Full wwPDB X-ray Structure Validation Report (i)

May 23, 2024 – 02:16 PM EDT

PDB ID	:	3ZZI
Title	:	Crystal structure of a tetrameric acetylglutamate kinase from Saccharomyces cerevisiae
Authors	:	de Cima, S.; Gil-Ortiz, F.; Crabeel, M.; Fita, I.; Rubio, V.
Deposited on	:	2011-09-01
Resolution	:	3.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

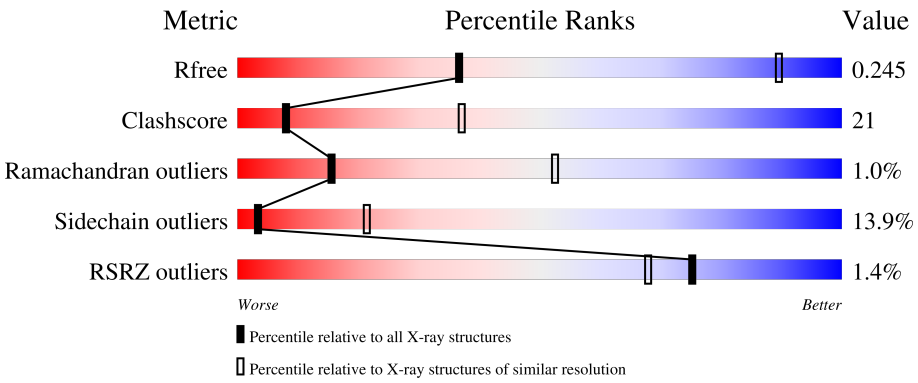
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	464	59% 29% 6% 6%
1	B	464	59% 29% 6% 6%
1	C	464	2% 58% 29% 6% 6%
1	D	464	% 55% 32% 6% 6%
1	E	464	% 53% 32% 8% • 6%

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Mol	Chain	Length	Quality of chain
1	F	464	%, 56%, 31%, 7%, 6%
1	G	464	3%, 61%, 26%, 6%, 6%
1	H	464	%, 53%, 34%, 7%, 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 27248 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 ACETYLGLUTAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3402	2167	571	655	9	0	0	0
1	B	436	3402	2167	571	655	9	0	0	0
1	C	436	3408	2170	574	655	9	0	0	0
1	D	436	3404	2167	573	655	9	0	0	0
1	E	436	3408	2170	574	655	9	0	0	0
1	F	436	3408	2170	574	655	9	0	0	0
1	G	436	3408	2170	574	655	9	0	0	0
1	H	436	3408	2170	574	655	9	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP Q01217
A	51	GLY	-	expression tag	UNP Q01217
A	52	HIS	-	expression tag	UNP Q01217
A	53	HIS	-	expression tag	UNP Q01217
A	54	HIS	-	expression tag	UNP Q01217
A	55	HIS	-	expression tag	UNP Q01217
A	56	HIS	-	expression tag	UNP Q01217
A	57	HIS	-	expression tag	UNP Q01217
B	50	MET	-	expression tag	UNP Q01217
B	51	GLY	-	expression tag	UNP Q01217
B	52	HIS	-	expression tag	UNP Q01217
B	53	HIS	-	expression tag	UNP Q01217
B	54	HIS	-	expression tag	UNP Q01217

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	HIS	-	expression tag	UNP Q01217
B	56	HIS	-	expression tag	UNP Q01217
B	57	HIS	-	expression tag	UNP Q01217
C	50	MET	-	expression tag	UNP Q01217
C	51	GLY	-	expression tag	UNP Q01217
C	52	HIS	-	expression tag	UNP Q01217
C	53	HIS	-	expression tag	UNP Q01217
C	54	HIS	-	expression tag	UNP Q01217
C	55	HIS	-	expression tag	UNP Q01217
C	56	HIS	-	expression tag	UNP Q01217
C	57	HIS	-	expression tag	UNP Q01217
D	50	MET	-	expression tag	UNP Q01217
D	51	GLY	-	expression tag	UNP Q01217
D	52	HIS	-	expression tag	UNP Q01217
D	53	HIS	-	expression tag	UNP Q01217
D	54	HIS	-	expression tag	UNP Q01217
D	55	HIS	-	expression tag	UNP Q01217
D	56	HIS	-	expression tag	UNP Q01217
D	57	HIS	-	expression tag	UNP Q01217
E	50	MET	-	expression tag	UNP Q01217
E	51	GLY	-	expression tag	UNP Q01217
E	52	HIS	-	expression tag	UNP Q01217
E	53	HIS	-	expression tag	UNP Q01217
E	54	HIS	-	expression tag	UNP Q01217
E	55	HIS	-	expression tag	UNP Q01217
E	56	HIS	-	expression tag	UNP Q01217
E	57	HIS	-	expression tag	UNP Q01217
F	50	MET	-	expression tag	UNP Q01217
F	51	GLY	-	expression tag	UNP Q01217
F	52	HIS	-	expression tag	UNP Q01217
F	53	HIS	-	expression tag	UNP Q01217
F	54	HIS	-	expression tag	UNP Q01217
F	55	HIS	-	expression tag	UNP Q01217
F	56	HIS	-	expression tag	UNP Q01217
F	57	HIS	-	expression tag	UNP Q01217
G	50	MET	-	expression tag	UNP Q01217
G	51	GLY	-	expression tag	UNP Q01217
G	52	HIS	-	expression tag	UNP Q01217
G	53	HIS	-	expression tag	UNP Q01217
G	54	HIS	-	expression tag	UNP Q01217
G	55	HIS	-	expression tag	UNP Q01217
G	56	HIS	-	expression tag	UNP Q01217

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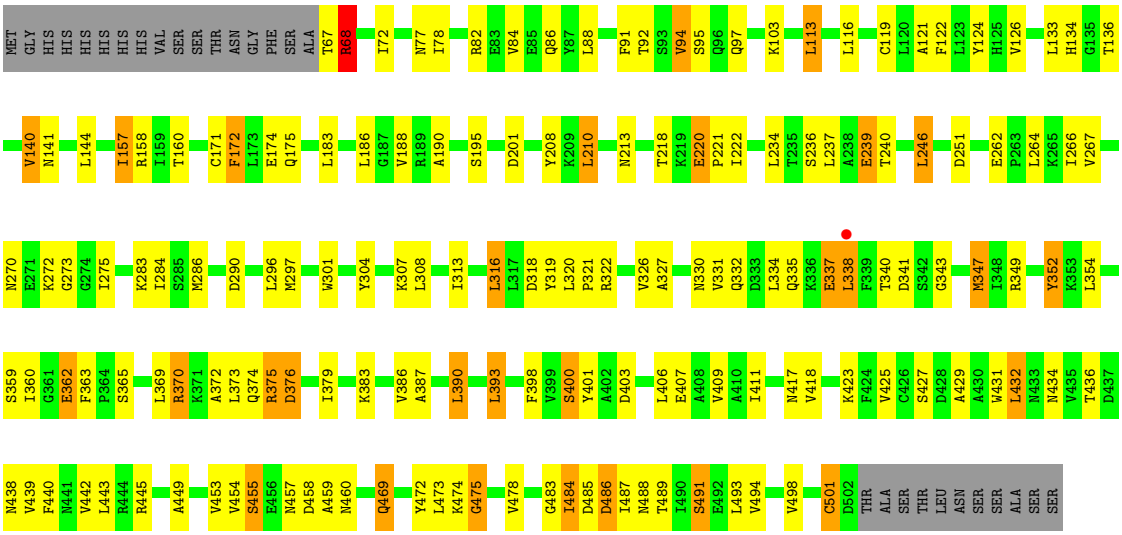
Chain	Residue	Modelled	Actual	Comment	Reference
G	57	HIS	-	expression tag	UNP Q01217
H	50	MET	-	expression tag	UNP Q01217
H	51	GLY	-	expression tag	UNP Q01217
H	52	HIS	-	expression tag	UNP Q01217
H	53	HIS	-	expression tag	UNP Q01217
H	54	HIS	-	expression tag	UNP Q01217
H	55	HIS	-	expression tag	UNP Q01217
H	56	HIS	-	expression tag	UNP Q01217
H	57	HIS	-	expression tag	UNP Q01217

