



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:43 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

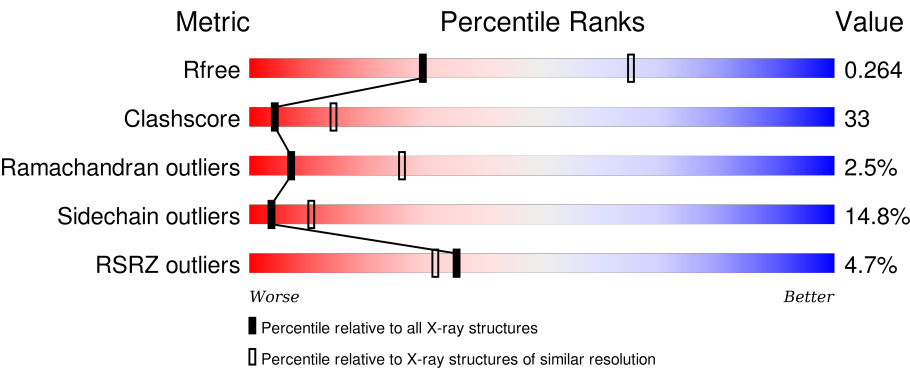
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance i

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}	91344	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (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 ≥ 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>5%</div><div><div>48%</div><div>42%</div><div>8%</div><div>..</div></div></div>
1	B	501	<div><div>4%</div><div><div>46%</div><div>44%</div><div>9%</div><div>..</div></div></div>
1	C	501	<div><div>7%</div><div><div>45%</div><div>44%</div><div>9%</div><div>.</div></div></div>
1	D	501	<div><div>4%</div><div><div>49%</div><div>41%</div><div>8%</div><div>.</div></div></div>
1	E	501	<div><div>4%</div><div><div>46%</div><div>44%</div><div>9%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	501	

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](#)

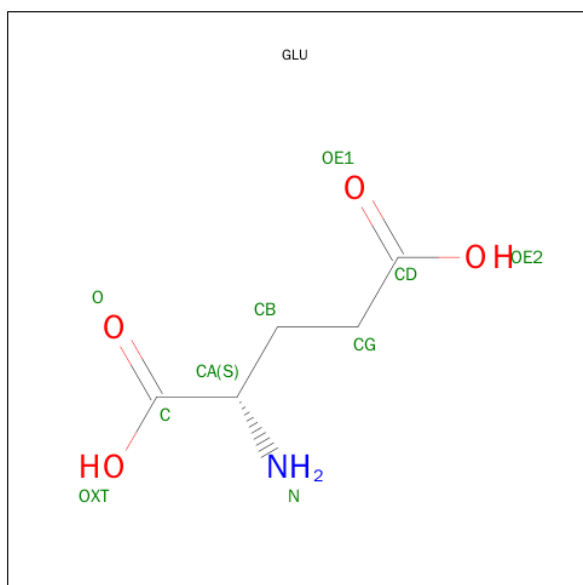
There are 5 unique types of molecules in this entry. The entry contains 23874 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

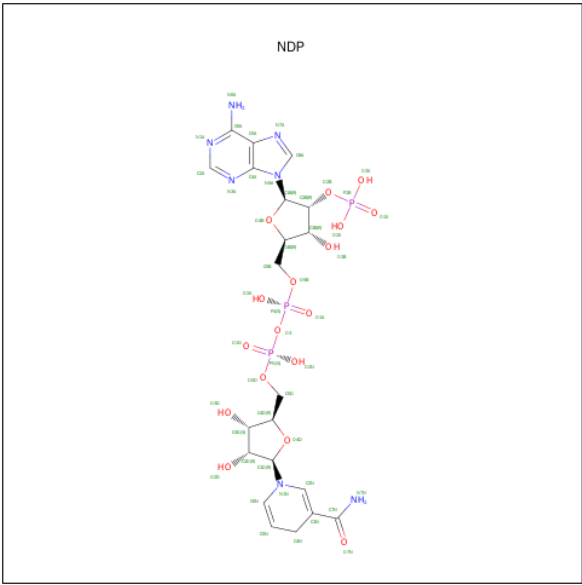
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	B	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	C	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	D	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	E	495	Total	C	N	O	S	0	0	0
			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: $C_5H_9NO_4$).



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: C₂₁H₃₀N₇O₁₇P₃).



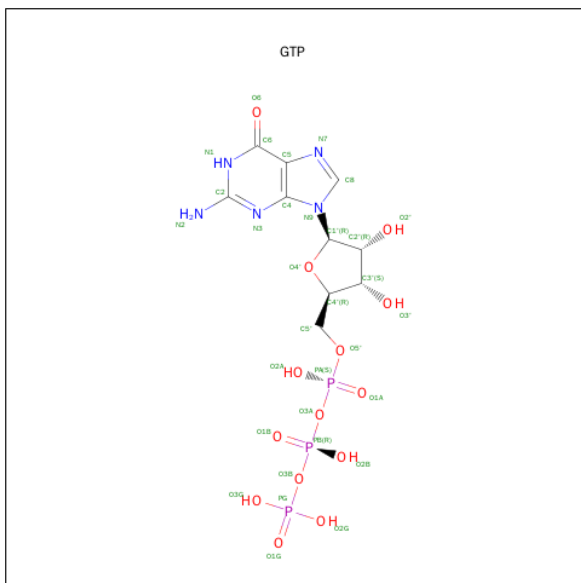
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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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: $C_{10}H_{16}N_5O_{14}P_3$).



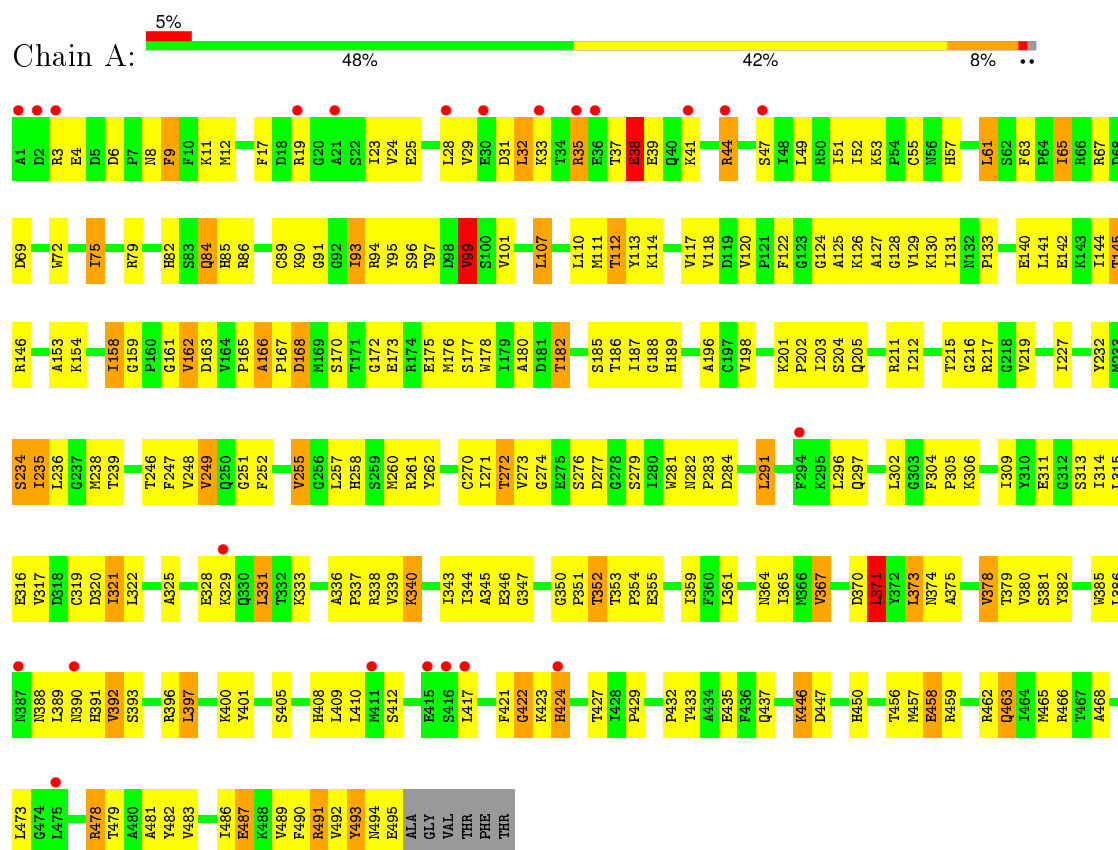
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	C	3	Total 3	Zn 3	0	0
5	A	2	Total 2	Zn 2	0	0
5	F	1	Total 1	Zn 1	0	0

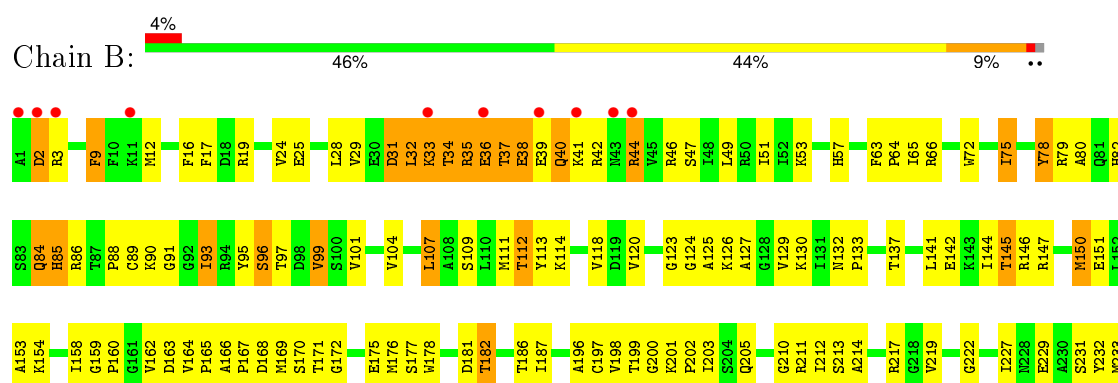
3 Residue-property plots

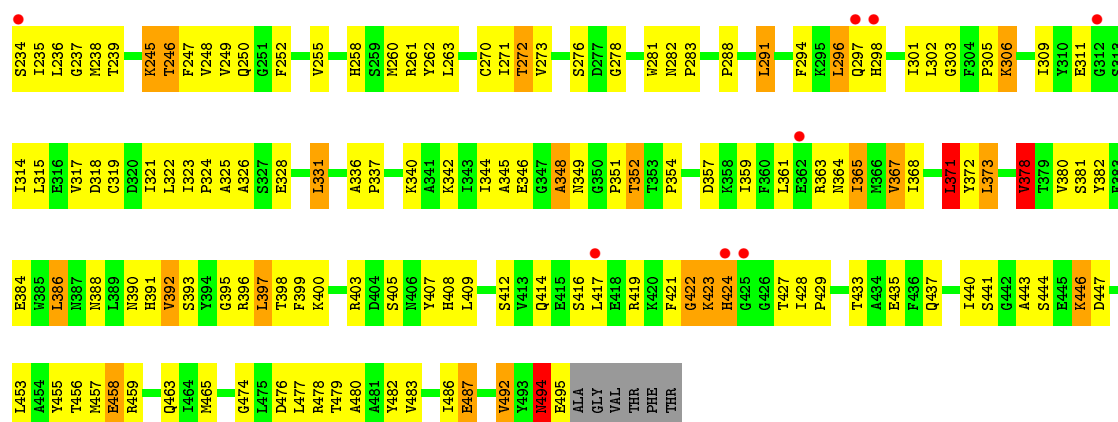
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

