255	VAL
1	F	272	THR
1	F	291	LEU
1	F	296	LEU
1	F	297	GLN
1	F	306	LYS

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Mol	Chain	Res	Type
1	F	311	GLU
1	F	321	ILE
1	F	331	LEU
1	F	340	LYS
1	F	342	LYS
1	F	352	THR
1	F	361	LEU
1	F	364	ASN
1	F	365	ILE
1	F	367	VAL
1	F	368	ILE
1	F	371	LEU
1	F	373	LEU
1	F	378	VAL
1	F	386	LEU
1	F	392	VAL
1	F	393	SER
1	F	397	LEU
1	F	398	THR
1	F	400	LYS
1	F	410	LEU
1	F	424	HIS
1	F	446	LYS
1	F	458	GLU
1	F	487	GLU
1	F	495	GLU
1	F	498	VAL
1	F	500	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	82	HIS
1	A	84	GLN
1	A	139	ASN
1	A	258	HIS
1	A	388	ASN
1	A	406	ASN
1	A	494	ASN
1	B	82	HIS
1	B	84	GLN

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Mol	Chain	Res	Type
1	B	258	HIS
1	B	388	ASN
1	B	406	ASN
1	B	494	ASN
1	C	82	HIS
1	C	84	GLN
1	C	139	ASN
1	C	258	HIS
1	C	388	ASN
1	D	82	HIS
1	D	84	GLN
1	D	388	ASN
1	E	40	GLN
1	E	82	HIS
1	E	84	GLN
1	E	258	HIS
1	E	297	GLN
1	E	388	ASN
1	E	406	ASN
1	E	494	ASN
1	F	40	GLN
1	F	82	HIS
1	F	84	GLN
1	F	139	ASN
1	F	258	HIS
1	F	264	HIS
1	F	388	ASN
1	F	406	ASN
1	F	494	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	GLU	A	502	-	1,9,9	0.31	0	1,11,11	0.38	0
4	GTP	A	503	5	27,34,34	1.31	3 (11%)	27,54,54	2.02	7 (25%)
3	NDP	A	552	-	43,52,52	1.49	5 (11%)	49,80,80	1.63	4 (8%)
2	GLU	B	502	-	1,9,9	0.23	0	1,11,11	0.10	0
4	GTP	B	503	5	27,34,34	1.10	2 (7%)	27,54,54	2.06	9 (33%)
3	NDP	B	552	-	43,52,52	1.55	4 (9%)	49,80,80	1.76	2 (4%)
2	GLU	C	502	-	1,9,9	0.55	0	1,11,11	0.29	0
4	GTP	C	503	5	27,34,34	0.94	1 (3%)	27,54,54	1.69	4 (14%)
3	NDP	C	552	-	43,52,52	1.60	4 (9%)	49,80,80	1.66	2 (4%)
2	GLU	D	502	-	1,9,9	0.08	0	1,11,11	0.67	0
4	GTP	D	503	5	27,34,34	0.96	1 (3%)	27,54,54	1.74	6 (22%)
3	NDP	D	552	-	43,52,52	1.52	4 (9%)	49,80,80	1.72	4 (8%)
2	GLU	E	502	-	1,9,9	0.20	0	1,11,11	0.10	0
4	GTP	E	503	5	27,34,34	1.04	2 (7%)	27,54,54	1.95	8 (29%)
3	NDP	E	552	-	43,52,52	1.56	5 (11%)	49,80,80	1.75	3 (6%)
2	GLU	F	502	-	1,9,9	0.40	0	1,11,11	0.17	0
4	GTP	F	503	5	27,34,34	1.00	1 (3%)	27,54,54	1.80	6 (22%)
3	NDP	F	552	-	43,52,52	1.50	3 (6%)	49,80,80	1.66	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	A	502	-	-	0/3/9/9	0/0/0/0
4	GTP	A	503	5	-	0/18/38/38	0/3/3/3
3	NDP	A	552	-	-	0/30/77/77	0/5/5/5