3 Residue-property plots (i)

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

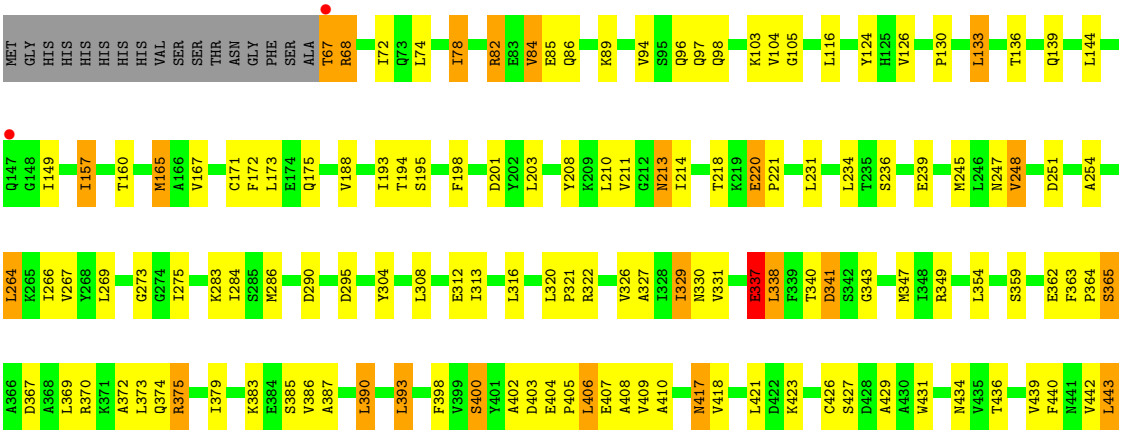
• Molecule 1: ACETYLGLUTAMATE KINASE

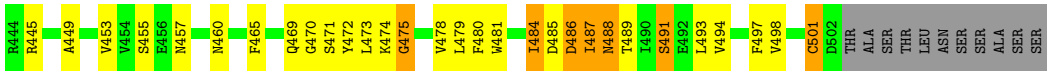
Chain A: 59% 29% 6% 6%



• Molecule 1: ACETYLGLUTAMATE KINASE

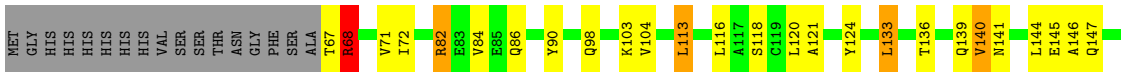
Chain B: 59% 29% 6% 6%

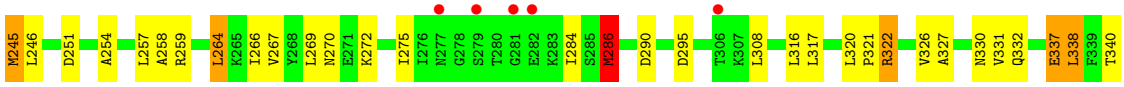


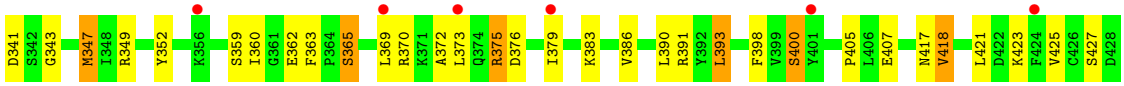


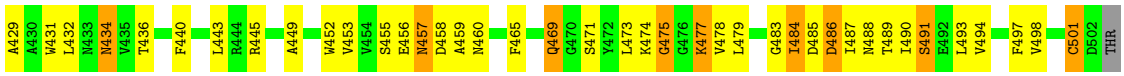
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain C:



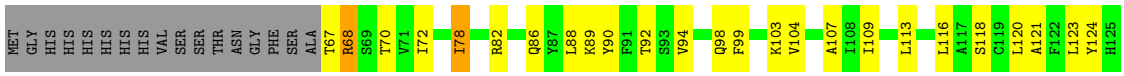


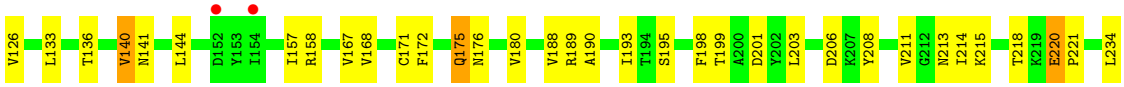


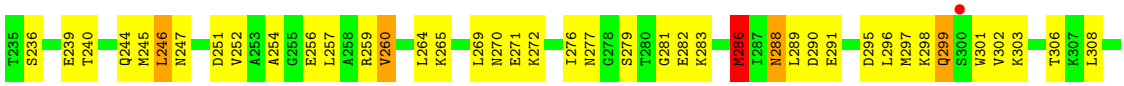


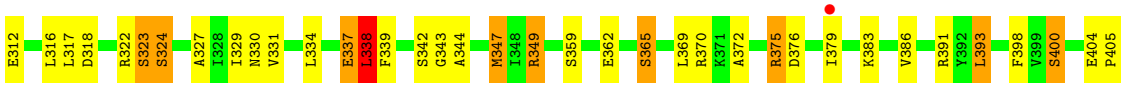
• Molecule 1: ACETYLGLUTAMATE KINASE

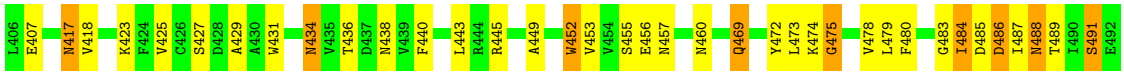
Chain D:

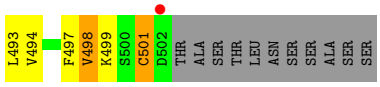






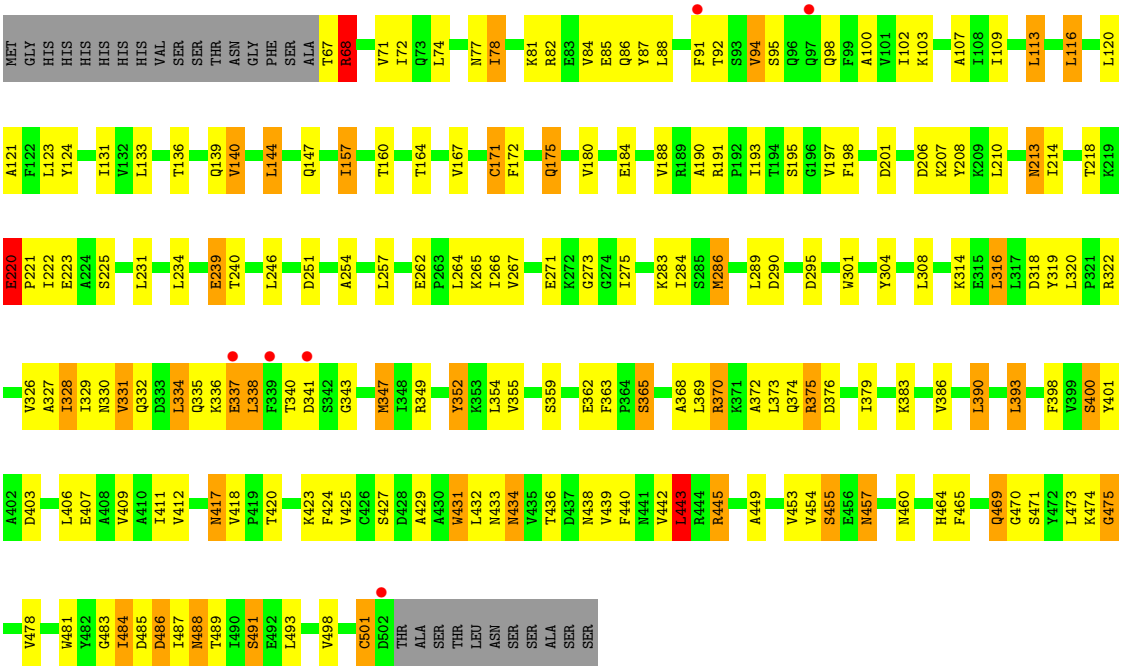






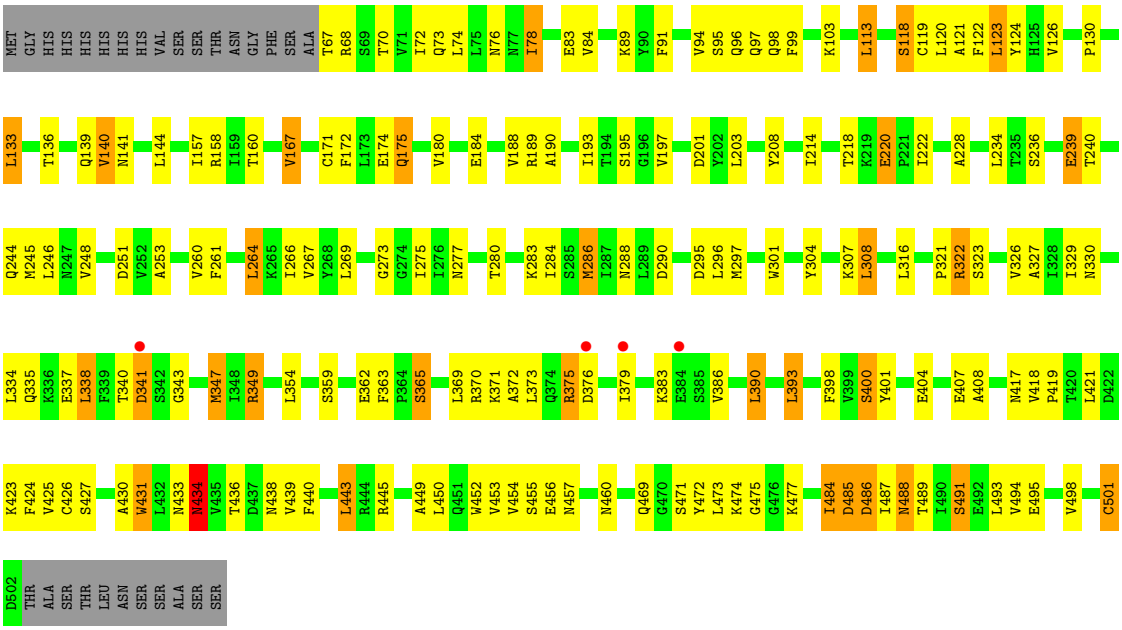
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain E:



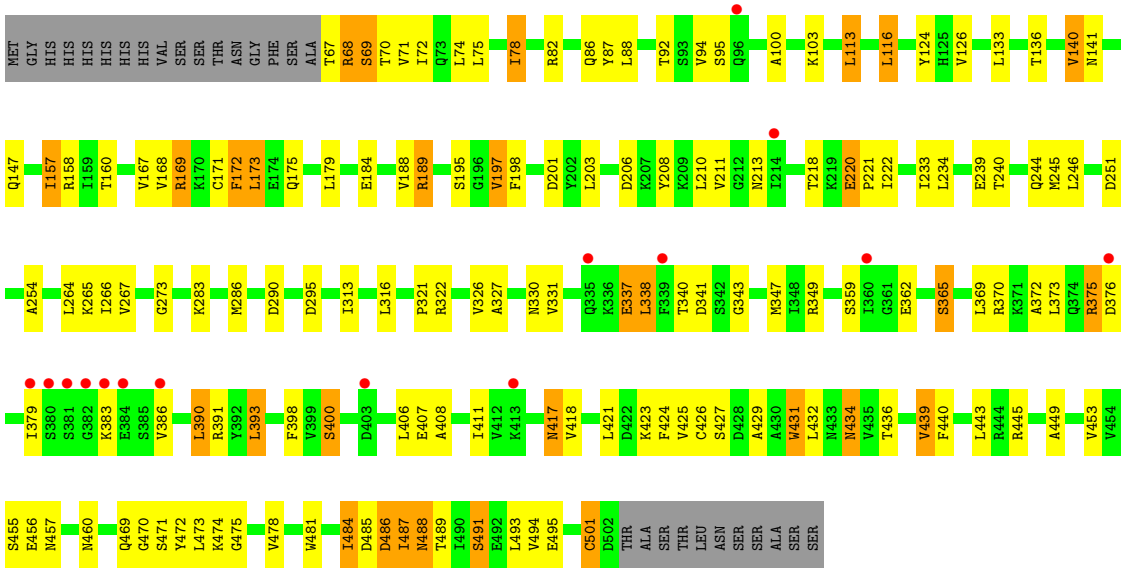
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain F:



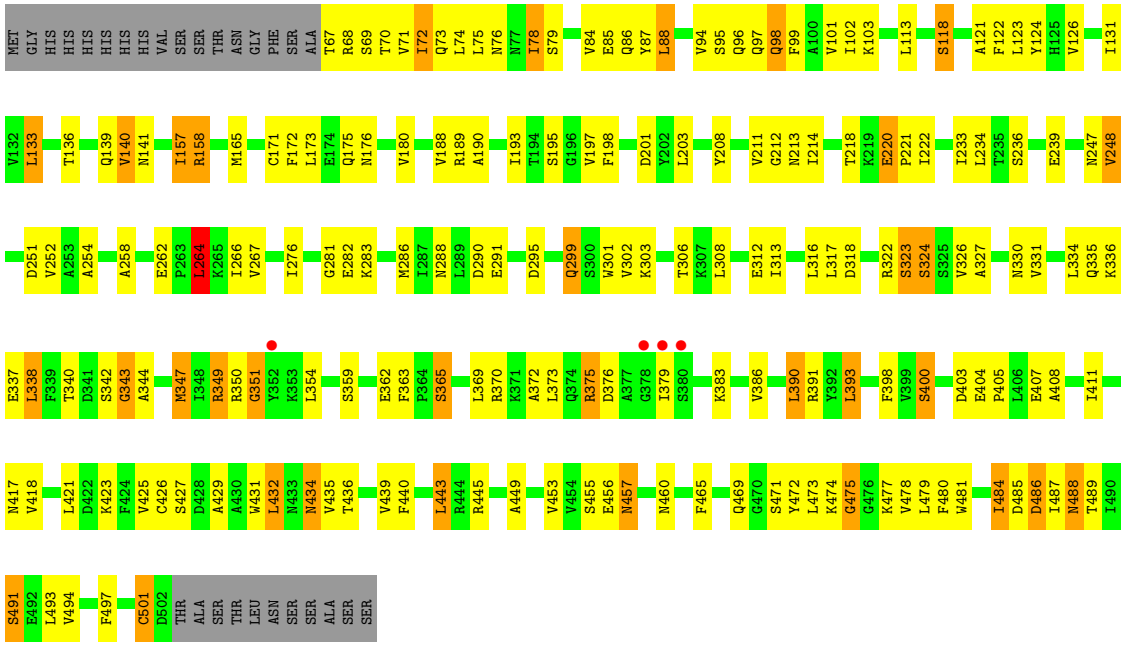
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain G:



- Molecule 1: ACETYLGLUTAMATE KINASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.24Å 111.29Å 113.14Å 75.77° 89.29° 69.12°	Depositor
Resolution (Å)	109.11 – 3.80 66.22 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (109.11-3.80) 96.3 (66.22-3.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.236 0.200 , 0.245	Depositor DCC
R_{free} test set	2003 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	136.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 79.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27248	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.86	3/3460 (0.1%)	0.95	9/4686 (0.2%)
1	B	0.86	3/3460 (0.1%)	0.92	3/4686 (0.1%)
1	C	0.77	0/3466	0.89	9/4693 (0.2%)
1	D	0.80	2/3462 (0.1%)	0.93	8/4689 (0.2%)
1	E	0.94	6/3466 (0.2%)	1.00	12/4693 (0.3%)
1	F	0.86	5/3466 (0.1%)	0.92	2/4693 (0.0%)
1	G	0.75	2/3466 (0.1%)	0.84	1/4693 (0.0%)
1	H	0.83	4/3466 (0.1%)	0.99	11/4693 (0.2%)
All	All	0.83	25/27712 (0.1%)	0.93	55/37526 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	2
1	G	0	2
1	H	0	1
All	All	0	7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	GLU	CD-OE1	8.55	1.35	1.25
1	H	239	GLU	CD-OE1	7.00	1.33	1.25
1	H	282	GLU	CG-CD	6.51	1.61	1.51
1	H	481	TRP	CD2-CE2	6.05	1.48	1.41
1	E	223	GLU	CD-OE1	6.04	1.32	1.25
1	F	341	ASP	CB-CG	5.83	1.64	1.51
1	E	431	TRP	CD2-CE2	5.77	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	301	TRP	CD2-CE2	5.72	1.48	1.41
1	E	301	TRP	CD2-CE2	5.68	1.48	1.41
1	F	431	TRP	CD2-CE2	5.39	1.47	1.41
1	B	337	GLU	CD-OE1	5.38	1.31	1.25
1	B	312	GLU	CD-OE2	5.35	1.31	1.25
1	A	301	TRP	CD2-CE2	5.31	1.47	1.41
1	A	362	GLU	CD-OE1	5.30	1.31	1.25
1	A	239	GLU	CD-OE1	5.27	1.31	1.25
1	E	220	GLU	CD-OE2	5.26	1.31	1.25
1	B	341	ASP	CB-CG	5.25	1.62	1.51
1	F	301	TRP	CD2-CE2	5.24	1.47	1.41
1	E	239	GLU	CD-OE1	5.20	1.31	1.25
1	F	239	GLU	CD-OE2	5.19	1.31	1.25
1	E	220	GLU	CD-OE1	5.15	1.31	1.25
1	F	220	GLU	CD-OE2	5.11	1.31	1.25
1	G	431	TRP	CD2-CE2	5.07	1.47	1.41
1	D	452	TRP	CD2-CE2	5.06	1.47	1.41
1	G	189	ARG	CZ-NH2	5.02	1.39	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	316	LEU	CB-CG-CD1	-8.74	96.14	111.00
1	C	68	ARG	CB-CA-C	-7.61	95.19	110.40
1	A	316	LEU	CB-CG-CD1	-7.41	98.41	111.00
1	E	334	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	H	295	ASP	CB-CG-OD2	6.83	124.45	118.30
1	D	318	ASP	CB-CG-OD2	6.72	124.35	118.30
1	H	351	GLY	CA-C-N	-6.71	102.44	117.20
1	A	423	LYS	CD-CE-NZ	6.61	126.90	111.70
1	A	352	TYR	CB-CA-C	-6.42	97.57	110.40
1	B	67	THR	N-CA-C	-6.34	93.89	111.00
1	F	286	MET	CG-SD-CE	6.31	110.30	100.20
1	H	318	ASP	CB-CG-OD2	6.05	123.75	118.30
1	E	286	MET	CG-SD-CE	6.01	109.82	100.20
1	H	282	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	E	328	ILE	CG1-CB-CG2	-5.96	98.28	111.40
1	D	239	GLU	CG-CD-OE2	-5.79	106.72	118.30
1	F	347	MET	CG-SD-CE	5.77	109.43	100.20
1	H	264	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	98	GLN	CB-CA-C	-5.75	98.91	110.40
1	H	165	MET	CG-SD-CE	-5.72	91.05	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	183	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	H	158	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	376	ASP	CB-CG-OD1	5.67	123.41	118.30
1	H	351	GLY	O-C-N	5.64	131.72	122.70
1	D	286	MET	CG-SD-CE	5.62	109.20	100.20
1	D	291	GLU	CG-CD-OE1	5.60	129.50	118.30
1	E	352	TYR	N-CA-C	5.58	126.06	111.00
1	E	68	ARG	CB-CA-C	-5.57	99.27	110.40
1	C	477	LYS	CD-CE-NZ	-5.53	98.97	111.70
1	C	286	MET	CG-SD-CE	5.50	109.00	100.20
1	C	347	MET	CG-SD-CE	5.45	108.91	100.20
1	G	169	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	231	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	H	291	GLU	CG-CD-OE2	-5.41	107.49	118.30
1	E	116	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	245	MET	CG-SD-CE	5.35	108.75	100.20
1	H	239	GLU	CG-CD-OE2	-5.34	107.61	118.30
1	A	68	ARG	CB-CA-C	-5.34	99.72	110.40
1	A	352	TYR	N-CA-C	5.32	125.37	111.00
1	D	338	LEU	CB-CA-C	5.31	120.30	110.20
1	D	291	GLU	CG-CD-OE2	-5.28	107.75	118.30
1	E	120	LEU	CB-CG-CD2	5.26	119.94	111.00
1	D	98	GLN	CB-CA-C	-5.25	99.89	110.40
1	H	291	GLU	CG-CD-OE1	5.23	128.76	118.30
1	D	158	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	406	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	370	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	370	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	186	LEU	CB-CG-CD2	5.14	119.75	111.00
1	B	329	ILE	CB-CA-C	-5.14	101.32	111.60
1	E	370	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	259	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	98	GLN	CB-CA-C	-5.06	100.28	110.40
1	C	158	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	E	123	LEU	CB-CG-CD1	5.02	119.53	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	VAL	Peptide
1	B	417	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	94	VAL	Peptide
1	E	95	SER	Peptide
1	G	501	CYS	Peptide
1	G	95	SER	Peptide
1	H	351	GLY	Peptide