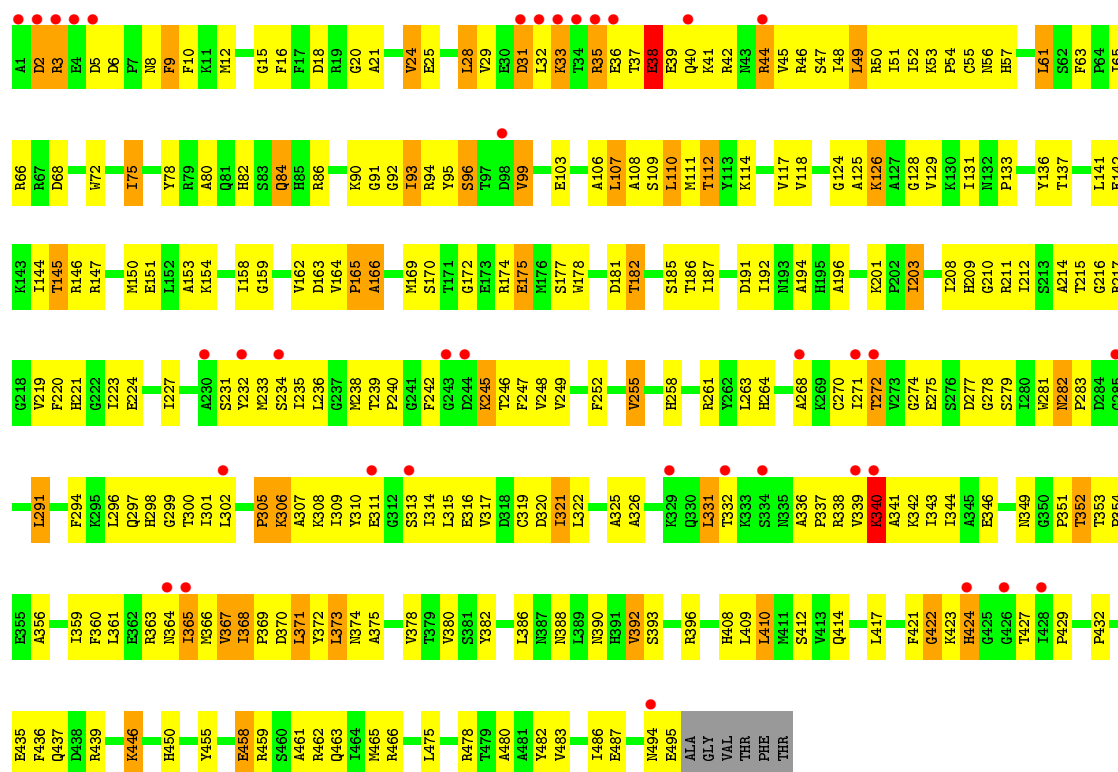


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

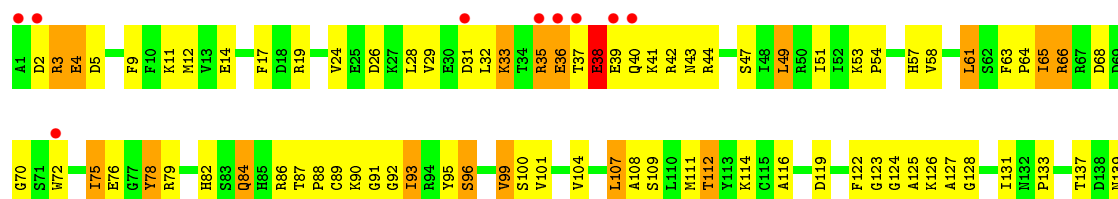


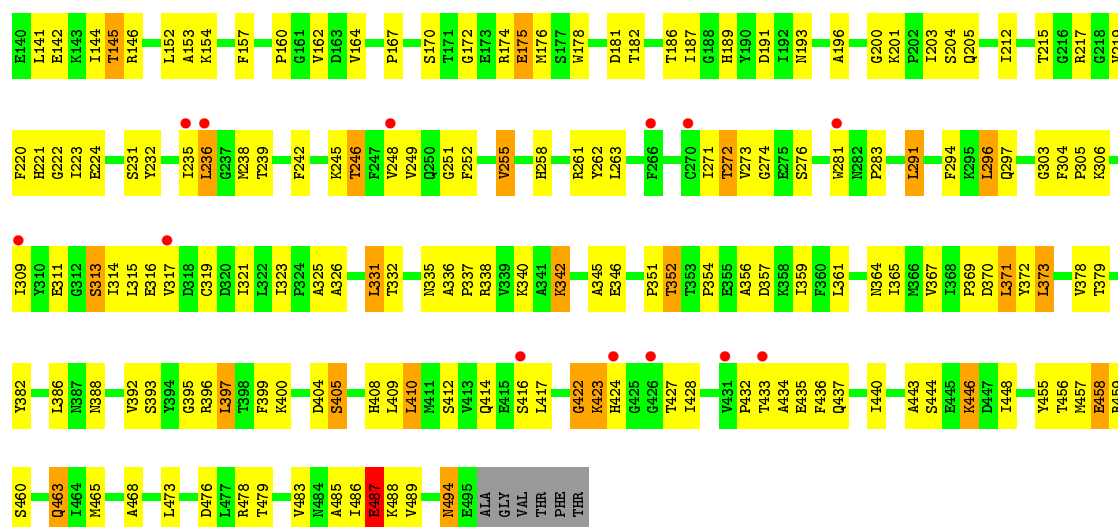


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

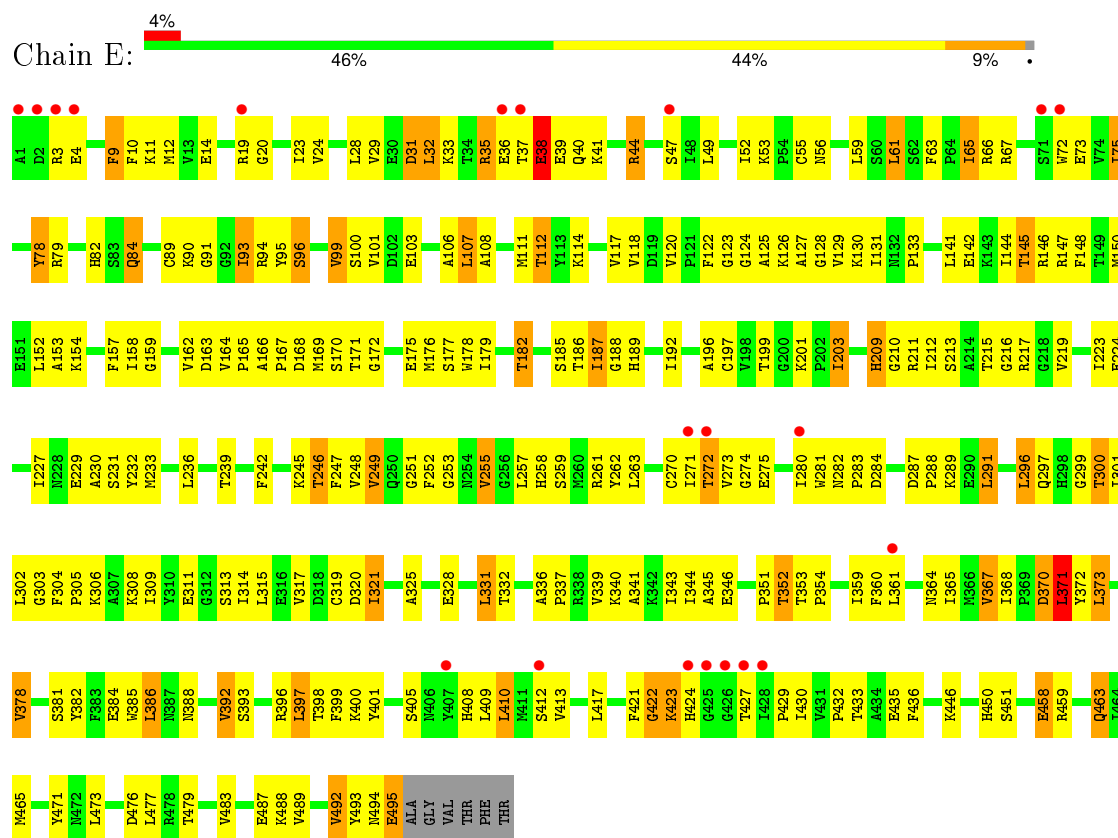


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

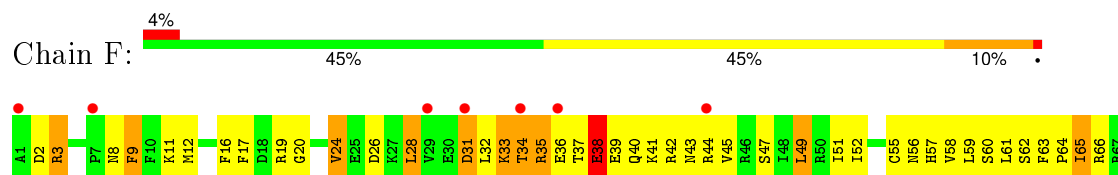




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



Y455	V378	E311	Y219	K143	D68
T456	T379	G312	I227	I144	
M457	V380	S313		T145	W72
E458	S381	I314	A230	R146	I75
R459	Y382	I315	S231	F147	E76
S460	F383	E316	Y232	T148	
A461	E384	V317	T233	T149	E77
R462	T385	D318	S234	M150	Y78
	L386	C319	L235	E151	R79
M465	N387	D320	L236	A153	H82
R466	N388	I321			
		L322	T239	I158	S83
L475	V392			G159	O84
	S393	A325	F242		H85
R478	G394			V162	H86
T479	G395	E328	D244	D163	C89
A480	R396	L397	K245	V164	X90
A481	L397		T246	P165	G91
A482	T398	L331	F247	A166	G92
V483	F399		V248	P167	I93
	K400	A336	V249		R94
I486	Y401	R337		S170	Y95
E487	E402	R338	F252	T171	S96
	R403	V339		G172	T97
R491		K340	V255	E173	D98
		A341	G256	R174	Y99
M494	R408	R342		E175	S100
E495	L409	I343	H258	M176	V101
A496	L410	I344		S177	D102
A497	M411	A345	R261	W178	E103
C497	S412	E346	T262		
V498		C347	L263	D181	L107
T499	S416	A348	H264	T182	A108
F500	L417	N349			S109
T501	E418	G350	C270	T186	L110
	R419	P351	I271	I187	M111
	K420	T352	T272	G188	T112
	F421	T353	V273	H189	Y113
	G422	P354			K114
	K423		I280	A196	
	H424	D357	N281	C197	V117
		K358	N282	V198	V118
	G425	I359	P283	T199	
	T427	F360	I286	G200	G123
	T428	L361	D287	K201	G124
	P429	E362	N288	P202	A125
	T430	R363	P288	I203	K126
	V431	N364		S204	A127
	P432	I365	L291	G128	
	T433	M366		V129	
	A434	V367	F294	G210	K130
	E435	I368	K295	R211	I131
	F436	P369	L296	I212	N132
	Q437	D370	Q297	S213	P133
	D438	Y371	H298	A214	
	R439	Y372		T215	T137
		L373	F304	G216	
	K446	N374	P305	R217	L141
	D447	A375	K306	G218	E142
	T448				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	34.5	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 75931 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23874	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