2	GLU	B	502	-	-	0/3/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	B	503	5	-	0/18/38/38	0/3/3/3
3	NDP	B	552	-	-	0/30/77/77	0/5/5/5
2	GLU	C	502	-	-	0/3/9/9	0/0/0/0
4	GTP	C	503	5	-	0/18/38/38	0/3/3/3
3	NDP	C	552	-	-	0/30/77/77	0/5/5/5
2	GLU	D	502	-	-	0/3/9/9	0/0/0/0
4	GTP	D	503	5	-	0/18/38/38	0/3/3/3
3	NDP	D	552	-	-	0/30/77/77	0/5/5/5
2	GLU	E	502	-	-	0/3/9/9	0/0/0/0
4	GTP	E	503	5	-	0/18/38/38	0/3/3/3
3	NDP	E	552	-	-	0/30/77/77	0/5/5/5
2	GLU	F	502	-	-	0/3/9/9	0/0/0/0
4	GTP	F	503	5	-	0/18/38/38	0/3/3/3
3	NDP	F	552	-	-	0/30/77/77	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	GTP	O4'-C4'	-2.31	1.39	1.45
4	B	503	GTP	C2-N1	2.01	1.39	1.35
3	A	552	NDP	C2N-C3N	2.06	1.40	1.34
4	E	503	GTP	C2-N1	2.06	1.39	1.35
3	E	552	NDP	C2N-C3N	2.15	1.41	1.34
3	B	552	NDP	C2A-N1A	2.18	1.38	1.33
3	C	552	NDP	C2A-N1A	2.24	1.38	1.33
3	A	552	NDP	C2A-N1A	2.27	1.38	1.33
3	D	552	NDP	C2A-N1A	2.34	1.38	1.33
4	A	503	GTP	C2-N1	2.63	1.40	1.35
3	E	552	NDP	C2A-N1A	2.67	1.38	1.33
4	F	503	GTP	C6-N1	2.82	1.38	1.33
4	D	503	GTP	C6-N1	2.85	1.38	1.33
4	C	503	GTP	C6-N1	2.87	1.38	1.33
3	B	552	NDP	C6N-C5N	2.88	1.38	1.33
3	E	552	NDP	C6N-C5N	2.88	1.38	1.33
3	D	552	NDP	C6N-C5N	2.98	1.38	1.33
3	F	552	NDP	C6N-C5N	3.24	1.39	1.33
3	B	552	NDP	C2A-N3A	3.33	1.37	1.32
4	E	503	GTP	C6-N1	3.35	1.39	1.33
3	A	552	NDP	C6N-C5N	3.38	1.39	1.33
4	B	503	GTP	C6-N1	3.40	1.39	1.33
3	A	552	NDP	C2A-N3A	3.44	1.37	1.32
3	E	552	NDP	C2A-N3A	3.66	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	552	NDP	C2A-N3A	3.72	1.38	1.32
3	C	552	NDP	C6N-C5N	3.76	1.40	1.33
3	C	552	NDP	C2A-N3A	3.92	1.38	1.32
3	F	552	NDP	C2A-N3A	3.96	1.38	1.32
4	A	503	GTP	C6-N1	4.10	1.40	1.33
3	F	552	NDP	O7N-C7N	6.39	1.40	1.24
3	A	552	NDP	O7N-C7N	6.53	1.40	1.24
3	D	552	NDP	O7N-C7N	6.63	1.41	1.24
3	C	552	NDP	O7N-C7N	6.87	1.41	1.24
3	E	552	NDP	O7N-C7N	6.99	1.41	1.24
3	B	552	NDP	O7N-C7N	7.10	1.42	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NDP	N3A-C2A-N1A	-10.62	119.61	128.86
3	E	552	NDP	N3A-C2A-N1A	-10.26	119.92	128.86
3	D	552	NDP	N3A-C2A-N1A	-9.94	120.20	128.86
3	F	552	NDP	N3A-C2A-N1A	-9.73	120.39	128.86
3	C	552	NDP	N3A-C2A-N1A	-9.63	120.47	128.86
3	A	552	NDP	N3A-C2A-N1A	-9.30	120.76	128.86
4	A	503	GTP	N3-C2-N1	-5.81	118.98	127.46
4	B	503	GTP	N3-C2-N1	-5.53	119.39	127.46