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	3402	0	3429	130	0
1	B	3402	0	3429	147	1
1	C	3408	0	3440	143	0
1	D	3404	0	3429	142	0
1	E	3408	0	3440	197	0
1	F	3408	0	3440	183	0
1	G	3408	0	3440	140	1
1	H	3408	0	3440	180	0
All	All	27248	0	27487	1169	1

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 21.

All (1169) 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:E:354:LEU:HD11	1:E:438:ASN:ND2	1.54	1.22
1:B:327:ALA:HB2	1:B:347:MET:CE	1.75	1.14
1:B:327:ALA:HB2	1:B:347:MET:HE3	1.29	1.12
1:E:418:VAL:HG21	1:E:493:LEU:HD11	1.25	1.11
1:D:418:VAL:HG21	1:D:493:LEU:HD11	1.12	1.11
1:E:267:VAL:HG21	1:E:338:LEU:HD11	1.25	1.10
1:G:327:ALA:HB2	1:G:347:MET:CE	1.82	1.10
1:A:266:ILE:HD13	1:A:316:LEU:HD21	1.34	1.09
1:D:334:LEU:HD11	1:D:338:LEU:HD12	1.32	1.09
1:E:77:ASN:ND2	1:E:335:GLN:HE21	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ASP:OD1	1:H:323:SER:HB2	1.53	1.08
1:D:334:LEU:CD1	1:D:338:LEU:HD12	1.84	1.07
1:G:267:VAL:HG21	1:G:338:LEU:HD11	1.31	1.04
1:D:334:LEU:HD11	1:D:338:LEU:CD1	1.89	1.01
1:B:267:VAL:HG21	1:B:338:LEU:HD11	1.40	1.01
1:E:267:VAL:CG2	1:E:338:LEU:HD11	1.89	1.01
1:G:327:ALA:HB2	1:G:347:MET:HE2	1.42	1.01
1:A:267:VAL:HG21	1:A:338:LEU:HD11	1.41	1.00
1:A:370:ARG:HG3	1:A:386:VAL:HG11	1.43	0.97
1:F:73:GLN:NE2	1:F:335:GLN:OE1	1.97	0.95
1:H:418:VAL:HG21	1:H:493:LEU:HD11	1.49	0.95
1:D:418:VAL:CG2	1:D:493:LEU:HD11	1.96	0.94
1:E:84:VAL:HG21	1:H:78:ILE:CG2	1.98	0.94
1:E:84:VAL:HG21	1:H:78:ILE:HG22	1.47	0.94
1:F:417:ASN:O	1:F:418:VAL:HG22	1.69	0.93
1:C:418:VAL:HG21	1:C:493:LEU:HD11	1.52	0.92
1:F:273:GLY:O	1:F:283:LYS:NZ	2.01	0.92
1:E:78:ILE:HG22	1:H:84:VAL:HG21	1.52	0.92
1:F:379:ILE:HG21	1:F:386:VAL:HG23	1.51	0.91
1:G:418:VAL:HG21	1:G:493:LEU:HD11	1.52	0.91
1:D:418:VAL:HG21	1:D:493:LEU:CD1	1.99	0.91
1:E:77:ASN:HD22	1:E:335:GLN:HE21	1.02	0.91
1:G:313:ILE:HD13	1:G:326:VAL:HG11	1.53	0.91
1:H:70:THR:HG23	1:H:122:PHE:CD1	2.05	0.90
1:B:327:ALA:CB	1:B:347:MET:HE3	2.02	0.90
1:F:97:GLN:OE1	1:F:264:LEU:HD22	1.72	0.90
1:E:354:LEU:HD11	1:E:438:ASN:HD22	1.31	0.90
1:B:417:ASN:O	1:B:418:VAL:HG22	1.72	0.90
1:E:354:LEU:CD1	1:E:438:ASN:ND2	2.36	0.89
1:C:146:ALA:HB1	1:F:323:SER:HB2	1.55	0.88
1:B:379:ILE:HG21	1:B:386:VAL:HG23	1.56	0.88
1:B:133:LEU:HD21	1:B:236:SER:HB3	1.55	0.88
1:C:136:THR:HG23	1:C:136:THR:O	1.72	0.88
1:B:103:LYS:HE3	1:B:251:ASP:OD1	1.73	0.88
1:A:417:ASN:O	1:A:418:VAL:HG22	1.73	0.88
1:C:327:ALA:HB2	1:C:347:MET:CE	2.04	0.88
1:H:97:GLN:OE1	1:H:264:LEU:HD13	1.73	0.87
1:E:418:VAL:CG2	1:E:493:LEU:HD11	2.04	0.87
1:H:313:ILE:HD13	1:H:326:VAL:HG11	1.56	0.87
1:G:234:LEU:N	1:G:234:LEU:HD12	1.89	0.86
1:E:77:ASN:ND2	1:E:335:GLN:NE2	2.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:370:ARG:HG3	1:H:386:VAL:HG11	1.58	0.86
1:E:85:GLU:HB3	1:E:432:LEU:HD22	1.55	0.86
1:E:88:LEU:HD11	1:H:76:ASN:OD1	1.76	0.85
1:E:91:PHE:HB3	1:H:72:ILE:CD1	2.06	0.85
1:B:387:ALA:HB3	1:H:262:GLU:CD	1.96	0.85
1:C:317:LEU:HD21	1:C:326:VAL:HG23	1.56	0.85
1:F:97:GLN:OE1	1:F:264:LEU:CD2	2.24	0.85
1:F:327:ALA:HB2	1:F:347:MET:CE	2.06	0.85
1:G:417:ASN:O	1:G:418:VAL:HG22	1.77	0.85
1:H:103:LYS:HE3	1:H:251:ASP:OD1	1.75	0.85
1:E:91:PHE:HB3	1:H:72:ILE:HD13	1.59	0.84
1:F:288:ASN:HD22	1:F:438:ASN:ND2	1.74	0.84
1:H:86:GLN:OE1	1:H:340:THR:CB	2.26	0.84
1:B:157:ILE:HD12	1:B:208:TYR:CE1	2.13	0.84
1:B:387:ALA:HB3	1:H:262:GLU:OE2	1.78	0.83
1:C:147:GLN:HG3	1:F:322:ARG:HB3	1.60	0.83
1:B:385:SER:HB3	1:H:262:GLU:OE1	1.78	0.83
1:E:144:LEU:HD21	1:E:164:THR:HG23	1.60	0.83
1:E:418:VAL:HG21	1:E:493:LEU:CD1	2.08	0.83
1:G:103:LYS:HE3	1:G:251:ASP:OD1	1.77	0.83
1:D:94:VAL:O	1:D:94:VAL:HG12	1.77	0.83
1:F:349:ARG:NH2	1:F:433:ASN:O	2.11	0.83
1:E:273:GLY:O	1:E:283:LYS:NZ	2.11	0.83
1:C:146:ALA:CB	1:F:323:SER:HB2	2.08	0.82
1:H:73:GLN:HG2	1:H:335:GLN:OE1	1.79	0.82
1:C:222:ILE:HD11	1:C:234:LEU:HD11	1.62	0.82
1:E:136:THR:HA	1:E:139:GLN:HE22	1.45	0.82
1:F:327:ALA:HB2	1:F:347:MET:HE1	1.62	0.82
1:C:103:LYS:HE3	1:C:251:ASP:OD1	1.80	0.82
1:B:213:ASN:HD22	1:B:214:ILE:N	1.78	0.82
1:A:157:ILE:HD12	1:A:208:TYR:CE1	2.15	0.81
1:B:273:GLY:O	1:B:283:LYS:NZ	2.14	0.81
1:G:267:VAL:CG2	1:G:338:LEU:HD11	2.10	0.81
1:B:363:PHE:CG	1:B:369:LEU:HD12	2.16	0.81
1:D:176:ASN:O	1:D:180:VAL:HG23	1.81	0.81
1:G:234:LEU:N	1:G:234:LEU:CD1	2.43	0.80
1:A:474:LYS:NZ	1:A:501:CYS:SG	2.54	0.80
1:C:68:ARG:O	1:C:72:ILE:CD1	2.30	0.80
1:G:370:ARG:HG3	1:G:386:VAL:HG11	1.61	0.79
1:A:487:ILE:HD11	1:D:491:SER:HA	1.63	0.79
1:F:379:ILE:HD11	1:F:423:LYS:NZ	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HE3	1:A:251:ASP:OD1	1.82	0.79
1:E:376:ASP:HB2	1:E:425:VAL:HG22	1.65	0.79
1:B:213:ASN:HD22	1:B:213:ASN:C	1.86	0.79
1:D:90:TYR:OH	1:D:265:LYS:NZ	2.15	0.79
1:C:68:ARG:O	1:C:72:ILE:HD12	1.83	0.79