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:D:93:ILE:HD11	1:D:95:TYR:CE1	2.02	0.95
1:C:337:PRO:HD3	1:C:359:ILE:HD13	1.47	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:C:93:ILE:HD11	1:C:95:TYR:HE1	1.33	0.90
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: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:E:201:LYS:NZ	1:E:388:ASN:HD21	1.74	0.85
1:B:91:GLY:HA3	1:B:125:ALA:O	1.75	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:F:112:THR:HG22	1:F:124:GLY:HA3	1.58	0.84
1:E:112:THR:HG22	1:E:124:GLY:N	1.92	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:D:346:GLU:HG2	1:D:351:PRO:HG2	1.60	0.82
1:C:248:VAL:HG23	1:C:272:THR:O	1.80	0.82
1:A:35:ARG:H	1:A:35:ARG:HD3	1.45	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:142:GLU:O	1:A:146:ARG:HG3	1.81	0.81
1:A:118:VAL:HG23	1:A:120:VAL:HG23	1.62	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:E:458:GLU:HG3	1:E:459:ARG:N	1.98	0.79
1:D:271:ILE:HD12	1:D:272:THR:HG22	1.63	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:E:258:HIS:CD2	1:E:261:ARG:HH11	2.00	0.79
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.17	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: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:A:346:GLU:OE1	1:A:352:THR:HG23	1.83	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:E:432:PRO:HB3	1:E:436:PHE:HD2	1.49	0.77
1:D:178:TRP:HE1	1:F:498:VAL:CG2	1.96	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:F:93:ILE:CD1	1:F:95:TYR:CE1	2.66	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:432:PRO:HB2	1:F:437:GLN:HG2	1.65	0.77
1:C:141:LEU:O	1:C:145:THR:HG23	1.84	0.77
1:A:90:LYS:HD3	1:A:122:PHE:CE1	2.19	0.77
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.19	0.77
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.65	0.76
1:B:93:ILE:HD11	1:B:95:TYR:HE1	1.50	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:C:65:ILE:HG13	1:C:144:ILE:HG12	1.68	0.76
1:A:12:MET:HG3	1:A:354:PRO:HD3	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:C:38:GLU:CG	1:C:39:GLU:H	1.85	0.75
1:B:336:ALA:N	1:B:337:PRO:HD2	2.02	0.75
1:E:38:GLU:CG	1:E:39:GLU:N	2.45	0.75
1:A:217:ARG:HB2	1:A:262:TYR:CE1	2.21	0.75
1:E:417:LEU:HD13	1:F:417:LEU:HD21	1.67	0.74
1:F:112:THR:HG22	1:F:124:GLY:CA	2.17	0.74
1:A:353:THR:HB	1:A:354:PRO:HD2	1.68	0.74
1:F:20:GLY:O	1:F:24:VAL:HG22	1.87	0.74
1:F:82:HIS:CD2	1:F:112:THR:CG2	2.69	0.74
1:A:201:LYS:NZ	1:A:388:ASN:HD21	1.84	0.74
1:A:25:GLU:O	1:A:29:VAL:HG23	1.88	0.74
1:A:91:GLY:HA3	1:A:125:ALA:O	1.87	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:F:346:GLU:HG2	1:F:351:PRO:HG2	1.69	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:D:201:LYS:NZ	1:D:388:ASN:HD21	1.87	0.73
1:A:19:ARG:HG2	1:A:479:THR:HG21	1.71	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:82:HIS:HD2	1:E:112:THR:HG21	1.52	0.72
1:E:246:THR:HG22	1:E:320:ASP:H	1.54	0.72
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.24	0.72
1:E:19:ARG:HG2	1:E:479:THR:HG21	1.71	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:F:372:TYR:OH	1:F:461:ALA:HB2	1.88	0.72
1:A:408:HIS:NE2	1:B:435:GLU:HG2	2.03	0.72
1:C:82:HIS:CD2	1:C:112:THR:CG2	2.73	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.18	0.72
1:B:247:PHE:CZ	1:B:270:CYS:HB2	2.22	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:281:TRP:O	1:C:307:ALA:HB1	1.90	0.71
1:C:247:PHE:CZ	1:C:270:CYS:HB2	2.25	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:B:417:LEU:HD21	1:C:417:LEU:CD1	2.21	0.71
1:C:346:GLU:HG2	1:C:351:PRO:HG2	1.73	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:F:252:PHE:CE2	1:F:291:LEU:HD13	2.26	0.70
1:A:315:LEU:HD13	1:A:331:LEU:HD13	1.72	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:F:65:ILE:HG13	1:F:144:ILE:CG1	2.21	0.70
1:D:457:MET:HA	1:D:457:MET:CE	2.21	0.70
1:B:344:ILE:HB	1:B:367:VAL:HG12	1.72	0.70
1:E:24:VAL:HG11	1:E:483:VAL:HG13	1.73	0.70
1:C:72:TRP:HB2	1:F:47:SER:HB3	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:F:107:LEU:HG	1:F:126:LYS:HE3	1.73	0.69
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.36	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:271:ILE:HD12	1:E:272:THR:HG23	1.74	0.69
1:D:303:GLY:H	1:D:309:ILE:HD11	1.58	0.69
1:B:213:SER:HB2	1:B:258:HIS:CD2	2.27	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:B:271:ILE:HD11	1:B:319:CYS:HB3	1.73	0.69
1:C:346:GLU:OE1	1:C:352:THR:HG23	1.92	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:C:126:LYS:NZ	2:C:502:GLU:N	2.41	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: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:C:107:LEU:HB3	1:C:126:LYS:HG2	1.74	0.68
1:A:257:LEU:O	1:A:257:LEU:HD12	1.92	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:O	1:B:9:PHE:HD2	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:336:ALA:N	1:C:337:PRO:HD2	2.09	0.68
1:C:246:THR:OG1	1:C:271:ILE:HG12	1.94	0.68
1:D:139:ASN:OD1	1:F:501:THR:HG21	1.92	0.68
1:C:322:LEU:HB3	1:C:344:ILE:CD1	2.23	0.68
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.75	0.68
1:D:95:TYR:HB3	1:D:133:PRO:HG3	1.76	0.68
1:A:79:ARG:HD2	1:A:127:ALA:HB2	1.76	0.68
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.75	0.68
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:107:LEU:HG	1:E:126:LYS:HE3	1.76	0.67
1:A:112:THR:CG2	1:A:124:GLY:H	2.06	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:B:196:ALA:HA	1:B:388:ASN:HD22	1.60	0.67
1:A:6:ASP:OD1	1:A:329:LYS:HD2	1.95	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:C:75:ILE:C	1:C:75:ILE:HD13	2.14	0.67
1:B:392:VAL:HG11	1:B:397:LEU:HD11	1.75	0.67
1:E:259:SER:O	1:E:263:LEU:HD12	1.94	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:A:159:GLY:HA3	1:A:162:VAL:HG13	1.77	0.67
1:D:32:LEU:HD13	1:D:494:ASN:OD1	1.95	0.66
1:C:99:VAL:HA	1:C:103:GLU:OE2	1.95	0.66
1:C:158:ILE:HG12	1:C:159:GLY:N	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:B:303:GLY:N	1:B:309:ILE:HD11	2.10	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:F:478:ARG:HH11	1:F:478:ARG:HG3	1.59	0.66
1:E:353:THR:HB	1:E:354:PRO:HD2	1.76	0.66
1:E:75:ILE:C	1:E:75:ILE:HD13	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:C:248:VAL:HB	1:C:272:THR:HG23	1.78	0.65
1:D:409:LEU:HD11	1:F:409:LEU:HD13	1.78	0.65
1:A:427:THR:O	1:A:429:PRO:HD3	1.96	0.65
1:E:52:ILE:HG12	1:E:493:TYR:CE1	2.32	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:D:112:THR:HG22	1:D:124:GLY:CA	2.26	0.65
1:C:219:VAL:HA	1:C:373:LEU:CD2	2.27	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:F:65:ILE:HG13	1:F:144:ILE:HG13	1.79	0.64
1:B:315:LEU:HD13	1:B:331:LEU:HD13	1.79	0.64
1:B:263:LEU:CD1	1:B:323:ILE:HD11	2.28	0.64
1:B:47:SER:O	1:B:51:ILE:HG13	1.96	0.64
1:E:413:VAL:HG12	1:E:430:ILE:HG13	1.78	0.64
1:C:55:CYS:O	1:F:62:SER:HB2	1.97	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:B:112:THR:CG2	1:B:124:GLY:H	2.11	0.64
1:B:114:LYS:HA	1:B:371:LEU:CD2	2.28	0.64
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.45	0.64
1:A:435:GLU:HG2	1:C:408:HIS:NE2	2.13	0.64
1:E:75:ILE:O	1:E:75:ILE:HD13	1.97	0.64
1:D:175:GLU:HA	1:D:178:TRP:CE3	2.33	0.64
1:C:322:LEU:HB3	1:C:344:ILE:HD13	1.80	0.64
1:B:37:THR:O	1:B:38:GLU:CG	2.41	0.64
1:D:53:LYS:O	1:D:82:HIS:HE1	1.80	0.64
1:B:32:LEU:HD13	1:B:494:ASN:HD21	1.62	0.64
1:C:332:THR:HG22	1:C:353:THR:CG2	2.28	0.64
1:F:95:TYR:OH	1:F:145:THR:HB	1.97	0.63
1:C:261:ARG:NH2	4:C:503:GTP:C8	2.66	0.63
1:E:196:ALA:HA	1:E:388:ASN:HD22	1.63	0.63
1:A:272:THR:CG2	1:A:317:VAL:HG11	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ASP:O	1:C:302:LEU:HD11	1.99	0.63
1:E:346:GLU:HG2	1:E:351:PRO:HG2	1.79	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:B:210:GLY:O	1:B:214:ALA:HB2	1.98	0.63
1:E:258:HIS:HD2	1:E:261:ARG:NH1	1.95	0.63
1:A:232:TYR:HE2	1:A:465:MET:HG2	1.63	0.63
1:C:315:LEU:HD13	1:C:331:LEU:HD12	1.79	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:C:223:ILE:HD12	1:C:263:LEU:HD11	1.81	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:C:93:ILE:HG13	1:C:93:ILE:O	1.99	0.62
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.46	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:E:63:PHE:CD1	1:E:147:ARG:HG3	2.35	0.62
1:C:3:ARG:H	1:C:3:ARG:CD	2.10	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: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:D:107:LEU:HG	1:D:126:LYS:HE3	1.81	0.62
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.29	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:D:172:GLY:H	1:D:175:GLU:HG2	1.64	0.61
1:B:214:ALA:HB1	1:B:380:VAL:HG21	1.83	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:F:255:VAL:HG22	1:F:325:ALA:HB1	1.81	0.61
1:D:47:SER:O	1:D:51:ILE:HG13	2.01	0.61
1:D:485:ALA:O	1:D:489:VAL:HG23	2.01	0.61
1:C:92:GLY:O	1:C:126:LYS:HD3	2.00	0.61
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.31	0.61
1:C:117:VAL:HG21	1:C:371:LEU:HD22	1.83	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:57:HIS:HD2	1:E:61:LEU:HD12	1.66	0.61
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.30	0.61
1:E:201:LYS:NZ	1:E:388:ASN:ND2	2.48	0.60
1:A:153:ALA:HB1	1:A:187:ILE:HG13	1.81	0.60
1:B:126:LYS:HG3	1:B:127:ALA:N	2.16	0.60
1:A:91:GLY:O	1:A:165:PRO:HA	2.01	0.60
1:E:117:VAL:CG2	1:E:371:LEU:HD22	2.30	0.60
1:A:392:VAL:HG22	1:B:386:LEU:HD11	1.83	0.60
1:D:167:PRO:HD3	1:D:200:GLY:HA3	1.83	0.60
1:C:217:ARG:CZ	1:C:450:HIS:CD2	2.85	0.60
1:B:164:VAL:HG13	1:B:198:VAL:HA	1.83	0.60
1:D:92:GLY:O	1:D:126:LYS:HD3	2.02	0.60
1:D:395:GLY:HA3	1:D:399:PHE:CZ	2.37	0.60
1:C:20:GLY:O	1:C:24:VAL:HG22	2.01	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:F:37:THR:O	1:F:38:GLU:HB3	2.01	0.60
1:A:446:LYS:HG3	1:A:447:ASP:H	1.67	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
1:B:408:HIS:HB3	1:C:436:PHE:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:LEU:HD21	1:F:417:LEU:HD13	1.83	0.60
1:C:211:ARG:HD2	1:C:211:ARG:O	2.00	0.60
1:B:153:ALA:HB1	1:B:187:ILE:HG13	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:F:82:HIS:CG	1:F:109:SER:HA	2.37	0.60
1:F:219:VAL:HA	1:F:373:LEU:HD22	1.82	0.60
1:F:8:ASN:OD1	1:F:11:LYS:HG3	2.02	0.60
1:C:427:THR:O	1:C:429:PRO:HD3	2.02	0.60
1:C:315:LEU:HD13	1:C:331:LEU:HD13	1.83	0.59
1:E:336:ALA:N	1:E:337:PRO:HD2	2.15	0.59
1:B:64:PRO:O	1:B:65:ILE:HD13	2.02	0.59
1:F:369:PRO:HG3	1:F:478:ARG:HA	1.82	0.59
1:C:24:VAL:HG13	1:C:483:VAL:HG22	1.83	0.59
1:E:203:ILE:HD11	1:E:209:HIS:HA	1.83	0.59
1:F:199:THR:HG22	1:F:384:GLU:HG2	1.82	0.59
1:B:146:ARG:HG2	1:B:182:THR:HG21	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:B:390:ASN:O	1:B:392:VAL:HG23	2.01	0.59
1:E:219:VAL:HA	1:E:373:LEU:HD22	1.84	0.59
1:A:24:VAL:HG11	1:A:483:VAL:HG13	1.82	0.59
1:E:229:GLU:HG3	1:E:231:SER:HB3	1.84	0.59
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.84	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:B:96:SER:O	1:B:99:VAL:CG1	2.50	0.59
1:A:247:PHE:CZ	1:A:270:CYS:HB2	2.38	0.59
1:D:457:MET:HE2	1:D:457:MET:HA	1.83	0.59
1:B:24:VAL:HG11	1:B:483:VAL:HG13	1.84	0.59
1:A:63:PHE:CZ	1:A:75:ILE:CD1	2.85	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:A:446:LYS:HG3	1:A:447:ASP:N	2.17	0.59
1:F:112:THR:HG22	1:F:124:GLY:N	2.18	0.59
1:F:9:PHE:CE1	1:F:107:LEU:HD13	2.38	0.59
1:E:227:ILE:HD11	1:E:245:LYS:HG2	1.85	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:E:422:GLY:C	1:E:423:LYS:HD2	2.23	0.59
1:C:298:HIS:O	1:C:300:THR:N	2.36	0.59
1:D:397:LEU:O	1:F:448:ILE:HD12	2.02	0.59
1:B:408:HIS:ND1	1:C:439:ARG:HD2	2.18	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:246:THR:O	1:C:320:ASP:HB2	2.03	0.58
1:C:63:PHE:CZ	1:C:75:ILE:CD1	2.86	0.58
1:A:433:THR:HG23	1:C:412:SER:OG	2.03	0.58
1:C:18:ASP:O	1:C:21:ALA:HB3	2.03	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:B:271:ILE:HD12	1:B:272:THR:HG23	1.86	0.58
1:A:490:PHE:O	1:A:491:ARG:CB	2.51	0.58
1:C:321:ILE:HG23	1:C:343:ILE:HB	1.84	0.58
1:F:322:LEU:HB3	1:F:344:ILE:HD12	1.86	0.58
1:D:422:GLY:C	1:D:423:LYS:HD2	2.23	0.58
1:D:95:TYR:OH	1:D:145:THR:HB	2.03	0.58
1:F:32:LEU:HD13	1:F:494:ASN:ND2	2.15	0.58
1:C:258:HIS:HD2	1:C:261:ARG:NH1	2.01	0.58
1:A:422:GLY:C	1:A:423:LYS:HD2	2.24	0.58
1:E:118:VAL:HG23	1:E:120:VAL:HG23	1.84	0.58
1:A:257:LEU:C	1:A:257:LEU:HD12	2.24	0.58
1:C:68:ASP:OD1	1:C:137:THR:HG21	2.03	0.58
1:F:172:GLY:H	1:F:175:GLU:HG2	1.69	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:E:95:TYR:OH	1:E:145:THR:HG22	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:D:152:LEU:HD22	1:D:157:PHE:HB3	1.85	0.58
1:E:150:MET:O	1:E:154:LYS:HG3	2.04	0.58
1:E:246:THR:CG2	1:E:320:ASP:H	2.15	0.58
1:A:85:HIS:CD2	1:A:86:ARG:HG2	2.38	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:E:432:PRO:HB3	1:E:436:PHE:CD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:LYS:N	1:D:342:LYS:HD3	2.19	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:C:215:THR:O	1:C:219:VAL:HG23	2.04	0.57
1:A:232:TYR:CE2	1:A:465:MET:HG2	2.38	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:463:GLN:OE1	1:E:488:LYS:NZ	2.35	0.57
1:E:23:ILE:HG22	1:E:471:TYR:CD1	2.40	0.57
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.40	0.57
1:D:248:VAL:HG12	1:D:319:CYS:SG	2.45	0.57
1:C:63:PHE:CZ	1:C:75:ILE:HD12	2.40	0.57
1:B:250:GLN:NE2	1:B:315:LEU:HD21	2.20	0.57
1:F:368:ILE:HB	1:F:373:LEU:HD12	1.85	0.57
1:E:308:LYS:HG3	1:E:309:ILE:O	2.05	0.57
1:E:427:THR:HG23	1:E:427:THR:O	2.04	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: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:E:196:ALA:HB2	1:E:388:ASN:HB2	1.87	0.57
1:D:370:ASP:OD1	1:D:371:LEU:N	2.34	0.57
1:C:37:THR:HG22	1:C:41:LYS:HE3	1.85	0.56
1:B:38:GLU:CG	1:B:39:GLU:N	2.61	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:F:93:ILE:CD1	1:F:95:TYR:HE1	2.11	0.56
1:E:29:VAL:HG13	1:E:41:LYS:HB3	1.87	0.56
1:A:114:LYS:HA	1:A:371:LEU:CD2	2.35	0.56
1:F:346:GLU:HG2	1:F:351:PRO:CG	2.35	0.56
1:F:258:HIS:HD2	1:F:261:ARG:NH1	1.97	0.56
1:D:107:LEU:HB3	1:D:126:LYS:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:PRO:O	1:D:65:ILE:HD13	2.05	0.56
1:F:59:LEU:O	1:F:78:TYR:HA	2.05	0.56
1:B:233:MET:HA	1:B:233:MET:HE2	1.86	0.56
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.87	0.56
1:F:24:VAL:HG13	1:F:483:VAL:HG13	1.88	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:B:260:MET:HE1	1:B:288:PRO:HA	1.86	0.56
1:F:382:TYR:O	1:F:386:LEU:HD22	2.05	0.56
1:F:227:ILE:HD11	1:F:245:LYS:HG2	1.86	0.56
1:C:146:ARG:HE	1:C:182:THR:CG2	2.18	0.56
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.87	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:E:75:ILE:HD11	1:E:129:VAL:HG13	1.87	0.56
1:C:466:ARG:HB2	1:C:466:ARG:NH1	2.20	0.56
1:A:107:LEU:CG	1:A:126:LYS:HE3	2.30	0.56
1:E:272:THR:OG1	1:E:314:ILE:HD11	2.04	0.56
1:C:371:LEU:HD12	1:C:482:TYR:CE1	2.41	0.56
1:A:432:PRO:HB2	1:A:437:GLN:HG2	1.87	0.56
1:A:37:THR:HG22	1:A:41:LYS:HE3	1.87	0.56
1:D:205:GLN:NE2	1:F:496:ALA:HB2	2.20	0.56
1:F:271:ILE:C	1:F:272:THR:HG22	2.26	0.56
1:F:63:PHE:CZ	1:F:75:ILE:CD1	2.89	0.56
1:B:38:GLU:H	1:B:41:LYS:HD2	1.71	0.56
1:A:370:ASP:OD1	1:A:371:LEU:N	2.29	0.56
1:E:23:ILE:CG2	1:E:471:TYR:CD1	2.89	0.56
1:D:3:ARG:HD2	1:D:4:GLU:N	2.20	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:211:ARG:HH22	3:A:552:NDP:H72N	1.53	0.55
1:F:374:ASN:HB2	3:F:552:NDP:C5N	2.36	0.55
1:A:196:ALA:HB2	1:A:388:ASN:HB2	1.88	0.55
1:E:90:LYS:HD3	1:E:122:PHE:CD1	2.41	0.55
1:F:201:LYS:HZ2	1:F:388:ASN:HD21	1.52	0.55
1:E:175:GLU:H	1:E:175:GLU:CD	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:GLN:C	1:F:86:ARG:H	2.08	0.55
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.88	0.55
1:F:457:MET:HA	1:F:457:MET:CE	2.37	0.55
1:F:150:MET:HA	1:F:150:MET:HE3	1.88	0.55
1:D:17:PHE:CE1	1:D:486:ILE:HG12	2.42	0.55
1:F:211:ARG:HH22	3:F:552:NDP:H72N	1.55	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:A:23:ILE:HD12	1:A:473:LEU:HD21	1.88	0.55
1:A:113:TYR:C	1:A:371:LEU:HD21	2.27	0.55
1:F:496:ALA:HB3	1:F:498:VAL:O	2.05	0.55
1:B:409:LEU:HD11	1:C:409:LEU:HD13	1.87	0.55
1:F:75:ILE:HG12	1:F:76:GLU:N	2.20	0.55
1:C:39:GLU:C	1:C:41:LYS:H	2.09	0.55
1:F:495:GLU:O	1:F:497:GLY:N	2.37	0.55
1:C:368:ILE:HB	1:C:373:LEU:HD12	1.88	0.55
1:F:201:LYS:HZ2	1:F:388:ASN:ND2	2.04	0.55
1:D:167:PRO:CD	1:D:200:GLY:HA3	2.37	0.55
1:D:315:LEU:HD13	1:D:331:LEU:HD13	1.88	0.55
1:A:281:TRP:CZ2	1:A:283:PRO:CG	2.90	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:A:427:THR:O	1:A:427:THR:HG23	2.06	0.55
1:C:203:ILE:HD11	1:C:209:HIS:HA	1.89	0.55
1:E:489:VAL:O	1:E:492:VAL:HG13	2.07	0.55
1:E:79:ARG:NH2	1:E:163:ASP:OD2	2.39	0.55
1:D:186:THR:O	1:D:189:HIS:ND1	2.30	0.55
1:D:346:GLU:HG2	1:D:351:PRO:CG	2.34	0.55
1:D:248:VAL:CG2	1:D:272:THR:HG23	2.37	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:96:SER:O	1:B:99:VAL:HG13	2.06	0.55
1:F:95:TYR:HB3	1:F:133:PRO:HG3	1.88	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:B:177:SER:HB2	1:B:202:PRO:HG2	1.89	0.55
1:E:63:PHE:CZ	1:E:75:ILE:HD12	2.42	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:F:478:ARG:NH1	1:F:478:ARG:HG3	2.22	0.54
1:A:232:TYR:O	1:A:236:LEU:HB2	2.07	0.54
1:F:131:ILE:O	1:F:133:PRO:HD3	2.07	0.54
1:B:90:LYS:HD2	1:B:164:VAL:O	2.06	0.54
1:B:273:VAL:HG21	1:B:291:LEU:CD1	2.35	0.54
1:A:154:LYS:HD2	1:E:189:HIS:HB3	1.88	0.54
1:B:444:SER:O	1:B:447:ASP:HB2	2.07	0.54
1:D:146:ARG:NH2	1:D:181:ASP:OD2	2.40	0.54
1:F:271:ILE:HD12	1:F:272:THR:HG22	1.90	0.54
1:F:146:ARG:NH2	1:F:181:ASP:OD2	2.40	0.54
1:C:24:VAL:HB	1:C:28:LEU:HD22	1.90	0.54
1:F:174:ARG:O	1:F:177:SER:HB3	2.08	0.54
1:F:294:PHE:CE2	1:F:298:HIS:ND1	2.75	0.54
1:E:166:ALA:HB1	1:E:167:PRO:HD2	1.88	0.54
1:B:248:VAL:HG23	1:B:272:THR:OG1	2.08	0.54
1:F:84:GLN:C	1:F:86:ARG:N	2.61	0.54
1:B:408:HIS:CE1	1:C:435:GLU:HG2	2.43	0.54
1:C:37:THR:O	1:C:38:GLU:HB3	2.08	0.54
1:B:378:VAL:HA	1:B:381:SER:HB2	1.87	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:F:32:LEU:CD1	1:F:494:ASN:HD21	2.19	0.54
1:D:201:LYS:HZ1	1:D:388:ASN:HD21	1.55	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:F:219:VAL:HA	1:F:373:LEU:CD2	2.38	0.54
1:B:95:TYR:HB3	1:B:133:PRO:HG3	1.89	0.54
1:E:90:LYS:HD2	1:E:164:VAL:HB	1.90	0.54
1:A:490:PHE:O	1:A:491:ARG:HB3	2.07	0.54
1:C:90:LYS:HD2	1:C:164:VAL:HB	1.89	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:F:427:THR:HG23	1:F:427:THR:O	2.08	0.54
1:E:114:LYS:HA	1:E:371:LEU:HD23	1.89	0.54
1:C:158:ILE:HG12	1:C:159:GLY:H	1.72	0.54
1:E:346:GLU:OE1	1:E:352:THR:HG23	2.08	0.54
1:C:108:ALA:O	1:C:111:MET:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:LYS:HG3	1:C:309:ILE:O	2.07	0.54
1:B:19:ARG:HG2	1:B:479:THR:HG21	1.90	0.54
1:F:112:THR:HG22	1:F:124:GLY:H	1.71	0.53
1:C:114:LYS:HA	1:C:371:LEU:HD23	1.89	0.53
1:F:2:ASP:O	1:F:3:ARG:HB2	2.07	0.53
1:A:400:LYS:HB2	1:B:455:TYR:HB2	1.89	0.53
1:B:272:THR:HG21	1:B:317:VAL:HG21	1.90	0.53
1:D:201:LYS:HZ2	1:D:388:ASN:HD21	1.56	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:C:21:ALA:HA	1:C:486:ILE:HD13	1.90	0.53
1:C:186:THR:OG1	1:C:187:ILE:N	2.36	0.53
1:F:68:ASP:OD1	1:F:137:THR:HG21	2.09	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:B:146:ARG:NE	1:B:182:THR:HG22	2.24	0.53
1:E:39:GLU:C	1:E:41:LYS:H	2.10	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:F:47:SER:O	1:F:51:ILE:HG13	2.09	0.53
1:D:2:ASP:CG	1:D:3:ARG:N	2.61	0.53
1:F:232:TYR:CE2	1:F:465:MET:HG2	2.43	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:172:GLY:H	1:B:175:GLU:HG2	1.73	0.53
1:D:53:LYS:O	1:D:82:HIS:CE1	2.62	0.53
1:D:314:ILE:HA	1:D:317:VAL:HG23	1.90	0.53
1:D:19:ARG:HG2	1:D:479:THR:CG2	2.37	0.53
1:D:432:PRO:HB2	1:D:437:GLN:HG2	1.89	0.53
1:B:446:LYS:NZ	1:B:446:LYS:HB2	2.24	0.53
1:B:82:HIS:HD2	1:B:112:THR:CG2	2.03	0.53
1:D:346:GLU:CG	1:D:351:PRO:HG2	2.37	0.53
1:A:248:VAL:CB	1:A:272:THR:HG23	2.37	0.53
1:C:114:LYS:NZ	2:C:502:GLU:O	2.42	0.53
1:C:374:ASN:HB2	3:C:552:NDP:C5N	2.39	0.53
1:E:255:VAL:HG22	1:E:325:ALA:HB1	1.90	0.53
1:D:222:GLY:HA2	1:D:372:TYR:OH	2.08	0.53
1:D:24:VAL:HG11	1:D:483:VAL:HG13	1.90	0.53
1:B:166:ALA:HA	1:B:199:THR:O	2.08	0.53
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.91	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:E:201:LYS:HZ2	1:E:388:ASN:ND2	2.07	0.53
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:246:THR:O	1:E:320:ASP:HB2	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:A:328:GLU:HB2	1:A:350:GLY:O	2.09	0.52
1:C:255:VAL:HG22	1:C:325:ALA:HB1	1.91	0.52
1:E:432:PRO:HA	1:F:412:SER:HB3	1.91	0.52
1:D:417:LEU:HD21	1:F:417:LEU:CD1	2.39	0.52
1:A:17:PHE:CE2	1:A:53:LYS:HG3	2.44	0.52
1:E:378:VAL:HA	1:E:381:SER:HB2	1.91	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:B:171:THR:HB	1:B:175:GLU:HG3	1.91	0.52
2:E:502:GLU:HA	3:E:552:NDP:H41N	1.92	0.52
1:A:67:ARG:HD2	1:A:140:GLU:OE1	2.10	0.52
1:E:199:THR:HA	1:E:384:GLU:OE1	2.09	0.52
1:B:346:GLU:HG2	1:B:351:PRO:HG2	1.90	0.52
1:E:346:GLU:HG2	1:E:351:PRO:CG	2.40	0.52
1:D:75:ILE:HG12	1:D:76:GLU:N	2.24	0.52
1:B:38:GLU:HG2	1:B:40:GLN:HG2	1.91	0.52
1:A:55:CYS:HA	1:A:82:HIS:HA	1.91	0.52
1:E:291:LEU:CD2	1:E:301:ILE:HG22	2.40	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:A:371:LEU:HD12	1:A:482:TYR:CD1	2.44	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:B:478:ARG:HG3	1:B:478:ARG:HH11	1.75	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:C:462:ARG:NH1	1:C:465:MET:HE1	2.25	0.52
1:C:217:ARG:NH2	1:C:450:HIS:CD2	2.78	0.52
1:C:220:PHE:CD2	1:C:221:HIS:N	2.78	0.52
1:C:10:PHE:HA	1:C:106:ALA:HB2	1.90	0.52
1:B:346:GLU:HG2	1:B:351:PRO:CG	2.40	0.52
1:B:457:MET:HA	1:B:457:MET:HE1	1.92	0.52
1:B:107:LEU:HB3	1:B:126:LYS:HG2	1.93	0.51
1:B:213:SER:CB	1:B:258:HIS:CD2	2.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:O	1:A:302:LEU:HD11	2.09	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:E:103:GLU:O	1:E:107:LEU:HB2	2.10	0.51
1:E:53:LYS:O	1:E:82:HIS:CE1	2.62	0.51
1:B:248:VAL:O	1:B:248:VAL:HG13	2.10	0.51
1:A:90:LYS:HE3	1:A:381:SER:HB3	1.92	0.51
1:E:245:LYS:HA	1:E:320:ASP:OD1	2.10	0.51
1:F:272:THR:OG1	1:F:273:VAL:N	2.42	0.51
1:F:372:TYR:CZ	1:F:461:ALA:HB2	2.46	0.51
1:C:236:LEU:HD21	1:C:343:ILE:HG12	1.92	0.51
1:B:446:LYS:HZ3	1:B:446:LYS:CB	2.24	0.51
1:F:321:ILE:HG23	1:F:343:ILE:HB	1.92	0.51
1:D:248:VAL:HG21	1:D:314:ILE:HG12	1.91	0.51
1:B:84:GLN:O	1:B:86:ARG:N	2.44	0.51
1:C:214:ALA:CB	1:C:380:VAL:HG21	2.39	0.51
1:B:414:GLN:HG3	1:B:428:ILE:O	2.10	0.51
1:C:39:GLU:C	1:C:41:LYS:N	2.62	0.51
1:F:37:THR:O	1:F:38:GLU:CB	2.58	0.51
1:B:107:LEU:CG	1:B:126:LYS:HE3	2.39	0.51
1:C:96:SER:O	1:C:99:VAL:CG1	2.59	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:E:345:ALA:HB1	1:E:373:LEU:CD1	2.41	0.51
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.93	0.51
1:C:374:ASN:HB2	3:C:552:NDP:H5N	1.91	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: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:359:ILE:O	1:C:363:ARG:HB2	2.11	0.51
1:F:211:ARG:NH2	2:F:502:GLU:HG3	2.26	0.51
1:A:142:GLU:OE2	1:A:146:ARG:NH1	2.44	0.51
1:C:248:VAL:HG22	1:C:249:VAL:N	2.25	0.51
1:F:232:TYR:HE2	1:F:465:MET:HG2	1.74	0.51
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.46	0.51
1:E:392:VAL:HG11	1:E:397:LEU:HD11	1.92	0.51
1:C:245:LYS:HA	1:C:320:ASP:OD1	2.11	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:E:473:LEU:HB3	1:E:476:ASP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.58	0.51
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.93	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:214:ALA:HB1	1:F:380:VAL:HG21	1.92	0.51
1:C:95:TYR:OH	1:C:145:THR:HB	2.11	0.50
1:B:337:PRO:HD3	1:B:359:ILE:CD1	2.41	0.50
1:F:118:VAL:HG11	1:F:375:ALA:HB3	1.91	0.50
1:E:421:PHE:CD2	1:E:421:PHE:N	2.77	0.50
1:B:211:ARG:HD2	1:B:211:ARG:O	2.11	0.50
1:E:370:ASP:CG	1:E:371:LEU:H	2.13	0.50
1:B:32:LEU:HD11	1:B:44:ARG:HH12	1.75	0.50
1:F:214:ALA:CB	1:F:380:VAL:HG21	2.40	0.50
1:A:291:LEU:O	1:A:291:LEU:HD22	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:B:75:ILE:O	1:B:75:ILE:HD13	2.11	0.50
1:A:478:ARG:HH11	1:A:478:ARG:CG	2.03	0.50
1:C:349:ASN:ND2	2:C:502:GLU:OXT	2.37	0.50
1:E:219:VAL:HA	1:E:373:LEU:CD2	2.41	0.50
1:F:416:SER:HA	1:F:419:ARG:NH1	2.26	0.50
1:E:166:ALA:HB1	1:E:167:PRO:CD	2.41	0.50
1:E:111:MET:SD	2:E:502:GLU:OXT	2.69	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:232:TYR:CE2	1:C:465:MET:HG2	2.42	0.50
1:E:217:ARG:HA	1:E:262:TYR:CD1	2.46	0.50
1:B:483:VAL:O	1:B:487:GLU:HB2	2.10	0.50
1:A:185:SER:O	1:E:154:LYS:HD3	2.11	0.50
1:C:165:PRO:O	1:C:166:ALA:HB2	2.10	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:E:492:VAL:O	1:F:205:GLN:NE2	2.44	0.50
1:F:114:LYS:HA	1:F:371:LEU:CD2	2.41	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:483:VAL:O	1:A:487:GLU:HB2	2.12	0.50
1:A:248:VAL:HG13	1:A:322:LEU:HD12	1.92	0.50
1:B:336:ALA:HB3	1:B:359:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:SER:HA	1:D:463:GLN:CG	2.42	0.50
1:C:421:PHE:O	1:C:422:GLY:C	2.50	0.50
1:B:245:LYS:HD2	1:B:245:LYS:N	2.26	0.50
1:B:75:ILE:HD11	1:B:129:VAL:HG13	1.93	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: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:339:VAL:O	1:A:340:LYS:HB2	2.12	0.50
1:A:189:HIS:HE1	1:E:187:ILE:HD12	1.77	0.49
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:E:56:ASN:HD22	1:E:84:GLN:NE2	2.10	0.49
1:B:113:TYR:C	1:B:371:LEU:HD21	2.33	0.49
1:F:271:ILE:HD11	1:F:319:CYS:HB3	1.94	0.49
1:E:423:LYS:N	1:E:423:LYS:HD2	2.26	0.49
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.12	0.49
1:F:366:MET:HG3	1:F:475:LEU:HD22	1.94	0.49
1:F:264:HIS:CD2	1:F:288:PRO:HD3	2.47	0.49
1:B:88:PRO:HG3	1:B:160:PRO:O	2.12	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:F:84:GLN:O	1:F:86:ARG:N	2.45	0.49
1:D:107:LEU:CB	1:D:126:LYS:HE3	2.43	0.49
1:A:446:LYS:O	1:A:447:ASP:C	2.50	0.49
1:C:44:ARG:NH2	1:C:494:ASN:HB2	2.26	0.49
1:A:412:SER:HA	1:B:433:THR:HG23	1.93	0.49
1:F:199:THR:HA	1:F:384:GLU:OE1	2.13	0.49
1:D:252:PHE:CZ	1:D:291:LEU:HD13	2.47	0.49
1:A:321:ILE:HG23	1:A:343:ILE:CG2	2.42	0.49
1:F:495:GLU:C	1:F:497:GLY:H	2.16	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:B:199:THR:HA	1:B:384:GLU:OE1	2.11	0.49
1:E:433:THR:HG23	1:F:412:SER:OG	2.13	0.49
1:D:427:THR:O	1:D:427:THR:HG23	2.12	0.49
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.94	0.49
1:D:272:THR:HG21	1:D:317:VAL:HG21	1.94	0.49
1:D:276:SER:HB2	3:D:552:NDP:O2X	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:GLU:CD	1:C:338:ARG:HD2	2.32	0.49
1:F:19:ARG:HG2	1:F:479:THR:HG21	1.95	0.49
1:B:163:ASP:OD2	1:B:163:ASP:C	2.51	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:F:92:GLY:O	1:F:126:LYS:HD3	2.12	0.49
1:D:142:GLU:OE1	1:F:498:VAL:HG21	2.12	0.49
1:E:427:THR:O	1:E:429:PRO:CD	2.60	0.49
1:D:215:THR:O	1:D:219:VAL:HG23	2.13	0.49
1:C:223:ILE:CD1	1:C:263:LEU:HD11	2.43	0.49
1:A:337:PRO:HD3	1:A:359:ILE:HD13	1.95	0.49
1:E:67:ARG:NE	1:E:73:GLU:OE1	2.46	0.49
1:B:399:PHE:HA	1:B:441:SER:O	2.13	0.49