4	E	503	GTP	N3-C2-N1	-5.14	119.95	127.46
4	C	503	GTP	N3-C2-N1	-4.98	120.19	127.46
4	F	503	GTP	N3-C2-N1	-4.78	120.48	127.46
4	D	503	GTP	N3-C2-N1	-4.57	120.78	127.46
4	E	503	GTP	C5-C6-N1	-3.62	118.33	123.48
4	A	503	GTP	C1'-N9-C4	-3.34	120.87	126.64
4	B	503	GTP	C5-C6-N1	-3.31	118.77	123.48
4	E	503	GTP	C1'-N9-C4	-3.20	121.10	126.64
4	C	503	GTP	C5-C6-N1	-3.12	119.04	123.48
4	A	503	GTP	C5-C6-N1	-2.97	119.26	123.48
4	F	503	GTP	O3'-C3'-C2'	-2.92	102.47	111.83
4	D	503	GTP	C5-C6-N1	-2.85	119.43	123.48
4	F	503	GTP	C5-C6-N1	-2.80	119.50	123.48
4	A	503	GTP	C6-C5-C4	-2.75	118.11	120.84
3	A	552	NDP	C1D-N1N-C6N	-2.71	114.88	120.77
4	D	503	GTP	C4-C5-N7	-2.70	106.80	109.41
3	E	552	NDP	C1D-N1N-C6N	-2.67	114.97	120.77
4	B	503	GTP	C1'-N9-C4	-2.60	122.15	126.64
3	D	552	NDP	C3N-C2N-N1N	-2.47	119.50	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NDP	C1D-N1N-C6N	-2.45	115.45	120.77
4	F	503	GTP	C6-C5-C4	-2.43	118.43	120.84
4	E	503	GTP	C4-C5-N7	-2.38	107.11	109.41
3	A	552	NDP	C4A-C5A-N7A	-2.36	107.13	109.41
3	D	552	NDP	C4A-C5A-N7A	-2.23	107.26	109.41
3	E	552	NDP	C4A-C5A-N7A	-2.20	107.28	109.41
3	F	552	NDP	C4A-C5A-N7A	-2.16	107.32	109.41
4	E	503	GTP	C6-C5-C4	-2.15	118.70	120.84
4	B	503	GTP	O5'-PA-O1A	-2.14	100.62	109.25
4	B	503	GTP	C4-C5-N7	-2.12	107.36	109.41
4	B	503	GTP	O3'-C3'-C4'	-2.07	105.05	111.09
3	D	552	NDP	O4D-C1D-N1N	2.06	112.23	108.07
3	A	552	NDP	O4D-C1D-N1N	2.21	112.52	108.07
3	C	552	NDP	C2B-C3B-C4B	2.38	107.36	101.95
4	D	503	GTP	N2-C2-N1	2.46	121.17	117.24
4	D	503	GTP	C6-N1-C2	2.52	119.69	116.06
4	C	503	GTP	C6-N1-C2	3.00	120.38	116.06
4	F	503	GTP	C6-N1-C2	3.01	120.39	116.06
4	B	503	GTP	N2-C2-N1	3.10	122.19	117.24
4	A	503	GTP	C6-N1-C2	3.22	120.69	116.06
4	B	503	GTP	C6-N1-C2	3.22	120.69	116.06
4	E	503	GTP	N2-C2-N1	3.25	122.43	117.24
4	E	503	GTP	C6-N1-C2	3.39	120.93	116.06
4	E	503	GTP	C2-N3-C4	3.51	119.26	115.16
4	A	503	GTP	C2-N3-C4	3.52	119.27	115.16
4	F	503	GTP	C2-N3-C4	3.60	119.36	115.16
4	C	503	GTP	C2-N3-C4	3.82	119.62	115.16
4	D	503	GTP	C2-N3-C4	4.05	119.89	115.16
4	A	503	GTP	N2-C2-N1	4.06	123.74	117.24
4	B	503	GTP	C2-N3-C4	4.20	120.06	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	GLU	3	0
4	A	503	GTP	1	0
3	A	552	NDP	4	0