1:F:495:GLU:HG3	1:G:487:ILE:HD13	1.65	0.79
1:E:82:ARG:HD2	1:E:432:LEU:O	1.83	0.78
1:F:103:LYS:HE3	1:F:251:ASP:OD1	1.84	0.78
1:D:103:LYS:HE3	1:D:251:ASP:OD1	1.83	0.78
1:D:193:ILE:HB	1:D:234:LEU:HD13	1.65	0.78
1:E:370:ARG:HG3	1:E:386:VAL:HG11	1.66	0.78
1:F:120:LEU:HA	1:F:123:LEU:HD12	1.67	0.77
1:H:342:SER:O	1:H:344:ALA:N	2.17	0.77
1:F:157:ILE:HD12	1:F:208:TYR:CE1	2.19	0.77
1:E:136:THR:HA	1:E:139:GLN:NE2	2.00	0.76
1:C:379:ILE:HG21	1:C:386:VAL:HG23	1.66	0.76
1:H:197:VAL:HG21	1:H:234:LEU:HD21	1.66	0.76
1:A:313:ILE:HD13	1:A:326:VAL:HG11	1.68	0.76
1:B:474:LYS:NZ	1:B:501:CYS:SG	2.57	0.76
1:E:487:ILE:HD11	1:H:491:SER:HB3	1.66	0.76
1:A:417:ASN:O	1:A:418:VAL:CG2	2.34	0.76
1:F:491:SER:O	1:G:487:ILE:HD11	1.86	0.75
1:G:417:ASN:O	1:G:418:VAL:CG2	2.34	0.75
1:D:203:LEU:HD22	1:D:208:TYR:CE2	2.21	0.75
1:H:133:LEU:HD21	1:H:236:SER:HB3	1.66	0.75
1:A:97:GLN:NE2	1:A:262:GLU:O	2.20	0.75
1:D:327:ALA:HB2	1:D:347:MET:CE	2.15	0.75
1:D:379:ILE:HG21	1:D:386:VAL:HG23	1.68	0.75
1:B:370:ARG:NH2	1:H:323:SER:OG	2.19	0.74
1:F:244:GLN:HE21	1:F:245:MET:N	1.85	0.74
1:G:369:LEU:O	1:G:369:LEU:HD23	1.88	0.74
1:D:342:SER:O	1:D:344:ALA:N	2.20	0.74
1:F:140:VAL:CG1	1:F:141:ASN:N	2.50	0.74
1:A:240:THR:CG2	1:A:246:LEU:HD11	2.18	0.74
1:C:267:VAL:HG21	1:C:338:LEU:HD11	1.67	0.74
1:G:233:ILE:C	1:G:234:LEU:HD12	2.07	0.74
1:H:140:VAL:CG1	1:H:141:ASN:N	2.50	0.74
1:C:157:ILE:HD12	1:C:208:TYR:CE1	2.23	0.73
1:F:386:VAL:CG1	1:F:390:LEU:HD22	2.17	0.73
1:A:273:GLY:O	1:A:283:LYS:NZ	2.19	0.73
1:F:119:CYS:SG	1:F:335:GLN:HB3	2.27	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ALA:HB2	1:D:347:MET:HE3	1.68	0.73
1:F:487:ILE:HD11	1:G:491:SER:HA	1.70	0.73
1:H:136:THR:HG23	1:H:136:THR:O	1.87	0.73
1:H:363:PHE:CG	1:H:369:LEU:HD12	2.24	0.73
1:H:313:ILE:CD1	1:H:326:VAL:HG11	2.19	0.73
1:C:490:ILE:O	1:C:494:VAL:HG23	1.88	0.72
1:D:417:ASN:O	1:D:418:VAL:HG22	1.88	0.72
1:E:103:LYS:HE3	1:E:251:ASP:OD1	1.89	0.72
1:G:267:VAL:HG21	1:G:338:LEU:CD1	2.15	0.72
1:C:327:ALA:HB2	1:C:347:MET:HE3	1.70	0.72
1:D:256:GLU:O	1:D:260:VAL:HG12	1.89	0.72
1:F:133:LEU:HD21	1:F:236:SER:HB3	1.71	0.72
1:C:327:ALA:HB2	1:C:347:MET:HE2	1.70	0.72
1:D:120:LEU:HD23	1:D:123:LEU:HD12	1.71	0.72
1:A:491:SER:HA	1:D:487:ILE:HD11	1.70	0.72
1:G:421:LEU:HD22	1:G:443:LEU:HD21	1.71	0.72
1:A:270:ASN:ND2	1:A:272:LYS:HB2	2.04	0.71
1:C:90:TYR:CE2	1:C:264:LEU:HD12	2.25	0.71
1:F:417:ASN:O	1:F:418:VAL:CG2	2.39	0.71
1:C:133:LEU:HD21	1:C:236:SER:HB3	1.71	0.71
1:A:418:VAL:HG21	1:A:493:LEU:HD11	1.70	0.71
1:E:94:VAL:HG12	1:E:94:VAL:O	1.91	0.71
1:E:213:ASN:HD22	1:E:214:ILE:N	1.88	0.71
1:F:140:VAL:HG12	1:F:141:ASN:N	2.05	0.71
1:H:180:VAL:HG13	1:H:190:ALA:HB3	1.71	0.71
1:H:140:VAL:HG12	1:H:141:ASN:N	2.04	0.71
1:D:474:LYS:NZ	1:D:501:CYS:SG	2.63	0.70
1:H:70:THR:HG23	1:H:122:PHE:HD1	1.54	0.70
1:B:267:VAL:HG21	1:B:338:LEU:CD1	2.20	0.70
1:B:327:ALA:CB	1:B:347:MET:CE	2.62	0.70
1:B:369:LEU:HD23	1:B:373:LEU:HD11	1.73	0.70
1:H:157:ILE:HD12	1:H:208:TYR:CE1	2.25	0.70
1:B:418:VAL:HG21	1:B:493:LEU:HD11	1.74	0.70
1:A:266:ILE:HD13	1:A:316:LEU:CD2	2.19	0.70
1:G:82:ARG:O	1:G:86:GLN:HG2	1.92	0.70
1:H:122:PHE:O	1:H:126:VAL:HG22	1.91	0.70
1:E:222:ILE:HD11	1:E:234:LEU:HD11	1.73	0.69
1:F:354:LEU:HD21	1:F:439:VAL:CG2	2.22	0.69
1:C:163:HIS:NE2	1:F:404:GLU:OE2	2.24	0.69
1:A:369:LEU:CD2	1:A:373:LEU:HD11	2.22	0.69
1:E:74:LEU:CD2	1:H:71:VAL:HG13	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:ILE:HG21	1:G:386:VAL:HG23	1.74	0.69
1:B:417:ASN:O	1:B:418:VAL:CG2	2.39	0.69
1:A:266:ILE:CD1	1:A:316:LEU:HD21	2.19	0.69
1:D:417:ASN:O	1:D:418:VAL:CG2	2.41	0.69
1:A:157:ILE:HD12	1:A:208:TYR:CZ	2.27	0.69
1:H:267:VAL:HG21	1:H:338:LEU:HD21	1.75	0.69
1:A:363:PHE:CD1	1:A:369:LEU:HD12	2.28	0.69
1:F:286:MET:SD	1:F:434:ASN:ND2	2.65	0.68
1:F:354:LEU:HD21	1:F:439:VAL:HG23	1.75	0.68
1:A:449:ALA:HB1	1:A:484:ILE:HG22	1.74	0.68
1:G:327:ALA:CB	1:G:347:MET:CE	2.67	0.68
1:H:99:PHE:CZ	1:H:338:LEU:HD12	2.28	0.68
1:F:144:LEU:HD22	1:F:167:VAL:HG11	1.75	0.68
1:G:169:ARG:HD2	1:G:245:MET:CE	2.23	0.68
1:E:84:VAL:HG11	1:H:78:ILE:O	1.94	0.68
1:D:379:ILE:HG21	1:D:386:VAL:CG2	2.23	0.68
1:E:376:ASP:HB2	1:E:425:VAL:CG2	2.24	0.68
1:F:418:VAL:HG11	1:F:493:LEU:HD11	1.76	0.68
1:G:313:ILE:CD1	1:G:326:VAL:HG11	2.24	0.68
1:B:385:SER:CB	1:H:262:GLU:OE1	2.42	0.67
1:B:144:LEU:HD22	1:B:167:VAL:HG11	1.75	0.67
1:B:193:ILE:HB	1:B:234:LEU:HD22	1.75	0.67
1:B:369:LEU:CD2	1:B:373:LEU:HD11	2.24	0.67
1:G:157:ILE:HD12	1:G:208:TYR:CE1	2.29	0.67
1:E:157:ILE:HD12	1:E:208:TYR:CE1	2.29	0.67
1:A:84:VAL:HG21	1:D:78:ILE:HG21	1.77	0.67
1:C:144:LEU:HD22	1:C:167:VAL:HG11	1.75	0.67
1:D:82:ARG:O	1:D:86:GLN:HG2	1.94	0.67
1:H:363:PHE:CD1	1:H:369:LEU:HD12	2.30	0.67
1:D:473:LEU:HD13	1:D:478:VAL:HG22	1.77	0.67