1:A:211:ARG:HD3	1:A:380:VAL:HG12	1.94	0.48
1:D:95:TYR:HB3	1:D:133:PRO:CG	2.41	0.48
1:E:55:CYS:HA	1:E:82:HIS:HA	1.95	0.48
1:E:35:ARG:CD	1:E:35:ARG:H	2.08	0.48
1:F:374:ASN:CB	3:F:552:NDP:H5N	2.43	0.48
1:E:258:HIS:CD2	1:E:261:ARG:NH1	2.73	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:E:271:ILE:HD12	1:E:272:THR:HG22	1.92	0.48
1:A:408:HIS:CD2	1:B:435:GLU:HB3	2.48	0.48
1:F:75:ILE:HD11	1:F:129:VAL:HG13	1.95	0.48
1:A:456:THR:OG1	1:C:396:ARG:NH2	2.45	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:F:35:ARG:O	1:F:37:THR:HG23	2.14	0.48
1:A:353:THR:HB	1:A:354:PRO:CD	2.42	0.48
1:C:494:ASN:OD1	1:C:495:GLU:N	2.46	0.48
1:B:324:PRO:HD2	1:B:345:ALA:O	2.13	0.48
1:F:186:THR:OG1	1:F:187:ILE:N	2.44	0.48
1:F:12:MET:CE	1:F:16:PHE:HE1	2.25	0.48
1:D:232:TYR:CE2	1:D:465:MET:HG2	2.48	0.48
1:C:341:ALA:O	1:C:365:ILE:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:178:TRP:HE1	1:F:498:VAL:HG22	1.78	0.48
1:A:9:PHE:HD2	1:A:9:PHE:O	1.96	0.48
1:B:278:GLY:HA3	1:B:302:LEU:HD21	1.96	0.48
1:A:493:TYR:O	1:A:494:ASN:ND2	2.47	0.48
1:E:93:ILE:HD11	1:E:95:TYR:HE1	1.70	0.48
1:B:317:VAL:CG1	1:B:318:ASP:N	2.77	0.48
1:C:248:VAL:CG2	1:C:249:VAL:N	2.76	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:E:315:LEU:HD13	1:E:331:LEU:CD1	2.44	0.48
1:E:325:ALA:O	3:E:552:NDP:H51N	2.14	0.48
1:B:97:THR:HG23	1:B:132:ASN:HB2	1.95	0.48
1:C:41:LYS:O	1:C:45:VAL:HG23	2.13	0.48
1:E:37:THR:O	1:E:38:GLU:HB3	2.14	0.48
1:C:131:ILE:O	1:C:133:PRO:HD3	2.14	0.48
1:A:371:LEU:HD12	1:A:482:TYR:CE1	2.49	0.48
1:E:82:HIS:CD2	1:E:112:THR:CG2	2.92	0.48
1:E:186:THR:OG1	1:E:187:ILE:N	2.47	0.48
1:D:174:ARG:HD2	1:D:178:TRP:CH2	2.49	0.48
1:A:75:ILE:HD11	1:A:129:VAL:HG13	1.96	0.48
1:E:339:VAL:HG11	1:E:344:ILE:HD11	1.95	0.48
1:E:275:GLU:HG3	1:E:301:ILE:CD1	2.44	0.48
1:B:84:GLN:C	1:B:86:ARG:N	2.67	0.48
1:B:167:PRO:HD3	1:B:200:GLY:HA3	1.96	0.48
1:E:93:ILE:HB	1:E:127:ALA:HB3	1.95	0.48
1:D:408:HIS:CE1	1:F:435:GLU:HG2	2.49	0.48
1:A:186:THR:OG1	1:A:187:ILE:N	2.47	0.48
1:D:248:VAL:HG21	1:D:314:ILE:CG1	2.44	0.48
1:F:272:THR:HG21	1:F:317:VAL:HG21	1.96	0.48
1:E:382:TYR:OH	1:F:392:VAL:HG13	2.14	0.48
1:C:278:GLY:HA3	1:C:302:LEU:HD21	1.96	0.48
1:E:291:LEU:O	1:E:291:LEU:HD22	2.14	0.48
1:B:342:LYS:HD3	1:B:342:LYS:N	2.29	0.48
1:D:160:PRO:O	1:E:192:ILE:HD12	2.14	0.48
1:F:186:THR:O	1:F:189:HIS:ND1	2.47	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:F:165:PRO:HD2	1:F:197:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:35:ARG:O	1:B:37:THR:N	2.46	0.47
1:E:282:ASN:C	1:E:282:ASN:OD1	2.52	0.47
1:D:88:PRO:HD2	1:D:122:PHE:CE2	2.49	0.47
1:D:396:ARG:O	1:D:396:ARG:HD2	2.13	0.47
1:D:236:LEU:HA	1:D:236:LEU:HD12	1.67	0.47
1:A:47:SER:CB	1:D:72:TRP:HB2	2.36	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:C:339:VAL:HG21	1:C:360:PHE:CZ	2.49	0.47
1:C:339:VAL:HG12	1:C:341:ALA:H	1.79	0.47
1:F:126:LYS:NZ	2:F:502:GLU:N	2.62	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:A:99:VAL:O	1:A:99:VAL:HG22	2.13	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:B:294:PHE:CE2	1:B:298:HIS:ND1	2.76	0.47
1:B:82:HIS:N	1:B:124:GLY:O	2.47	0.47
1:F:336:ALA:N	1:F:337:PRO:CD	2.75	0.47
1:E:175:GLU:HA	1:E:178:TRP:CE3	2.49	0.47
1:F:56:ASN:HD22	1:F:84:GLN:HE21	1.60	0.47
1:A:173:GLU:OE2	1:A:202:PRO:HA	2.14	0.47
1:D:263:LEU:HD11	1:D:323:ILE:HD11	1.97	0.47
1:F:378:VAL:HA	1:F:381:SER:HB2	1.96	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:B:2:ASP:HB3	1:B:3:ARG:H	1.51	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: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:C:153:ALA:HB1	1:C:187:ILE:HG13	1.96	0.47
1:A:96:SER:O	1:A:130:LYS:HA	2.15	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
1:E:152:LEU:O	1:E:153:ALA:C	2.53	0.47
1:E:271:ILE:O	1:E:272:THR:HG22	2.15	0.47
1:A:409:LEU:C	1:A:409:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:CD	1:A:127:ALA:HB2	2.43	0.47
1:F:49:LEU:HA	1:F:49:LEU:HD12	1.64	0.47
1:E:158:ILE:HG12	1:E:159:GLY:N	2.30	0.47
1:F:448:ILE:HD13	1:F:448:ILE:HA	1.72	0.47
1:C:211:ARG:HA	1:C:380:VAL:HG11	1.96	0.47
1:B:291:LEU:HD21	1:B:301:ILE:HG22	1.97	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:B:421:PHE:N	1:B:421:PHE:CD2	2.81	0.47
1:A:118:VAL:HG23	1:A:120:VAL:CG2	2.41	0.47
1:B:248:VAL:HG13	1:B:322:LEU:HD12	1.96	0.47
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.97	0.47
1:F:272:THR:OG1	1:F:314:ILE:HD11	2.15	0.47
1:E:19:ARG:CG	1:E:479:THR:HG21	2.44	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:C:246:THR:CG2	1:C:319:CYS:HA	2.45	0.47
1:A:163:ASP:C	1:A:163:ASP:OD2	2.53	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:B:9:PHE:O	1:B:9:PHE:CD2	2.63	0.47
1:B:99:VAL:HG22	1:B:99:VAL:O	2.13	0.47
1:A:433:THR:HG23	1:C:412:SER:HA	1.97	0.47
1:C:313:SER:HB3	1:C:316:GLU:HG3	1.96	0.47
1:A:304:PHE:CD1	1:A:305:PRO:HD2	2.50	0.47
1:B:371:LEU:HD12	1:B:482:TYR:CE1	2.49	0.46
1:A:37:THR:HG22	1:A:41:LYS:CE	2.46	0.46
1:D:112:THR:HG22	1:D:124:GLY:N	2.30	0.46
1:D:82:HIS:CG	1:D:109:SER:HA	2.50	0.46
1:C:478:ARG:HG2	1:C:482:TYR:CE1	2.50	0.46
1:F:153:ALA:HA	1:F:158:ILE:CG2	2.45	0.46
1:A:72:TRP:HB2	1:D:47:SER:HB3	1.97	0.46
1:C:196:ALA:HA	1:C:388:ASN:ND2	2.28	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:E:103:GLU:OE1	1:E:328:GLU:OE1	2.33	0.46
1:E:242:PHE:CE1	1:E:263:LEU:HD23	2.51	0.46
1:D:196:ALA:HA	1:D:388:ASN:HD22	1.81	0.46
1:A:408:HIS:CE1	1:B:435:GLU:HG2	2.49	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:C:5:ASP:HB3	1:C:332:THR:HB	1.97	0.46
1:C:332:THR:HG22	1:C:353:THR:HG23	1.95	0.46
1:F:341:ALA:O	1:F:365:ILE:HG23	2.14	0.46
1:D:313:SER:HB3	1:D:316:GLU:HG3	1.98	0.46
1:A:51:ILE:O	1:A:51:ILE:HG22	2.14	0.46
1:A:201:LYS:NZ	1:A:388:ASN:ND2	2.59	0.46
1:E:142:GLU:O	1:E:146:ARG:HG3	2.14	0.46
1:A:236:LEU:HA	1:A:236:LEU:HD12	1.62	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:C:172:GLY:H	1:C:175:GLU:HG2	1.80	0.46
1:C:33:LYS:HB2	1:C:33:LYS:HE3	1.82	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:E:172:GLY:H	1:E:175:GLU:CG	2.27	0.46
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.98	0.46
1:C:84:GLN:C	1:C:86:ARG:H	2.18	0.46
1:C:84:GLN:C	1:C:86:ARG:N	2.68	0.46
1:D:400:LYS:HB2	1:F:455:TYR:HB2	1.97	0.46
1:F:89:CYS:HA	1:F:123:GLY:O	2.15	0.46
1:C:141:LEU:O	1:C:145:THR:CG2	2.61	0.46
1:F:28:LEU:O	1:F:31:ASP:HB2	2.15	0.46
1:B:328:GLU:HA	1:B:351:PRO:HA	1.96	0.46
1:D:114:LYS:HA	1:D:371:LEU:CD2	2.46	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:C:315:LEU:HB3	1:C:331:LEU:HD11	1.96	0.46
1:D:246:THR:CG2	1:D:319:CYS:HA	2.46	0.46
1:F:248:VAL:HB	1:F:272:THR:HG23	1.97	0.46
1:A:79:ARG:CG	1:A:127:ALA:HB2	2.45	0.46
1:C:332:THR:HA	1:C:356:ALA:HB2	1.96	0.46
1:B:33:LYS:O	1:B:34:THR:C	2.54	0.46
1:F:94:ARG:O	1:F:128:GLY:HA2	2.16	0.46
1:E:39:GLU:C	1:E:41:LYS:N	2.68	0.46
1:B:36:GLU:O	1:B:37:THR:O	2.34	0.46
1:F:281:TRP:O	1:F:282:ASN:HB2	2.16	0.46
1:C:409:LEU:C	1:C:409:LEU:HD23	2.35	0.46
1:B:213:SER:HA	1:B:258:HIS:CG	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:271:ILE:C	1:A:272:THR:HG22	2.36	0.46
1:F:245:LYS:HD2	1:F:245:LYS:N	2.31	0.46
1:C:275:GLU:HG3	1:C:301:ILE:HD13	1.98	0.46
1:C:15:GLY:O	1:C:16:PHE:C	2.53	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: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:342:LYS:O	1:B:365:ILE:HG22	2.15	0.46
1:F:112:THR:CG2	1:F:124:GLY:H	2.29	0.45
1:D:141:LEU:O	1:D:145:THR:CG2	2.63	0.45
1:F:150:MET:HA	1:F:150:MET:CE	2.43	0.45
1:C:187:ILE:HD13	1:C:187:ILE:N	2.31	0.45
1:D:217:ARG:HA	1:D:262:TYR:CD1	2.51	0.45
1:B:477:LEU:O	1:B:480:ALA:HB3	2.16	0.45
1:E:40:GLN:HE21	1:E:40:GLN:HB3	1.60	0.45
1:E:131:ILE:HG13	1:E:131:ILE:O	2.16	0.45
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.98	0.45
1:A:57:HIS:HE1	1:A:84:GLN:NE2	2.14	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:A:321:ILE:HG23	1:A:343:ILE:HB	1.98	0.45
1:C:131:ILE:HB	1:C:136:TYR:CE2	2.51	0.45
1:D:186:THR:OG1	1:D:187:ILE:N	2.47	0.45
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.15	0.45
1:B:202:PRO:O	1:B:203:ILE:C	2.55	0.45
1:D:248:VAL:CB	1:D:272:THR:HG23	2.45	0.45
1:E:165:PRO:HD2	1:E:197:CYS:O	2.16	0.45
1:A:52:ILE:HD13	1:A:489:VAL:CG1	2.45	0.45
1:A:459:ARG:O	1:A:463:GLN:HG2	2.17	0.45
1:F:178:TRP:O	1:F:182:THR:CG2	2.65	0.45
1:D:336:ALA:N	1:D:337:PRO:CD	2.78	0.45
1:E:65:ILE:HG13	1:E:144:ILE:HG12	1.98	0.45
1:B:381:SER:O	1:B:384:GLU:N	2.49	0.45
1:F:347:GLY:O	1:F:374:ASN:HB3	2.16	0.45
1:A:373:LEU:O	1:A:373:LEU:HD22	2.17	0.45
1:A:248:VAL:HG21	1:A:314:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ILE:O	1:D:317:VAL:HG23	2.16	0.45
1:C:216:GLY:O	1:C:219:VAL:HB	2.17	0.45
1:D:434:ALA:O	1:D:437:GLN:HB2	2.16	0.45
1:F:247:PHE:HB2	1:F:321:ILE:O	2.16	0.45
1:D:220:PHE:CE1	1:D:242:PHE:CE2	3.05	0.45
1:E:451:SER:HB2	1:F:400:LYS:HB3	1.97	0.45
1:B:416:SER:HA	1:B:419:ARG:NH1	2.31	0.45
2:A:502:GLU:HA	3:A:552:NDP:H41N	1.98	0.45
1:C:336:ALA:H	1:C:337:PRO:HD2	1.81	0.45
1:B:80:ALA:O	1:B:125:ALA:HA	2.17	0.45
1:A:258:HIS:HD2	1:A:261:ARG:NH1	2.11	0.45
1:B:409:LEU:O	1:B:412:SER:HB2	2.16	0.45
1:F:402:GLU:O	1:F:403:ARG:C	2.53	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:D:371:LEU:HD23	1:D:371:LEU:HA	1.75	0.45
1:B:16:PHE:O	1:B:19:ARG:HB3	2.17	0.45
1:B:19:ARG:HG2	1:B:479:THR:CG2	2.46	0.45
1:B:158:ILE:HG12	1:B:159:GLY:N	2.32	0.45
1:C:185:SER:O	1:D:154:LYS:HD3	2.16	0.45
1:D:455:TYR:HB2	1:E:400:LYS:HB2	1.98	0.45
1:D:79:ARG:CG	1:D:127:ALA:HB2	2.47	0.45
1:A:417:LEU:HD21	1:B:417:LEU:HD11	1.98	0.45
1:A:219:VAL:HA	1:A:373:LEU:HD21	1.94	0.45
1:A:189:HIS:CE1	1:E:187:ILE:HD12	2.51	0.45
1:D:255:VAL:HG13	3:D:552:NDP:O2N	2.16	0.45
1:A:204:SER:OG	1:A:205:GLN:HG2	2.16	0.45
1:F:58:VAL:HG11	1:F:101:VAL:HG23	1.99	0.45
1:A:424:HIS:ND1	1:A:424:HIS:N	2.65	0.45
1:E:319:CYS:O	1:E:341:ALA:HA	2.17	0.45
1:A:65:ILE:HG13	1:A:144:ILE:HG12	1.97	0.45
1:A:126:LYS:NZ	2:A:502:GLU:N	2.65	0.45
1:F:82:HIS:CE1	1:F:109:SER:HB3	2.52	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:A:282:ASN:OD1	1:A:284:ASP:HB2	2.17	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:75:ILE:C	1:D:75:ILE:HD13	2.37	0.44
1:D:249:VAL:HG22	1:D:251:GLY:O	2.16	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:273:VAL:HG12	1:D:274:GLY:N	2.32	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:A:316:GLU:OE2	1:A:338:ARG:HD2	2.17	0.44
1:F:421:PHE:O	1:F:422:GLY:C	2.55	0.44
1:C:91:GLY:O	1:C:165:PRO:HA	2.17	0.44
1:C:12:MET:HE2	1:C:16:PHE:HE1	1.83	0.44
1:F:446:LYS:CB	1:F:446:LYS:NZ	2.80	0.44
1:C:342:LYS:N	1:C:342:LYS:HD3	2.33	0.44
1:B:296:LEU:HD22	1:B:296:LEU:HA	1.79	0.44
1:D:272:THR:CG2	1:D:317:VAL:HG11	2.47	0.44
1:A:39:GLU:C	1:A:41:LYS:H	2.18	0.44
1:B:169:MET:CG	3:B:552:NDP:H3D	2.48	0.44
1:D:408:HIS:ND1	1:F:439:ARG:HD2	2.33	0.44
1:C:72:TRP:HB3	1:F:51:ILE:HD11	2.00	0.44
1:C:367:VAL:O	1:C:369:PRO:HD3	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: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:B:234:SER:O	1:B:237:GLY:N	2.50	0.44
1:D:444:SER:OG	1:D:446:LYS:HG3	2.17	0.44
1:A:309:ILE:HD12	1:A:309:ILE:N	2.33	0.44
1:C:446:LYS:CB	1:C:446:LYS:NZ	2.80	0.44
1:F:246:THR:O	1:F:320:ASP:HB2	2.16	0.44
1:B:9:PHE:C	1:B:9:PHE:CD2	2.90	0.44
1:D:337:PRO:HD3	1:D:359:ILE:HD13	1.99	0.44
1:B:99:VAL:HG13	1:B:130:LYS:HA	1.99	0.44
1:D:152:LEU:HD22	1:D:157:PHE:CB	2.46	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:F:93:ILE:O	1:F:93:ILE:HG13	2.15	0.44
1:E:95:TYR:HB3	1:E:133:PRO:CG	2.47	0.44
1:E:90:LYS:HB2	1:E:122:PHE:CG	2.53	0.44
1:C:242:PHE:CE1	1:C:263:LEU:CD2	3.00	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:A:161:GLY:CA	1:C:192:ILE:HG13	2.48	0.44
1:C:463:GLN:HB3	1:C:463:GLN:HE21	1.60	0.44
1:C:424:HIS:N	1:C:424:HIS:ND1	2.66	0.44
1:B:217:ARG:HA	1:B:262:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLU:O	1:B:29:VAL:HG23	2.18	0.44
1:F:82:HIS:ND1	1:F:109:SER:HB3	2.33	0.44
1:E:282:ASN:OD1	1:E:284:ASP:N	2.51	0.44
1:F:272:THR:HB	1:F:280:ILE:O	2.17	0.44
1:A:313:SER:HB3	1:A:316:GLU:CG	2.47	0.44
1:F:340:LYS:HE2	1:F:340:LYS:HB2	1.73	0.44
1:D:456:THR:HG22	1:D:457:MET:HE3	2.00	0.44
1:F:457:MET:CA	1:F:457:MET:HE2	2.46	0.44
1:F:12:MET:HE2	1:F:16:PHE:HE1	1.82	0.44
1:C:46:ARG:O	1:C:50:ARG:HB2	2.17	0.44
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.83	0.44
1:C:298:HIS:C	1:C:300:THR:H	2.21	0.44
1:F:26:ASP:HA	1:F:42:ARG:NH2	2.33	0.44
1:D:37:THR:HG22	1:D:41:LYS:CE	2.47	0.43
1:A:95:TYR:OH	1:A:145:THR:HB	2.18	0.43
1:D:93:ILE:HA	1:D:127:ALA:O	2.18	0.43
1:A:188:GLY:O	1:A:189:HIS:C	2.54	0.43
1:B:344:ILE:HB	1:B:367:VAL:CG1	2.45	0.43
1:D:242:PHE:O	1:D:245:LYS:HB2	2.18	0.43
1:C:10:PHE:CA	1:C:106:ALA:HB2	2.48	0.43
1:B:231:SER:O	1:B:235:ILE:HD13	2.18	0.43
1:D:68:ASP:OD1	1:D:137:THR:HG21	2.18	0.43
1:F:236:LEU:HD12	1:F:236:LEU:HA	1.84	0.43
1:D:33:LYS:HB2	1:D:33:LYS:HE3	1.81	0.43
1:D:37:THR:O	1:D:40:GLN:HG2	2.17	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:E:148:PHE:CE2	1:E:152:LEU:HD11	2.52	0.43
1:C:326:ALA:O	3:C:552:NDP:H4D	2.18	0.43
1:B:31:ASP:O	1:B:32:LEU:C	2.56	0.43
1:F:142:GLU:O	1:F:143:LYS:C	2.55	0.43
1:E:99:VAL:HG21	1:E:128:GLY:C	2.38	0.43
1:E:108:ALA:O	1:E:111:MET:HB2	2.19	0.43
1:C:37:THR:O	1:C:38:GLU:CB	2.66	0.43
1:B:348:ALA:HB3	1:B:351:PRO:HB3	2.01	0.43
1:D:272:THR:HG21	1:D:317:VAL:HG11	2.00	0.43
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.81	0.43
1:F:395:GLY:O	1:F:397:LEU:N	2.51	0.43
1:A:159:GLY:CA	1:A:162:VAL:HG13	2.44	0.43
1:D:17:PHE:HZ	1:D:49:LEU:HD12	1.83	0.43
1:C:95:TYR:HB3	1:C:133:PRO:HG3	1.99	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:79:ARG:HG3	1:B:127:ALA:HB2	2.01	0.43
1:F:423:LYS:N	1:F:423:LYS:HD2	2.33	0.43
1:B:331:LEU:HA	1:B:331:LEU:HD12	1.77	0.43
1:D:448:ILE:HA	1:D:448:ILE:HD13	1.81	0.43
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.66	0.43
1:B:165:PRO:C	1:B:198:VAL:HG23	2.39	0.43
1:C:245:LYS:CD	1:C:245:LYS:N	2.81	0.43
1:B:373:LEU:O	1:B:373:LEU:HD23	2.18	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:A:462:ARG:NH1	1:A:465:MET:HE1	2.34	0.43
1:B:187:ILE:HD12	1:F:189:HIS:HE1	1.83	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:C:264:HIS:HA	1:C:268:ALA:O	2.19	0.43
1:E:11:LYS:HA	1:E:14:GLU:HB2	2.01	0.43
1:F:424:HIS:N	1:F:424:HIS:ND1	2.65	0.43
1:B:29:VAL:HG13	1:B:41:LYS:HB3	2.00	0.43
1:A:255:VAL:HG13	3:A:552:NDP:O2N	2.19	0.43
1:A:84:GLN:C	1:A:86:ARG:N	2.72	0.43
1:E:188:GLY:O	1:E:189:HIS:C	2.57	0.43
1:A:99:VAL:HG21	1:A:128:GLY:C	2.39	0.43
1:E:299:GLY:O	1:E:300:THR:HB	2.18	0.43
1:A:180:ALA:HB2	1:A:198:VAL:CG1	2.49	0.43
1:A:450:HIS:CE1	4:A:503:GTP:O1B	2.72	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
2:B:502:GLU:CA	3:B:552:NDP:H41N	2.38	0.43
1:E:248:VAL:HG23	1:E:272:THR:OG1	2.18	0.43
1:E:172:GLY:O	1:E:176:MET:HG2	2.19	0.43
1:F:49:LEU:HD12	1:F:52:ILE:HD12	2.00	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:B:107:LEU:CB	1:B:126:LYS:HE3	2.48	0.43
1:C:126:LYS:HB2	1:C:126:LYS:HE2	1.85	0.43
1:A:85:HIS:HB2	1:A:492:VAL:HG11	2.00	0.43
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.76	0.43
1:D:114:LYS:HA	1:D:371:LEU:HD23	2.00	0.43
1:A:9:PHE:CD1	1:A:328:GLU:HG3	2.54	0.43
1:C:56:ASN:HD22	1:C:84:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:HIS:CE1	4:E:503:GTP:O1B	2.72	0.43
1:D:11:LYS:HA	1:D:14:GLU:HB2	2.01	0.43
1:C:29:VAL:HG22	1:C:45:VAL:HG21	2.00	0.43
1:B:371:LEU:HD12	1:B:482:TYR:CD1	2.54	0.43
1:B:282:ASN:C	1:B:282:ASN:OD1	2.57	0.43
1:B:78:TYR:O	1:B:127:ALA:HA	2.18	0.43
1:E:248:VAL:CG1	1:E:319:CYS:SG	3.06	0.43
1:A:459:ARG:O	1:A:462:ARG:HB3	2.19	0.43
1:D:242:PHE:CE1	1:D:263:LEU:CD2	3.02	0.43
1:C:446:LYS:HB2	1:C:446:LYS:HZ2	1.84	0.43
1:E:477:LEU:HA	1:E:477:LEU:HD23	1.75	0.43
1:F:496:ALA:C	1:F:498:VAL:N	2.66	0.43
1:E:246:THR:HG23	1:E:319:CYS:HA	2.01	0.43
1:F:65:ILE:CG1	1:F:144:ILE:HG12	2.48	0.43
1:E:44:ARG:HH12	1:E:494:ASN:ND2	2.17	0.43
1:A:257:LEU:O	1:A:260:MET:HB3	2.18	0.43
1:E:273:VAL:HG12	1:E:274:GLY:N	2.34	0.43
1:F:462:ARG:NH1	1:F:465:MET:CE	2.82	0.43
1:B:391:HIS:O	1:C:382:TYR:OH	2.28	0.43
1:E:215:THR:HG23	1:E:216:GLY:N	2.34	0.43
1:D:410:LEU:HA	1:D:410:LEU:HD12	1.64	0.43
1:A:37:THR:O	1:A:38:GLU:HB3	2.18	0.42
1:A:126:LYS:NZ	1:A:168:ASP:OD2	2.48	0.42
1:A:347:GLY:O	1:A:374:ASN:HB3	2.19	0.42
1:F:55:CYS:HA	1:F:82:HIS:HA	2.00	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:A:177:SER:HB2	1:A:202:PRO:HG2	2.01	0.42
1:B:146:ARG:CB	1:B:182:THR:HG21	2.48	0.42
1:B:146:ARG:NH2	1:B:181:ASP:OD2	2.52	0.42
1:C:191:ASP:HB3	1:C:194:ALA:HB2	2.00	0.42
1:C:150:MET:O	1:C:154:LYS:HG3	2.19	0.42
1:F:361:LEU:HA	1:F:361:LEU:HD22	1.77	0.42
1:C:390:ASN:O	1:C:392:VAL:HG23	2.19	0.42
1:C:82:HIS:CG	1:C:109:SER:HA	2.55	0.42
1:D:79:ARG:HA	1:D:127:ALA:HA	2.01	0.42
1:F:31:ASP:O	1:F:32:LEU:C	2.57	0.42
1:A:196:ALA:HA	1:A:388:ASN:HD22	1.85	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:E:171:THR:HB	1:E:175:GLU:HG3	2.01	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:B:476:ASP:OD2	1:B:479:THR:HG23	2.18	0.42
1:B:175:GLU:HA	1:B:178:TRP:CE3	2.53	0.42
1:A:273:VAL:HG21	1:A:291:LEU:HD12	2.01	0.42
1:A:249:VAL:HG22	1:A:251:GLY:O	2.19	0.42
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.53	0.42
1:A:37:THR:O	1:A:38:GLU:CB	2.68	0.42
1:A:95:TYR:OH	1:A:145:THR:CG2	2.68	0.42
1:A:215:THR:HG23	1:A:216:GLY:H	1.85	0.42
1:A:118:VAL:HG11	1:A:375:ALA:HB3	2.00	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:A:336:ALA:N	1:A:337:PRO:CD	2.82	0.42
1:E:331:LEU:HA	1:E:331:LEU:HD12	1.76	0.42
1:B:160:PRO:HD3	1:B:197:CYS:HB3	2.01	0.42
1:B:395:GLY:HA3	1:B:399:PHE:CZ	2.54	0.42
1:A:234:SER:O	1:A:235:ILE:C	2.57	0.42
1:A:389:LEU:O	1:A:391:HIS:ND1	2.52	0.42
1:F:39:GLU:C	1:F:41:LYS:H	2.23	0.42
1:E:196:ALA:HB1	1:E:385:TRP:CD1	2.54	0.42
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.78	0.42
1:A:313:SER:C	1:A:315:LEU:N	2.73	0.42
1:F:421:PHE:N	1:F:421:PHE:CD2	2.87	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:A:215:THR:HG23	1:A:216:GLY:N	2.35	0.42
1:E:272:THR:HG21	1:E:317:VAL:HG21	2.01	0.42
1:A:489:VAL:C	1:A:490:PHE:O	2.57	0.42
1:B:142:GLU:OE2	1:B:146:ARG:NH1	2.53	0.42
1:E:303:GLY:N	1:E:309:ILE:HD11	2.33	0.42
1:D:291:LEU:O	1:D:294:PHE:N	2.52	0.42
1:A:96:SER:O	1:A:99:VAL:CG1	2.67	0.42
1:F:328:GLU:HB2	1:F:350:GLY:O	2.19	0.42
1:D:131:ILE:O	1:D:131:ILE:HG13	2.17	0.42
1:E:38:GLU:HG3	1:E:39:GLU:HG2	2.00	0.42
1:D:29:VAL:HG13	1:D:41:LYS:HB3	2.02	0.42
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.73	0.42
1:E:196:ALA:HB2	1:E:388:ASN:CB	2.48	0.42
1:F:498:VAL:HB	1:F:499:THR:H	1.69	0.42
1:E:272:THR:CG2	1:E:281:TRP:HD1	2.29	0.42
1:A:409:LEU:O	1:A:409:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:GLY:HA3	1:D:125:ALA:O	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: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:E:37:THR:O	1:E:38:GLU:CB	2.67	0.42
1:A:93:ILE:HG13	1:A:94:ARG:N	2.27	0.42
1:F:215:THR:HB	3:F:552:NDP:H42N	2.01	0.42
1:C:248:VAL:CG2	1:C:314:ILE:HD11	2.49	0.42
1:A:378:VAL:HA	1:A:381:SER:HB2	2.02	0.42
1:E:370:ASP:OD1	1:E:371:LEU:N	2.47	0.42
1:F:117:VAL:HG21	1:F:371:LEU:HD22	2.02	0.42
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.73	0.42
1:C:51:ILE:HG23	1:F:64:PRO:HB3	2.02	0.42
1:A:75:ILE:HD11	1:A:129:VAL:CG1	2.49	0.42
1:E:344:ILE:HB	1:E:367:VAL:HG12	2.02	0.42
1:E:275:GLU:HG3	1:E:301:ILE:HD11	2.02	0.42
1:D:221:HIS:O	1:D:224:GLU:HB3	2.20	0.42
1:A:370:ASP:HB2	1:A:374:ASN:HD21	1.84	0.42
1:C:305:PRO:O	1:C:307:ALA:N	2.51	0.42
1:D:476:ASP:OD2	1:D:479:THR:HG23	2.20	0.42
1:F:337:PRO:HD3	1:F:359:ILE:HD13	2.01	0.42
1:D:142:GLU:OE2	1:D:146:ARG:NH1	2.53	0.42
1:C:208:ILE:HG22	1:C:211:ARG:HB2	2.02	0.42
1:C:446:LYS:HB2	1:C:446:LYS:NZ	2.35	0.42
1:F:33:LYS:O	1:F:34:THR:C	2.58	0.42
1:E:100:SER:O	1:E:101:VAL:C	2.59	0.42
1:C:53:LYS:N	1:C:54:PRO:CD	2.83	0.42
1:D:271:ILE:HD11	1:D:319:CYS:HB3	2.01	0.42
1:E:281:TRP:O	1:E:282:ASN:HB2	2.19	0.42
1:D:409:LEU:HD23	1:D:409:LEU:O	2.20	0.42
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.01	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:84:GLN:C	1:D:86:ARG:N	2.73	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:E:213:SER:CB	1:E:258:HIS:CD2	3.03	0.41
1:C:31:ASP:O	1:C:32:LEU:C	2.58	0.41
1:F:281:TRP:CZ2	1:F:283:PRO:CG	3.00	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:C:90:LYS:HD2	1:C:164:VAL:O	2.20	0.41
1:E:253:GLY:HA3	3:E:552:NDP:O5B	2.20	0.41
1:C:25:GLU:OE2	1:C:42:ARG:NH1	2.53	0.41
1:B:82:HIS:CG	1:B:109:SER:HA	2.55	0.41
1:E:169:MET:O	1:E:170:SER:HB2	2.20	0.41
1:D:79:ARG:HB2	1:D:127:ALA:HB2	2.03	0.41
1:D:248:VAL:CG2	1:D:314:ILE:HG12	2.50	0.41
1:A:201:LYS:HZ1	1:A:388:ASN:ND2	2.09	0.41
1:B:382:TYR:CE1	1:B:386:LEU:HD22	2.55	0.41
1:B:252:PHE:CE2	1:B:291:LEU:HD13	2.54	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:C:274:GLY:HA2	1:C:279:SER:HA	2.01	0.41
1:C:142:GLU:OE2	1:C:146:ARG:NH1	2.53	0.41
1:E:224:GLU:HB2	1:E:242:PHE:CE2	2.54	0.41
1:C:63:PHE:CD1	1:C:147:ARG:HG3	2.55	0.41
1:A:435:GLU:HG2	1:C:408:HIS:CE1	2.55	0.41
1:C:224:GLU:HB2	1:C:242:PHE:CE2	2.54	0.41
1:C:436:PHE:CG	1:C:436:PHE:O	2.74	0.41
1:F:368:ILE:HB	1:F:373:LEU:CD1	2.50	0.41
1:B:416:SER:O	1:B:419:ARG:HB3	2.20	0.41
1:C:227:ILE:HA	1:C:233:MET:SD	2.60	0.41
1:A:379:THR:O	1:A:382:TYR:HB3	2.20	0.41
1:F:79:ARG:HG3	1:F:127:ALA:HB2	2.01	0.41
1:B:38:GLU:CG	1:B:39:GLU:H	1.92	0.41
1:A:272:THR:HG21	1:A:317:VAL:HG21	2.02	0.41
1:C:65:ILE:HA	1:C:65:ILE:HD13	1.68	0.41
1:A:57:HIS:HD2	1:D:61:LEU:HD12	1.85	0.41
1:C:75:ILE:HD11	1:C:129:VAL:HG13	2.02	0.41
1:A:63:PHE:CZ	1:A:75:ILE:HD12	2.56	0.41
1:C:309:ILE:N	1:C:309:ILE:HD12	2.35	0.41
1:D:100:SER:O	1:D:101:VAL:C	2.59	0.41
1:F:487:GLU:OE2	1:F:491:ARG:NH1	2.53	0.41
1:E:9:PHE:HD2	1:E:9:PHE:O	2.04	0.41
1:F:35:ARG:O	1:F:37:THR:N	2.54	0.41
1:B:349:ASN:ND2	3:B:552:NDP:O2D	2.46	0.41
1:A:189:HIS:CE1	1:E:187:ILE:CD1	3.03	0.41
1:E:10:PHE:HD2	1:E:106:ALA:HA	1.86	0.41
1:B:453:LEU:O	1:B:453:LEU:HD12	2.20	0.41
1:F:28:LEU:HA	1:F:28:LEU:HD12	1.77	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:F:337:PRO:O	1:F:363:ARG:CZ	2.68	0.41
1:F:201:LYS:NZ	1:F:388:ASN:ND2	2.57	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:87:THR:HB	1:D:88:PRO:HA	2.02	0.41
1:D:78:TYR:CD1	1:D:78:TYR:N	2.88	0.41
1:A:246:THR:HG22	1:A:320:ASP:H	1.86	0.41
1:C:29:VAL:CG2	1:C:45:VAL:HG21	2.50	0.41
1:A:276:SER:OG	3:A:552:NDP:P2B	2.79	0.41
1:A:175:GLU:HA	1:A:178:TRP:CE3	2.55	0.41
1:E:386:LEU:HD21	1:F:392:VAL:HG13	2.01	0.41
1:C:344:ILE:HB	1:C:367:VAL:HG13	2.01	0.41
1:F:146:ARG:CA	1:F:182:THR:HG21	2.49	0.41
1:B:84:GLN:HE21	1:B:84:GLN:HB2	1.69	0.41
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.89	0.41
1:E:65:ILE:HD13	1:E:65:ILE:HA	1.63	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:F:39:GLU:C	1:F:41:LYS:N	2.72	0.41
1:B:35:ARG:HD3	1:B:35:ARG:N	2.14	0.41
1:F:374:ASN:OD1	1:F:374:ASN:C	2.59	0.41
1:B:346:GLU:HB2	1:B:368:ILE:O	2.19	0.41
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.55	0.41
1:A:63:PHE:CE1	1:A:75:ILE:HD12	2.56	0.41
1:E:162:VAL:O	1:E:163:ASP:HB2	2.21	0.41
1:B:17:PHE:CE2	1:B:53:LYS:CG	3.03	0.41
1:A:37:THR:HG22	1:A:41:LYS:NZ	2.35	0.41
1:E:107:LEU:HD12	1:E:107:LEU:HA	1.88	0.41
1:E:95:TYR:CD1	1:E:129:VAL:HB	2.56	0.41
1:C:339:VAL:HG21	1:C:360:PHE:CE1	2.55	0.41
1:C:281:TRP:O	1:C:282:ASN:CB	2.67	0.41
1:A:158:ILE:HA	1:A:163:ASP:O	2.20	0.41
1:B:314:ILE:HA	1:B:317:VAL:HG23	2.02	0.41
1:A:346:GLU:HG2	1:A:351:PRO:CG	2.50	0.41
1:E:90:LYS:HB2	1:E:122:PHE:CD1	2.56	0.41
1:A:111:MET:CA	1:A:111:MET:HE3	2.50	0.41
1:E:224:GLU:HA	1:E:227:ILE:HG22	2.03	0.41
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.89	0.41
1:D:460:SER:HA	1:D:463:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ALA:HB2	1:C:388:ASN:CB	2.51	0.41
1:D:167:PRO:HG3	1:D:176:MET:CG	2.50	0.41
1:D:486:ILE:O	1:D:487:GLU:C	2.58	0.41
1:F:371:LEU:HA	1:F:371:LEU:HD23	1.81	0.41
1:B:398:THR:O	1:B:399:PHE:C	2.59	0.41
1:A:65:ILE:HA	1:A:65:ILE:HD13	1.62	0.41
1:D:90:LYS:HD2	1:D:164:VAL:HB	2.03	0.41
1:D:191:ASP:C	1:D:193:ASN:H	2.23	0.41
1:F:159:GLY:HA3	1:F:162:VAL:HG13	2.03	0.41
1:D:119:ASP:O	1:E:396:ARG:NH1	2.53	0.41
1:F:257:LEU:HD12	1:F:257:LEU:O	2.21	0.41
1:D:79:ARG:CB	1:D:127:ALA:HB2	2.51	0.41
1:B:90:LYS:HE2	1:B:164:VAL:HG12	2.03	0.41
1:A:153:ALA:HA	1:A:158:ILE:HG22	2.03	0.41
1:D:175:GLU:HA	1:D:178:TRP:HE3	1.82	0.41
1:E:430:ILE:HA	1:F:416:SER:HB3	2.03	0.41
1:F:462:ARG:HG3	1:F:466:ARG:HH22	1.86	0.41
2:E:502:GLU:HA	3:E:552:NDP:C4N	2.51	0.41
1:F:96:SER:OG	1:F:98:ASP:HB2	2.21	0.41
1:A:32:LEU:HD11	1:A:44:ARG:NH1	2.36	0.41
1:E:289:LYS:HD2	1:E:289:LYS:HA	1.83	0.41
1:D:416:SER:CB	1:F:430:ILE:HA	2.50	0.41
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: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:F:201:LYS:HB2	1:F:201:LYS:HE2	1.85	0.40
1:F:65:ILE:HA	1:F:65:ILE:HD13	1.64	0.40
1:E:31:ASP:O	1:E:32:LEU:C	2.59	0.40
1:C:232:TYR:O	1:C:236:LEU:HB2	2.21	0.40
1:E:229:GLU:O	1:E:230:ALA:C	2.60	0.40
1:E:213:SER:HB2	1:E:258:HIS:CD2	2.56	0.40
1:A:196:ALA:HB1	1:A:385:TRP:CD1	2.56	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:A:409:LEU:O	1:A:412:SER:HB2	2.21	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:F:113:TYR:C	1:F:371:LEU:HD21	2.42	0.40
1:F:42:ARG:O	1:F:45:VAL:HB	2.21	0.40
1:F:286:ILE:HG23	1:F:304:PHE:HE2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:PHE:CD2	1:A:421:PHE:N	2.86	0.40
1:A:457:MET:CE	1:A:457:MET:HA	2.38	0.40
1:F:370:ASP:HB2	1:F:374:ASN:ND2	2.36	0.40
1:B:32:LEU:HD11	1:B:44:ARG:NH1	2.37	0.40
1:C:427:THR:HG23	1:C:427:THR:O	2.21	0.40
1:C:294:PHE:CE1	1:C:300:THR:O	2.74	0.40
1:F:371:LEU:HD13	1:F:481:ALA:HB1	2.03	0.40
1:A:96:SER:OG	1:A:97:THR:N	2.54	0.40
1:D:66:ARG:CZ	1:D:70:GLY:O	2.69	0.40
1:B:424:HIS:ND1	1:B:424:HIS:N	2.69	0.40
1:D:417:LEU:HB3	1:D:428:ILE:HD13	2.03	0.40
1:F:271:ILE:C	1:F:272:THR:CG2	2.90	0.40
1:E:175:GLU:N	1:E:175:GLU:CD	2.74	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:E:331:LEU:HG	1:E:360:PHE:HZ	1.86	0.40
1:D:2:ASP:OD1	1:D:5:ASP:O	2.39	0.40
1:E:255:VAL:HG11	3:E:552:NDP:O4D	2.21	0.40
1:A:466:ARG:NH1	1:A:466:ARG:HB2	2.37	0.40
1:F:107:LEU:HA	1:F:107:LEU:HD12	1.72	0.40
1:A:216:GLY:HA2	1:A:219:VAL:HB	2.03	0.40
1:A:118:VAL:HG11	1:A:375:ALA:CB	2.52	0.40
1:C:211:ARG:NH2	2:C:502:GLU:HG2	2.36	0.40
1:E:24:VAL:HG13	1:E:483:VAL:HG22	2.03	0.40
1:D:436:PHE:O	1:D:440:ILE:HB	2.22	0.40
1:B:186:THR:OG1	1:B:187:ILE:N	2.53	0.40
1:A:423:LYS:HD2	1:A:423:LYS:N	2.36	0.40
1:F:172:GLY:H	1:F:175:GLU:CG	2.34	0.40
1:E:273:VAL:HG21	1:E:291:LEU:HD12	2.02	0.40
1:E:301:ILE:HG13	1:E:302:LEU:N	2.37	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:E:296:LEU:HA	1:E:296:LEU:HD22	1.70	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%)	7	25
1	B	493/501 (98%)	429 (87%)	49 (10%)	15 (3%)	5	21
1	C	493/501 (98%)	424 (86%)	55 (11%)	14 (3%)	6	23
1	D	493/501 (98%)	427 (87%)	57 (12%)	9 (2%)	11	36
1	E	493/501 (98%)	427 (87%)	56 (11%)	10 (2%)	9	33
1	F	499/501 (100%)	424 (85%)	62 (12%)	13 (3%)	7	25
All	All	2964/3006 (99%)	2559 (86%)	331 (11%)	74 (2%)	7	26