2	B	502	GLU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	552	NDP	7	0
2	C	502	GLU	5	0
4	C	503	GTP	1	0
3	C	552	NDP	5	0
2	D	502	GLU	1	0
3	D	552	NDP	3	0
2	E	502	GLU	3	0
4	E	503	GTP	1	0
3	E	552	NDP	5	0
2	F	502	GLU	2	0
3	F	552	NDP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	495/501 (98%)	0.13	22 (4%)	35	33	15, 32, 68, 127	0
1	B	495/501 (98%)	0.13	17 (3%)	46	43	17, 34, 71, 128	0
1	C	495/501 (98%)	0.28	36 (7%)	16	13	18, 38, 71, 129	0
1	D	495/501 (98%)	0.10	21 (4%)	37	34	15, 32, 71, 131	0
1	E	495/501 (98%)	0.12	20 (4%)	39	37	16, 32, 71, 126	0
1	F	501/501 (100%)	-0.03	19 (3%)	41	39	14, 29, 73, 130	0
All	All	2976/3006 (99%)	0.12	135 (4%)	34	32	14, 32, 72, 131	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	HIS	8.1
1	B	2	ASP	7.5
1	C	3	ARG	7.2
1	E	424	HIS	7.0
1	F	424	HIS	6.5
1	C	4	GLU	5.7
1	B	39	GLU	5.7
1	E	425	GLY	5.6
1	C	424	HIS	5.3
1	F	498	VAL	5.3
1	A	1	ALA	5.3
1	C	32	LEU	4.9
1	F	425	GLY	4.9
1	B	425	GLY	4.8
1	E	1	ALA	4.7
1	A	424	HIS	4.6
1	E	3	ARG	4.6
1	A	3	ARG	4.5
1	C	230	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	33	LYS	4.5
1	C	334	SER	4.4
1	B	1	ALA	4.2
1	B	3	ARG	4.2
1	E	72	TRP	4.1
1	C	339	VAL	4.1
1	A	2	ASP	3.9
1	F	497	GLY	3.9
1	A	21	ALA	3.8
1	C	311	GLU	3.6
1	F	429	PRO	3.6
1	D	424	HIS	3.6
1	C	1	ALA	3.5
1	F	496	ALA	3.5
1	E	2	ASP	3.5
1	D	235	ILE	3.5
1	E	71	SER	3.4
1	D	36	GLU	3.4
1	C	36	GLU	3.3
1	D	309	ILE	3.3
1	C	272	THR	3.3
1	D	248	VAL	3.3
1	D	39	GLU	3.3
1	C	40	GLN	3.2
1	F	1	ALA	3.2
1	B	43	ASN	3.2
1	C	44	ARG	3.2
1	C	2	ASP	3.1
1	E	36	GLU	3.1
1	F	36	GLU	3.1
1	D	40	GLN	3.1
1	C	302	LEU	3.1
1	B	298	HIS	3.1
1	D	1	ALA	3.1
1	E	428	ILE	3.1
1	C	428	ILE	3.0
1	E	426	GLY	3.0
1	F	500	PHE	2.9
1	D	281	TRP	2.9
1	D	266	PHE	2.9
1	B	44	ARG	2.9
1	C	329	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	29	VAL	2.9
1	D	236	LEU	2.9
1	B	36	GLU	2.8
1	C	268	ALA	2.8
1	A	47	SER	2.8
1	A	33	LYS	2.8
1	C	426	GLY	2.8
1	A	390	ASN	2.8
1	B	297	GLN	2.8
1	C	364	ASN	2.8
1	B	312	GLY	2.7
1	A	417	LEU	2.7
1	C	5	ASP	2.7
1	C	285	GLY	2.7
1	F	499	THR	2.7
1	A	35	ARG	2.7
1	C	271	ILE	2.7
1	E	37	THR	2.7
1	E	272	THR	2.7
1	C	34	THR	2.7
1	C	35	ARG	2.6
1	E	427	THR	2.6
1	A	415	GLU	2.6
1	C	365	ILE	2.6
1	E	47	SER	2.6
1	D	270	CYS	2.6
1	D	431	VAL	2.5
1	D	433	THR	2.5
1	A	44	ARG	2.5
1	D	416	SER	2.5