1:E:77:ASN:HD22	1:E:335:GLN:NE2	1.81	0.67
1:E:369:LEU:CD2	1:E:373:LEU:HD11	2.25	0.67
1:E:78:ILE:CG2	1:H:84:VAL:HG21	2.23	0.67
1:H:86:GLN:OE1	1:H:340:THR:HB	1.94	0.67
1:H:417:ASN:O	1:H:418:VAL:CG2	2.43	0.67
1:F:386:VAL:HG12	1:F:390:LEU:HD22	1.77	0.66
1:G:473:LEU:HD13	1:G:478:VAL:HG22	1.78	0.66
1:E:417:ASN:O	1:E:418:VAL:HG22	1.94	0.66
1:C:370:ARG:HG3	1:C:386:VAL:HG11	1.76	0.66
1:A:267:VAL:CG2	1:A:338:LEU:HD11	2.21	0.66
1:E:213:ASN:HD22	1:E:213:ASN:C	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:THR:HG23	1:D:136:THR:O	1.95	0.66
1:E:88:LEU:CD1	1:H:76:ASN:OD1	2.42	0.66
1:H:70:THR:CG2	1:H:122:PHE:CD1	2.77	0.66
1:A:82:ARG:O	1:A:86:GLN:HG2	1.94	0.66
1:D:334:LEU:HD11	1:D:338:LEU:HD11	1.78	0.66
1:G:136:THR:O	1:G:136:THR:HG23	1.96	0.66
1:A:425:VAL:HG12	1:A:425:VAL:O	1.95	0.66
1:C:418:VAL:HG21	1:C:493:LEU:CD1	2.25	0.66
1:E:82:ARG:O	1:E:86:GLN:HG2	1.95	0.66
1:F:327:ALA:HB2	1:F:347:MET:HE2	1.78	0.66
1:E:379:ILE:HG21	1:E:386:VAL:HG23	1.76	0.66
1:E:457:ASN:ND2	1:E:457:ASN:H	1.94	0.65
1:G:94:VAL:HG12	1:G:94:VAL:O	1.95	0.65
1:G:70:THR:CG2	1:G:126:VAL:HG12	2.27	0.65
1:F:379:ILE:HD11	1:F:423:LYS:HZ2	1.61	0.65
1:E:180:VAL:HG13	1:E:190:ALA:HB3	1.78	0.65
1:E:379:ILE:HD11	1:E:423:LYS:NZ	2.12	0.65
1:F:99:PHE:HE2	1:F:123:LEU:HD22	1.60	0.65
1:H:327:ALA:HB2	1:H:347:MET:HE3	1.79	0.65
1:G:124:TYR:CG	1:G:188:VAL:HG13	2.32	0.65
1:H:393:LEU:HD22	1:H:398:PHE:CD1	2.32	0.65
1:E:484:ILE:HD11	1:E:493:LEU:HD22	1.80	0.64
1:H:176:ASN:ND2	1:H:233:ILE:HG22	2.12	0.64
1:H:323:SER:O	1:H:324:SER:C	2.35	0.64
1:C:82:ARG:O	1:C:86:GLN:HG2	1.96	0.64
1:F:94:VAL:CG1	1:F:96:GLN:NE2	2.60	0.64
1:G:169:ARG:HD2	1:G:245:MET:HE3	1.78	0.64
1:D:323:SER:O	1:D:324:SER:C	2.36	0.64
1:E:81:LYS:HG3	1:H:79:SER:O	1.98	0.64
1:A:386:VAL:HG12	1:A:387:ALA:N	2.11	0.64
1:B:354:LEU:HD21	1:B:439:VAL:HG23	1.79	0.64
1:C:469:GLN:HE21	1:C:483:GLY:H	1.44	0.64
1:D:488:ASN:HD22	1:D:489:THR:N	1.96	0.64
1:E:88:LEU:HD22	1:E:92:THR:HG23	1.80	0.64
1:F:136:THR:HG23	1:F:136:THR:O	1.97	0.64
1:G:424:PHE:HE1	1:G:439:VAL:HG11	1.63	0.64
1:C:266:ILE:HD13	1:C:316:LEU:HD21	1.80	0.64
1:A:124:TYR:CD2	1:A:188:VAL:HG22	2.32	0.63
1:B:82:ARG:O	1:B:86:GLN:HG2	1.98	0.63
1:C:327:ALA:CB	1:C:347:MET:HE3	2.28	0.63
1:E:304:TYR:CE1	1:E:308:LEU:HD13	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD11	1:A:236:SER:HB3	1.79	0.63
1:E:474:LYS:NZ	1:E:501:CYS:SG	2.67	0.63
1:F:327:ALA:CB	1:F:347:MET:HE2	2.29	0.63
1:F:327:ALA:CB	1:F:347:MET:CE	2.76	0.63
1:F:449:ALA:HB1	1:F:484:ILE:HG22	1.81	0.63
1:E:136:THR:HG23	1:E:136:THR:O	1.99	0.62
1:F:487:ILE:HD11	1:G:491:SER:CA	2.28	0.62
1:E:88:LEU:HD22	1:E:92:THR:CG2	2.29	0.62
1:F:340:THR:HG23	1:F:343:GLY:H	1.63	0.62
1:H:474:LYS:NZ	1:H:501:CYS:SG	2.69	0.62
1:C:473:LEU:HD13	1:C:478:VAL:HG22	1.81	0.62
1:H:386:VAL:CG1	1:H:390:LEU:HD22	2.30	0.62
1:C:90:TYR:HE2	1:C:264:LEU:HD12	1.63	0.62
1:A:297:MET:HE1	1:A:307:LYS:HA	1.81	0.62
1:B:213:ASN:C	1:B:213:ASN:ND2	2.53	0.62
1:E:68:ARG:O	1:E:72:ILE:HD12	2.00	0.62
1:C:68:ARG:O	1:C:72:ILE:HD13	1.99	0.61
1:F:133:LEU:C	1:F:133:LEU:HD22	2.20	0.61
1:C:473:LEU:HD13	1:C:478:VAL:CG2	2.30	0.61
1:G:266:ILE:HD13	1:G:316:LEU:HD21	1.81	0.61
1:B:68:ARG:O	1:B:72:ILE:HD12	2.00	0.61
1:B:369:LEU:HD23	1:B:373:LEU:CD1	2.30	0.61
1:B:393:LEU:HD22	1:B:398:PHE:CD1	2.36	0.61
1:F:222:ILE:HD11	1:F:234:LEU:HD11	1.80	0.61
1:F:418:VAL:HG21	1:F:493:LEU:HD11	1.83	0.61
1:H:417:ASN:O	1:H:418:VAL:HG22	2.00	0.61
1:C:474:LYS:NZ	1:C:501:CYS:SG	2.73	0.61
1:A:304:TYR:CE1	1:A:308:LEU:HD13	2.35	0.61
1:D:133:LEU:HD11	1:D:236:SER:HB3	1.82	0.61
1:F:393:LEU:HD22	1:F:398:PHE:CD1	2.35	0.61
1:A:240:THR:HG22	1:A:246:LEU:HD11	1.81	0.61
1:B:406:LEU:HD12	1:B:409:VAL:CG2	2.30	0.61
1:D:449:ALA:HB1	1:D:484:ILE:HG22	1.83	0.61
1:G:140:VAL:CG1	1:G:141:ASN:N	2.63	0.61
1:G:173:LEU:N	1:G:173:LEU:HD23	2.15	0.61
1:G:473:LEU:HD13	1:G:478:VAL:CG2	2.30	0.61
1:H:472:TYR:CD2	1:H:494:VAL:HG13	2.36	0.61
1:F:193:ILE:CG2	1:F:234:LEU:HD22	2.31	0.60
1:A:122:PHE:O	1:A:126:VAL:HG22	2.01	0.60
1:B:313:ILE:HD13	1:B:326:VAL:HG11	1.83	0.60
1:E:379:ILE:HD11	1:E:423:LYS:HZ2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HG23	1:A:136:THR:O	2.01	0.60
1:C:116:LEU:HD11	1:C:120:LEU:HD11	1.83	0.60
1:D:369:LEU:HD23	1:D:369:LEU:O	2.01	0.60
1:H:94:VAL:HG12	1:H:96:GLN:NE2	2.16	0.60
1:B:157:ILE:HD12	1:B:208:TYR:CZ	2.35	0.60
1:G:240:THR:CG2	1:G:246:LEU:HD11	2.32	0.60
1:F:160:THR:O	1:F:160:THR:HG22	2.01	0.60
1:B:363:PHE:CD1	1:B:369:LEU:CD1	2.85	0.60
1:H:87:TYR:OH	1:H:335:GLN:O	2.19	0.60
1:E:124:TYR:CD2	1:E:188:VAL:HG22	2.35	0.60
1:E:442:VAL:HG12	1:E:443:LEU:N	2.16	0.60
1:F:297:MET:HE1	1:F:307:LYS:CA	2.31	0.60
1:G:222:ILE:HD11	1:G:234:LEU:HD21	1.83	0.60
1:A:113:LEU:HD23	1:A:113:LEU:O	2.01	0.60
1:B:136:THR:O	1:B:136:THR:HG23	2.01	0.60