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	11
1	B	416/420 (99%)	353 (85%)	63 (15%)	3	10
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%)	4	11
1	F	420/420 (100%)	356 (85%)	64 (15%)	3	10
All	All	2500/2520 (99%)	2130 (85%)	370 (15%)	4	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	-	3,9,9	0.42	0	2,11,11	0.16	0
4	GTP	A	503	5	25,34,34	1.26	3 (12%)	34,54,54	1.99	9 (26%)
3	NDP	A	552	-	42,52,52	1.51	5 (11%)	55,80,80	1.89	6 (10%)
2	GLU	B	502	-	3,9,9	0.45	0	2,11,11	0.13	0
4	GTP	B	503	5	25,34,34	1.06	2 (8%)	34,54,54	1.98	12 (35%)
3	NDP	B	552	-	42,52,52	1.55	5 (11%)	55,80,80	1.93	3 (5%)
2	GLU	C	502	-	3,9,9	0.46	0	2,11,11	0.34	0
4	GTP	C	503	5	25,34,34	0.92	1 (4%)	34,54,54	1.72	6 (17%)
3	NDP	C	552	-	42,52,52	1.60	5 (11%)	55,80,80	1.79	3 (5%)
2	GLU	D	502	-	3,9,9	0.30	0	2,11,11	0.13	0
4	GTP	D	503	5	25,34,34	0.95	1 (4%)	34,54,54	1.74	8 (23%)
3	NDP	D	552	-	42,52,52	1.53	5 (11%)	55,80,80	1.95	5 (9%)
2	GLU	E	502	-	3,9,9	0.38	0	2,11,11	0.16	0
4	GTP	E	503	5	25,34,34	1.06	2 (8%)	34,54,54	1.97	10 (29%)
3	NDP	E	552	-	42,52,52	1.57	5 (11%)	55,80,80	1.97	6 (10%)
2	GLU	F	502	-	3,9,9	0.47	0	2,11,11	0.33	0
4	GTP	F	503	5	25,34,34	0.99	1 (4%)	34,54,54	1.97	10 (29%)
3	NDP	F	552	-	42,52,52	1.52	4 (9%)	55,80,80	1.80	3 (5%)