1	B	11	LYS	2.5
1	F	421	PHE	2.5
1	D	72	TRP	2.5
1	C	332	THR	2.5
1	C	31	ASP	2.4
1	E	4	GLU	2.4
1	A	36	GLU	2.4
1	B	417	LEU	2.4
1	F	430	ILE	2.4
1	F	501	THR	2.4
1	C	243	GLY	2.4
1	A	387	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	19	ARG	2.4
1	E	412	SER	2.4
1	A	28	LEU	2.3
1	E	280	ILE	2.3
1	A	30	GLU	2.3
1	A	475	LEU	2.3
1	D	2	ASP	2.3
1	E	19	ARG	2.2
1	D	426	GLY	2.2
1	B	234	SER	2.2
1	C	313	SER	2.2
1	D	35	ARG	2.2
1	F	7	PRO	2.2
1	C	98	ASP	2.2
1	C	244	ASP	2.1
1	E	271	ILE	2.1
1	C	232	TYR	2.1
1	A	294	PHE	2.1
1	C	340	LYS	2.1
1	F	31	ASP	2.1
1	F	417	LEU	2.1
1	B	33	LYS	2.1
1	F	44	ARG	2.1
1	A	329	LYS	2.1
1	C	234	SER	2.1
1	B	41	LYS	2.1
1	F	34	THR	2.1
1	D	317	VAL	2.1
1	A	411	MET	2.1
1	E	361	LEU	2.0
1	D	37	THR	2.0
1	A	41	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLU	F	502	10/10	0.95	0.19	1.36	19,20,26,26	0
2	GLU	D	502	10/10	0.94	0.19	0.96	20,24,26,33	0
2	GLU	C	502	10/10	0.95	0.17	0.68	25,31,33,34	0
2	GLU	B	502	10/10	0.95	0.17	0.26	22,26,31,31	0
5	ZN	C	506	1/1	0.96	0.19	0.03	46,46,46,46	0
2	GLU	E	502	10/10	0.94	0.17	-0.23	20,29,33,35	0
3	NDP	A	552	48/48	0.96	0.16	-0.30	18,27,36,44	0
2	GLU	A	502	10/10	0.95	0.16	-0.38	19,26,31,31	0
5	ZN	B	505	1/1	0.97	0.17	-0.41	43,43,43,43	0
5	ZN	F	504	1/1	0.97	0.18	-0.43	37,37,37,37	0
3	NDP	D	552	48/48	0.97	0.15	-0.45	17,27,38,46	0
3	NDP	F	552	48/48	0.97	0.15	-0.49	14,21,32,35	0
3	NDP	C	552	48/48	0.94	0.17	-0.58	23,39,55,60	0
3	NDP	B	552	48/48	0.97	0.14	-0.58	24,32,39,42	0
5	ZN	D	505	1/1	0.95	0.15	-0.70	42,42,42,42	0
4	GTP	D	503	32/32	0.96	0.16	-0.80	19,33,40,42	0
3	NDP	E	552	48/48	0.95	0.15	-0.98	22,30,44,54	0
4	GTP	E	503	32/32	0.96	0.15	-1.07	16,27,33,38	0
4	GTP	B	503	32/32	0.96	0.14	-1.25	24,36,43,48	0
4	GTP	A	503	32/32	0.96	0.14	-1.27	24,34,37,44	0
4	GTP	C	503	32/32	0.94	0.15	-1.44	27,41,51,62	0
4	GTP	F	503	32/32	0.97	0.12	-1.98	18,23,35,45	0
5	ZN	E	505	1/1	0.93	0.13	-2.13	37,37,37,37	0
5	ZN	A	505	1/1	0.98	0.11	-2.61	31,31,31,31	0
5	ZN	C	504	1/1	0.95	0.06	-3.74	63,63,63,63	0
5	ZN	C	505	1/1	0.95	0.05	-4.41	55,55,55,55	0
5	ZN	D	504	1/1	0.92	0.08	-	65,65,65,65	0
5	ZN	B	504	1/1	0.97	0.04	-	64,64,64,64	0
5	ZN	E	504	1/1	0.99	0.07	-	50,50,50,50	0
5	ZN	A	504	1/1	0.95	0.08	-	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.