1:C:240:THR:CG2	1:C:246:LEU:HD11	2.31	0.60
1:E:393:LEU:HD11	1:E:411:ILE:HD13	1.84	0.60
1:A:487:ILE:HD11	1:D:491:SER:CA	2.32	0.60
1:B:387:ALA:HB3	1:H:262:GLU:OE1	2.00	0.60
1:F:94:VAL:HG11	1:F:96:GLN:NE2	2.17	0.60
1:G:169:ARG:CD	1:G:245:MET:HE3	2.31	0.60
1:H:369:LEU:CD2	1:H:373:LEU:HD11	2.31	0.60
1:E:304:TYR:CZ	1:E:308:LEU:HD13	2.37	0.60
1:E:407:GLU:OE2	1:E:429:ALA:HB3	2.00	0.59
1:C:267:VAL:HG21	1:C:338:LEU:CD1	2.32	0.59
1:A:297:MET:HE1	1:A:307:LYS:CA	2.30	0.59
1:D:286:MET:HE3	1:D:347:MET:HB3	1.83	0.59
1:E:74:LEU:HD21	1:H:71:VAL:HG13	1.84	0.59
1:F:370:ARG:HG3	1:F:386:VAL:HG11	1.84	0.59
1:C:363:PHE:CD1	1:C:369:LEU:HD12	2.36	0.59
1:D:479:LEU:HD12	1:D:480:PHE:H	1.67	0.59
1:A:262:GLU:HA	1:A:320:LEU:HD22	1.84	0.59
1:E:354:LEU:CD1	1:E:438:ASN:HD21	2.12	0.59
1:H:86:GLN:OE1	1:H:340:THR:HA	2.02	0.59
1:G:379:ILE:HD11	1:G:423:LYS:NZ	2.17	0.59
1:G:486:ASP:CB	1:G:489:THR:HG23	2.33	0.59
1:F:297:MET:HE1	1:F:307:LYS:HA	1.84	0.59
1:A:407:GLU:OE2	1:A:429:ALA:HB3	2.03	0.59
1:E:77:ASN:HD21	1:E:335:GLN:HG3	1.68	0.58
1:G:474:LYS:NZ	1:G:501:CYS:SG	2.75	0.58
1:G:386:VAL:CG1	1:G:390:LEU:HD22	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:HB2	1:B:347:MET:HE2	1.75	0.58
1:H:258:ALA:HB3	1:H:316:LEU:HD11	1.85	0.58
1:C:417:ASN:O	1:C:418:VAL:CG2	2.51	0.58
1:D:370:ARG:HG3	1:D:386:VAL:HG11	1.86	0.58
1:E:197:VAL:HG21	1:E:234:LEU:HD13	1.86	0.58
1:E:418:VAL:HG11	1:E:493:LEU:HD21	1.84	0.58
1:F:76:ASN:OD1	1:G:88:LEU:HD11	2.04	0.58
1:F:203:LEU:C	1:F:203:LEU:HD13	2.24	0.58
1:F:474:LYS:NZ	1:F:501:CYS:SG	2.72	0.58
1:G:421:LEU:HD22	1:G:443:LEU:CD2	2.33	0.58
1:H:140:VAL:HG11	1:H:158:ARG:NH2	2.18	0.58
1:C:457:ASN:H	1:C:457:ASN:ND2	1.99	0.58
1:H:489:THR:O	1:H:493:LEU:HD13	2.03	0.58
1:G:273:GLY:O	1:G:283:LYS:NZ	2.27	0.58
1:E:84:VAL:CG2	1:H:78:ILE:HG22	2.30	0.58
1:C:486:ASP:CB	1:C:489:THR:HG23	2.34	0.58
1:D:252:VAL:HG22	1:D:312:GLU:CD	2.23	0.58
1:D:479:LEU:HD12	1:D:480:PHE:N	2.19	0.58
1:H:266:ILE:HD13	1:H:316:LEU:HD21	1.86	0.58
1:B:74:LEU:CD2	1:C:71:VAL:HG13	2.34	0.57
1:G:140:VAL:HG11	1:G:158:ARG:NH2	2.19	0.57
1:C:154:ILE:HD12	1:F:371:LYS:NZ	2.19	0.57
1:C:393:LEU:HD22	1:C:398:PHE:CD1	2.40	0.57
1:B:379:ILE:HG21	1:B:386:VAL:CG2	2.31	0.57
1:E:363:PHE:CD1	1:E:369:LEU:HD12	2.39	0.57
1:H:379:ILE:HG21	1:H:386:VAL:HG23	1.86	0.57
1:D:193:ILE:HG22	1:D:193:ILE:O	2.03	0.57
1:E:417:ASN:O	1:E:418:VAL:CG2	2.53	0.57
1:F:304:TYR:CZ	1:F:308:LEU:HD13	2.39	0.57
1:A:313:ILE:CD1	1:A:326:VAL:HG11	2.34	0.57
1:D:473:LEU:HD13	1:D:478:VAL:CG2	2.34	0.57
1:E:363:PHE:CG	1:E:369:LEU:HD12	2.40	0.57
1:G:160:THR:HG22	1:G:160:THR:O	2.04	0.57
1:B:354:LEU:HD22	1:B:439:VAL:HG22	1.87	0.57
1:B:363:PHE:CD1	1:B:369:LEU:HD12	2.39	0.57
1:H:124:TYR:CG	1:H:188:VAL:HG13	2.39	0.57
1:E:136:THR:CA	1:E:139:GLN:NE2	2.68	0.57
1:E:457:ASN:ND2	1:E:457:ASN:N	2.51	0.57
1:D:334:LEU:HD12	1:D:338:LEU:HD12	1.80	0.57
1:D:379:ILE:HD11	1:D:423:LYS:NZ	2.19	0.57
1:E:160:THR:HG22	1:E:160:THR:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:473:LEU:HD12	1:F:474:LYS:O	2.05	0.56
1:D:70:THR:CG2	1:D:126:VAL:HG12	2.34	0.56
1:D:299:GLN:HB2	1:D:302:VAL:HG23	1.87	0.56
1:E:74:LEU:HD22	1:H:71:VAL:HG13	1.88	0.56
1:F:408:ALA:HB1	1:F:426:CYS:SG	2.44	0.56
1:G:140:VAL:HG12	1:G:141:ASN:N	2.21	0.56
1:H:407:GLU:OE2	1:H:429:ALA:HB3	2.04	0.56
1:B:364:PRO:HB3	1:H:407:GLU:OE2	2.06	0.56
1:A:469:GLN:HE21	1:A:483:GLY:H	1.53	0.56
1:B:133:LEU:HD12	1:B:254:ALA:HA	1.88	0.56
1:C:154:ILE:HD12	1:F:371:LYS:HZ3	1.70	0.56
1:D:329:ILE:HD12	1:D:337:GLU:CG	2.34	0.56
1:D:400:SER:O	1:D:400:SER:OG	2.23	0.56
1:H:198:PHE:CD1	1:H:214:ILE:HD13	2.40	0.56
1:C:327:ALA:CB	1:C:347:MET:CE	2.80	0.56
1:C:363:PHE:CG	1:C:369:LEU:HD12	2.41	0.56
1:C:449:ALA:HB1	1:C:484:ILE:HG22	1.86	0.56
1:F:260:VAL:HG12	1:F:261:PHE:CD1	2.41	0.56
1:F:400:SER:O	1:F:400:SER:OG	2.24	0.56
1:B:97:GLN:OE1	1:B:264:LEU:HD23	2.06	0.56
1:E:449:ALA:HB1	1:E:484:ILE:HG22	1.87	0.56
1:H:124:TYR:CD1	1:H:188:VAL:HG13	2.40	0.56
1:A:222:ILE:HD11	1:A:234:LEU:HD21	1.88	0.55
1:B:340:THR:HG23	1:B:343:GLY:H	1.71	0.55
1:B:400:SER:O	1:B:400:SER:OG	2.25	0.55
1:D:168:VAL:HG11	1:D:247:ASN:HD22	1.71	0.55
1:A:88:LEU:HD22	1:A:92:THR:HG23	1.88	0.55
1:D:329:ILE:CD1	1:D:337:GLU:HB2	2.36	0.55
1:E:88:LEU:HD11	1:H:76:ASN:HA	1.88	0.55
1:B:363:PHE:CE1	1:B:369:LEU:HD11	2.41	0.55
1:C:136:THR:O	1:C:136:THR:CG2	2.45	0.55
1:F:376:ASP:HB2	1:F:425:VAL:HG22	1.89	0.55
1:B:104:VAL:HG12	1:B:105:GLY:O	2.07	0.55
1:C:146:ALA:HB3	1:F:323:SER:HB2	1.89	0.55
1:H:363:PHE:CD1	1:H:369:LEU:CD1	2.90	0.55
1:A:369:LEU:CD2	1:A:373:LEU:CD1	2.84	0.55
1:B:491:SER:CB	1:C:487:ILE:HD11	2.37	0.55
1:C:145:GLU:OE2	1:F:89:LYS:HE3	2.07	0.55
1:E:139:GLN:HG3	1:E:175:GLN:HE22	1.71	0.55
1:H:86:GLN:OE1	1:H:340:THR:OG1	2.23	0.55