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 (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	GTP	O4'-C4'	-2.27	1.39	1.45
4	B	503	GTP	C2-N1	2.04	1.39	1.35
3	D	552	NDP	C2N-C3N	2.08	1.39	1.34
3	C	552	NDP	C2N-C3N	2.08	1.39	1.34
4	E	503	GTP	C2-N1	2.09	1.39	1.35
3	B	552	NDP	C2A-N1A	2.16	1.38	1.33
3	C	552	NDP	C2A-N1A	2.22	1.38	1.33
3	B	552	NDP	C2N-C3N	2.24	1.40	1.34
3	A	552	NDP	C2A-N1A	2.25	1.38	1.33
3	D	552	NDP	C2A-N1A	2.31	1.38	1.33
3	F	552	NDP	C2N-C3N	2.36	1.40	1.34
3	A	552	NDP	C2N-C3N	2.47	1.40	1.34
3	E	552	NDP	C2N-C3N	2.58	1.41	1.34
3	E	552	NDP	C2A-N1A	2.64	1.38	1.33
4	A	503	GTP	C2-N1	2.67	1.40	1.35
4	F	503	GTP	C6-N1	2.72	1.38	1.33
3	B	552	NDP	C6N-C5N	2.74	1.38	1.33
3	E	552	NDP	C6N-C5N	2.74	1.38	1.33
4	D	503	GTP	C6-N1	2.75	1.38	1.33
4	C	503	GTP	C6-N1	2.77	1.38	1.33
3	D	552	NDP	C6N-C5N	2.84	1.38	1.33
3	F	552	NDP	C6N-C5N	3.08	1.39	1.33
3	B	552	NDP	C2A-N3A	3.13	1.37	1.32
3	A	552	NDP	C6N-C5N	3.22	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	552	NDP	C2A-N3A	3.23	1.37	1.32
4	E	503	GTP	C6-N1	3.24	1.39	1.33
4	B	503	GTP	C6-N1	3.28	1.39	1.33
3	E	552	NDP	C2A-N3A	3.43	1.38	1.32
3	D	552	NDP	C2A-N3A	3.49	1.38	1.32
3	C	552	NDP	C6N-C5N	3.57	1.40	1.33
3	C	552	NDP	C2A-N3A	3.68	1.38	1.32
3	F	552	NDP	C2A-N3A	3.72	1.38	1.32
4	A	503	GTP	C6-N1	3.96	1.40	1.33
3	F	552	NDP	O7N-C7N	6.36	1.40	1.24
3	A	552	NDP	O7N-C7N	6.50	1.40	1.24
3	D	552	NDP	O7N-C7N	6.60	1.41	1.24
3	C	552	NDP	O7N-C7N	6.84	1.41	1.24
3	E	552	NDP	O7N-C7N	6.96	1.41	1.24
3	B	552	NDP	O7N-C7N	7.07	1.42	1.24

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NDP	N3A-C2A-N1A	-12.13	119.61	128.89
3	E	552	NDP	N3A-C2A-N1A	-11.72	119.92	128.89
3	D	552	NDP	N3A-C2A-N1A	-11.36	120.20	128.89
3	F	552	NDP	N3A-C2A-N1A	-11.11	120.39	128.89
3	C	552	NDP	N3A-C2A-N1A	-11.00	120.47	128.89
3	A	552	NDP	N3A-C2A-N1A	-10.62	120.76	128.89
4	A	503	GTP	N3-C2-N1	-5.56	118.98	127.44
4	B	503	GTP	N3-C2-N1	-5.29	119.39	127.44
4	F	503	GTP	C2'-C1'-N9	-5.22	106.32	114.29
3	A	552	NDP	PN-O3-PA	-5.09	118.44	132.73
4	E	503	GTP	N3-C2-N1	-4.92	119.95	127.44
3	D	552	NDP	PN-O3-PA	-4.79	119.27	132.73
4	C	503	GTP	N3-C2-N1	-4.76	120.19	127.44
4	F	503	GTP	N3-C2-N1	-4.57	120.48	127.44
4	D	503	GTP	N3-C2-N1	-4.38	120.78	127.44
4	D	503	GTP	PB-O3B-PG	-4.34	118.12	132.67
3	E	552	NDP	PN-O3-PA	-4.04	121.39	132.73
4	A	503	GTP	C1'-N9-C4	-4.03	120.87	126.94
4	C	503	GTP	PB-O3B-PG	-3.99	119.29	132.67
4	E	503	GTP	C1'-N9-C4	-3.87	121.10	126.94
4	E	503	GTP	C5-C6-N1	-3.84	118.33	123.59
3	B	552	NDP	PN-O3-PA	-3.78	122.13	132.73
4	B	503	GTP	PB-O3B-PG	-3.71	120.23	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	GTP	C2'-C1'-N9	-3.71	108.63	114.29
4	B	503	GTP	C5-C6-N1	-3.53	118.77	123.59
4	E	503	GTP	PB-O3B-PG	-3.48	121.01	132.67
4	F	503	GTP	PA-O3A-PB	-3.45	123.03	132.73
4	C	503	GTP	C5-C6-N1	-3.33	119.04	123.59
4	C	503	GTP	C2'-C1'-N9	-3.31	109.23	114.29
4	B	503	GTP	C1'-N9-C4	-3.18	122.15	126.94
4	A	503	GTP	C5-C6-N1	-3.17	119.26	123.59
4	A	503	GTP	PB-O3B-PG	-3.05	122.45	132.67
4	D	503	GTP	C5-C6-N1	-3.04	119.43	123.59
4	F	503	GTP	PB-O3B-PG	-3.00	122.61	132.67
4	F	503	GTP	C5-C6-N1	-2.99	119.50	123.59
3	C	552	NDP	PN-O3-PA	-2.94	124.48	132.73
4	D	503	GTP	C4-C5-N7	-2.91	106.80	109.48
4	F	503	GTP	O3'-C3'-C2'	-2.88	102.47	111.83
3	E	552	NDP	O3-PN-O5D	-2.85	95.38	102.94
3	F	552	NDP	PN-O3-PA	-2.80	124.86	132.73
3	A	552	NDP	C1D-N1N-C6N	-2.65	114.88	120.81
3	E	552	NDP	C1D-N1N-C6N	-2.61	114.97	120.81
4	E	503	GTP	C4-C5-N7	-2.57	107.11	109.48
3	A	552	NDP	C4A-C5A-N7A	-2.55	107.13	109.48
3	D	552	NDP	C3N-C2N-N1N	-2.54	119.50	123.14
4	D	503	GTP	C1'-N9-C4	-2.49	123.19	126.94
3	D	552	NDP	C4A-C5A-N7A	-2.41	107.26	109.48
3	B	552	NDP	C1D-N1N-C6N	-2.39	115.45	120.81
3	E	552	NDP	C4A-C5A-N7A	-2.39	107.28	109.48
3	F	552	NDP	C4A-C5A-N7A	-2.35	107.32	109.48
4	A	503	GTP	C6-C5-C4	-2.34	118.11	120.90
4	E	503	GTP	PA-O3A-PB	-2.33	126.18	132.73
4	B	503	GTP	O5'-PA-O1A	-2.32	100.62	109.62
4	B	503	GTP	C4-C5-N7	-2.30	107.36	109.48
4	F	503	GTP	C1'-N9-C4	-2.27	123.51	126.94
3	E	552	NDP	P2B-O2B-C2B	-2.24	116.19	121.56
4	B	503	GTP	C2'-C1'-N9	-2.16	110.99	114.29
4	F	503	GTP	C6-C5-C4	-2.06	118.43	120.90
3	A	552	NDP	C3N-C2N-N1N	-2.06	120.19	123.14
4	E	503	GTP	C2'-C1'-N9	-2.04	111.17	114.29
4	B	503	GTP	PA-O3A-PB	-2.02	127.04	132.73
4	C	503	GTP	C4-C5-N7	-2.02	107.62	109.48
4	B	503	GTP	O3'-C3'-C4'	-2.00	105.05	111.05
4	D	503	GTP	O3A-PA-O5'	2.05	108.38	102.94
3	A	552	NDP	O4D-C1D-N1N	2.11	112.52	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	552	NDP	O4B-C1B-N9A	2.16	112.62	108.10
4	B	503	GTP	O3A-PA-O5'	2.31	109.08	102.94
3	C	552	NDP	C2B-C3B-C4B	2.32	107.36	101.85
4	A	503	GTP	O3A-PA-O5'	2.35	109.17	102.94
4	D	503	GTP	N2-C2-N1	2.40	121.17	117.20
4	F	503	GTP	O4'-C1'-N9	2.62	113.58	108.10
4	D	503	GTP	C6-N1-C2	2.70	119.69	115.94
4	B	503	GTP	N2-C2-N1	3.01	122.19	117.20
4	E	503	GTP	O3A-PA-O5'	3.04	110.99	102.94
4	E	503	GTP	N2-C2-N1	3.16	122.43	117.20
4	C	503	GTP	C6-N1-C2	3.20	120.38	115.94
4	F	503	GTP	C6-N1-C2	3.21	120.39	115.94
4	A	503	GTP	C6-N1-C2	3.42	120.69	115.94
4	B	503	GTP	C6-N1-C2	3.42	120.69	115.94
4	E	503	GTP	C6-N1-C2	3.60	120.93	115.94
4	A	503	GTP	N2-C2-N1	3.95	123.74	117.20

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
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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	495/501 (98%)	0.14	23 (4%)	36	32	15, 32, 68, 127	0
1	B	495/501 (98%)	0.15	18 (3%)	46	42	17, 34, 71, 128	0
1	C	495/501 (98%)	0.29	37 (7%)	17	13	18, 38, 71, 129	0
1	D	495/501 (98%)	0.12	22 (4%)	38	34	15, 32, 71, 131	0
1	E	495/501 (98%)	0.13	21 (4%)	40	36	16, 32, 71, 126	0
1	F	501/501 (100%)	-0.02	19 (3%)	44	40	14, 29, 73, 130	0
All	All	2976/3006 (99%)	0.13	140 (4%)	35	32	14, 32, 72, 131	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	HIS	8.2
1	B	2	ASP	7.7
1	E	424	HIS	7.1
1	C	3	ARG	6.9
1	F	424	HIS	6.6
1	C	4	GLU	5.9
1	B	39	GLU	5.9
1	E	425	GLY	5.7
1	C	424	HIS	5.4
1	F	498	VAL	5.3
1	A	1	ALA	5.2
1	C	32	LEU	5.0
1	F	425	GLY	4.9
1	B	425	GLY	4.9
1	A	424	HIS	4.7
1	E	1	ALA	4.6
1	C	33	LYS	4.6
1	C	334	SER	4.5
1	C	230	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	3	ARG	4.4
1	A	3	ARG	4.4
1	E	72	TRP	4.3
1	B	1	ALA	4.1
1	C	339	VAL	4.1
1	A	2	ASP	4.1
1	B	3	ARG	4.0
1	F	497	GLY	4.0
1	A	21	ALA	3.8
1	C	311	GLU	3.7
1	F	429	PRO	3.7
1	D	424	HIS	3.6
1	E	2	ASP	3.6
1	D	235	ILE	3.5
1	E	71	SER	3.5
1	C	1	ALA	3.5
1	D	36	GLU	3.5
1	F	496	ALA	3.5
1	C	36	GLU	3.4
1	C	272	THR	3.4
1	D	309	ILE	3.4
1	D	39	GLU	3.4
1	C	40	GLN	3.4
1	B	43	ASN	3.3
1	D	248	VAL	3.3
1	C	2	ASP	3.2
1	E	36	GLU	3.2
1	D	40	GLN	3.2
1	F	36	GLU	3.2
1	F	1	ALA	3.2
1	B	298	HIS	3.1
1	C	302	LEU	3.1
1	E	428	ILE	3.1
1	C	44	ARG	3.1
1	D	281	TRP	3.0
1	D	1	ALA	3.0
1	C	428	ILE	3.0
1	C	329	LYS	3.0
1	E	426	GLY	3.0
1	D	266	PHE	3.0
1	F	500	PHE	3.0
1	F	29	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	236	LEU	2.9
1	B	36	GLU	2.9
1	A	390	ASN	2.9
1	A	47	SER	2.9
1	B	297	GLN	2.9
1	C	364	ASN	2.9
1	A	33	LYS	2.9
1	C	426	GLY	2.8
1	C	5	ASP	2.8
1	B	44	ARG	2.8
1	C	268	ALA	2.8
1	A	417	LEU	2.8
1	F	499	THR	2.8
1	B	312	GLY	2.8
1	E	37	THR	2.8
1	E	272	THR	2.8
1	C	285	GLY	2.7
1	C	34	THR	2.7
1	E	427	THR	2.7
1	C	271	ILE	2.7
1	A	415	GLU	2.7
1	D	270	CYS	2.7
1	E	47	SER	2.7
1	C	365	ILE	2.6
1	D	433	THR	2.6
1	A	35	ARG	2.6
1	D	416	SER	2.6
1	D	72	TRP	2.6
1	C	332	THR	2.5
1	C	35	ARG	2.5
1	D	431	VAL	2.5
1	B	11	LYS	2.5
1	C	31	ASP	2.5
1	F	421	PHE	2.5
1	E	4	GLU	2.5
1	A	36	GLU	2.5
1	F	501	THR	2.5
1	A	387	ASN	2.5
1	B	417	LEU	2.4
1	F	430	ILE	2.4
1	E	412	SER	2.4
1	C	243	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	2.4
1	A	30	GLU	2.4
1	D	2	ASP	2.4
1	A	28	LEU	2.3
1	E	280	ILE	2.3
1	A	475	LEU	2.3
1	A	19	ARG	2.3
1	F	7	PRO	2.3
1	D	426	GLY	2.3
1	B	234	SER	2.3
1	C	313	SER	2.3
1	C	98	ASP	2.2
1	C	244	ASP	2.2
1	F	31	ASP	2.2
1	C	340	LYS	2.2
1	C	232	TYR	2.2
1	E	271	ILE	2.2
1	E	19	ARG	2.2
1	A	294	PHE	2.2
1	A	329	LYS	2.2
1	B	33	LYS	2.2
1	C	234	SER	2.1
1	F	34	THR	2.1
1	F	417	LEU	2.1
1	B	41	LYS	2.1
1	A	411	MET	2.1
1	D	37	THR	2.1
1	D	35	ARG	2.1
1	D	317	VAL	2.1
1	E	361	LEU	2.1
1	D	31	ASP	2.1
1	A	41	LYS	2.1
1	C	494	ASN	2.1
1	F	44	ARG	2.0
1	E	407	TYR	2.0
1	A	416	SER	2.0
1	B	362	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GLU	F	502	10/10	0.95	0.19	1.31	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	0.69	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	-0.26	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	-0.37	19,26,31,31	0
5	ZN	B	505	1/1	0.97	0.17	-0.40	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	-0.48	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	-4.43	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

There are no such residues in this entry.