1:A:94:VAL:HG12	1:A:94:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLN:HB3	1:F:96:GLN:NE2	2.21	0.55
1:F:94:VAL:HG12	1:F:96:GLN:NE2	2.22	0.55
1:D:180:VAL:HG13	1:D:190:ALA:CB	2.37	0.55
1:G:393:LEU:HD22	1:G:398:PHE:CE1	2.41	0.55
1:B:374:GLN:O	1:H:96:GLN:HG3	2.07	0.55
1:B:491:SER:HA	1:C:487:ILE:HD11	1.87	0.55
1:E:193:ILE:HB	1:E:234:LEU:HD22	1.87	0.55
1:H:449:ALA:HB1	1:H:484:ILE:HG22	1.89	0.55
1:C:407:GLU:OE2	1:C:429:ALA:HB3	2.07	0.55
1:F:369:LEU:HD23	1:F:369:LEU:O	2.06	0.55
1:F:267:VAL:HG21	1:F:338:LEU:HD11	1.88	0.54
1:C:376:ASP:HB2	1:C:425:VAL:HG22	1.89	0.54
1:F:123:LEU:HD13	1:F:130:PRO:HG3	1.90	0.54
1:G:386:VAL:HG12	1:G:390:LEU:HD22	1.88	0.54
1:B:487:ILE:HD11	1:C:491:SER:O	2.07	0.54
1:C:133:LEU:HD12	1:C:254:ALA:HA	1.90	0.54
1:C:400:SER:O	1:C:400:SER:OG	2.25	0.54
1:G:68:ARG:O	1:G:71:VAL:N	2.39	0.54
1:A:360:ILE:HD11	1:A:393:LEU:HD13	1.90	0.54
1:C:160:THR:HG22	1:C:160:THR:O	2.08	0.54
1:C:180:VAL:HG13	1:C:190:ALA:HB3	1.89	0.54
1:F:240:THR:CG2	1:F:246:LEU:HD11	2.38	0.54
1:G:140:VAL:HG21	1:G:168:VAL:HG22	1.90	0.54
1:H:363:PHE:CE1	1:H:369:LEU:HD11	2.43	0.54
1:A:363:PHE:CG	1:A:369:LEU:HD12	2.43	0.54
1:F:133:LEU:C	1:F:133:LEU:CD2	2.75	0.54
1:C:486:ASP:HB3	1:C:489:THR:HG23	1.89	0.54
1:E:84:VAL:CG2	1:H:78:ILE:CG2	2.81	0.54
1:G:472:TYR:CD2	1:G:494:VAL:HG13	2.43	0.54
1:D:198:PHE:CD1	1:D:214:ILE:HD13	2.42	0.54
1:G:393:LEU:CD2	1:G:398:PHE:CD1	2.91	0.54
1:G:400:SER:O	1:G:400:SER:OG	2.25	0.54
1:C:139:GLN:CB	1:F:96:GLN:HG3	2.38	0.53
1:F:244:GLN:HE21	1:F:245:MET:H	1.56	0.53
1:G:169:ARG:CD	1:G:245:MET:CE	2.87	0.53
1:A:140:VAL:HG12	1:A:141:ASN:N	2.24	0.53
1:E:84:VAL:HG21	1:H:78:ILE:HG21	1.84	0.53
1:C:113:LEU:HD23	1:C:113:LEU:O	2.08	0.53
1:D:94:VAL:HG23	1:E:147:GLN:HG3	1.89	0.53
1:D:193:ILE:CG2	1:D:234:LEU:CD1	2.86	0.53
1:H:327:ALA:HB2	1:H:347:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:SER:O	1:E:400:SER:OG	2.23	0.53
1:A:376:ASP:HB2	1:A:425:VAL:CG2	2.39	0.53
1:D:68:ARG:O	1:D:72:ILE:HD12	2.09	0.53
1:H:336:LYS:HG2	1:H:340:THR:CG2	2.39	0.53
1:B:379:ILE:HD13	1:B:386:VAL:HG22	1.90	0.53
1:H:197:VAL:HG21	1:H:234:LEU:CD2	2.34	0.53
1:E:393:LEU:HD22	1:E:398:PHE:CE1	2.44	0.53
1:E:473:LEU:HD13	1:E:478:VAL:CG2	2.39	0.53
1:H:86:GLN:OE1	1:H:340:THR:CA	2.56	0.53
1:A:77:ASN:ND2	1:A:335:GLN:NE2	2.57	0.53
1:B:370:ARG:HG3	1:B:386:VAL:HG11	1.90	0.53
1:D:140:VAL:HG12	1:D:141:ASN:N	2.22	0.53
1:D:379:ILE:HD11	1:D:423:LYS:HZ2	1.73	0.53
1:E:486:ASP:CB	1:E:489:THR:HG23	2.39	0.53
1:F:136:THR:HA	1:F:139:GLN:NE2	2.24	0.53
1:A:234:LEU:HD12	1:A:234:LEU:N	2.24	0.52
1:A:352:TYR:CD1	1:A:352:TYR:N	2.77	0.52
1:C:157:ILE:HD12	1:C:208:TYR:CZ	2.44	0.52
1:D:486:ASP:CB	1:D:489:THR:HG23	2.39	0.52
1:E:330:ASN:OD1	1:E:331:VAL:N	2.42	0.52
1:F:124:TYR:CG	1:F:188:VAL:HG13	2.44	0.52
1:B:94:VAL:HG12	1:B:96:GLN:HE21	1.75	0.52
1:C:457:ASN:ND2	1:C:457:ASN:N	2.54	0.52
1:D:124:TYR:CG	1:D:188:VAL:HG13	2.44	0.52
1:H:317:LEU:HD13	1:H:349:ARG:HA	1.91	0.52
1:F:203:LEU:HD12	1:F:208:TYR:CD2	2.44	0.52
1:F:473:LEU:CD1	1:F:477:LYS:O	2.57	0.52
1:F:386:VAL:HG13	1:F:390:LEU:HD22	1.91	0.52
1:E:87:TYR:HB3	1:H:75:LEU:HD13	1.90	0.52
1:H:212:GLY:O	1:H:248:VAL:HG13	2.10	0.52
1:B:78:ILE:CG2	1:C:84:VAL:HG21	2.39	0.52
1:H:211:VAL:HG13	1:H:247:ASN:O	2.10	0.52
1:E:369:LEU:CD2	1:E:373:LEU:CD1	2.88	0.52
1:E:393:LEU:CD2	1:E:398:PHE:CD1	2.93	0.52
1:F:157:ILE:HD12	1:F:208:TYR:CZ	2.43	0.52
1:B:160:THR:HG22	1:B:160:THR:O	2.10	0.52
1:D:193:ILE:HB	1:D:234:LEU:CD1	2.37	0.52
1:E:240:THR:HG22	1:E:246:LEU:HD11	1.91	0.52
1:E:334:LEU:HD11	1:E:338:LEU:HD22	1.92	0.52
1:F:363:PHE:CD1	1:F:369:LEU:HD12	2.45	0.52
1:E:401:TYR:CE1	1:E:442:VAL:HG11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:479:LEU:HD12	1:H:480:PHE:H	1.75	0.52
1:A:407:GLU:HG3	1:A:427:SER:HB3	1.92	0.51
1:C:198:PHE:CD1	1:C:214:ILE:HD13	2.45	0.51
1:D:94:VAL:O	1:D:94:VAL:CG1	2.48	0.51
1:D:220:GLU:N	1:D:221:PRO:CD	2.74	0.51
1:E:107:ALA:HB1	1:E:271:GLU:OE1	2.10	0.51
1:E:222:ILE:CD1	1:E:234:LEU:HD11	2.40	0.51
1:E:354:LEU:HD21	1:E:439:VAL:HG23	1.93	0.51
1:F:94:VAL:HG12	1:F:96:GLN:CD	2.31	0.51
1:F:418:VAL:HG23	1:F:418:VAL:O	2.10	0.51
1:B:201:ASP:OD1	1:B:201:ASP:N	2.43	0.51
1:C:418:VAL:CG1	1:C:484:ILE:HG21	2.40	0.51
1:G:157:ILE:HD12	1:G:208:TYR:CZ	2.46	0.51
1:A:400:SER:O	1:A:400:SER:OG	2.24	0.51
1:E:124:TYR:CD1	1:E:188:VAL:HG13	2.44	0.51
1:F:486:ASP:CB	1:F:489:THR:HG23	2.40	0.51
1:H:418:VAL:HG21	1:H:493:LEU:CD1	2.33	0.51
1:B:68:ARG:O	1:B:72:ILE:CD1	2.58	0.51
1:B:354:LEU:HD21	1:B:439:VAL:CG2	2.40	0.51
1:E:213:ASN:C	1:E:213:ASN:ND2	2.61	0.51
1:H:484:ILE:HD11	1:H:493:LEU:HD22	1.91	0.51
1:A:133:LEU:HD12	1:A:134:HIS:N	2.25	0.51
1:G:88:LEU:HD22	1:G:92:THR:HG23	1.91	0.51
1:G:486:ASP:HB3	1:G:489:THR:HG23	1.91	0.51
1:D:203:LEU:HD22	1:D:208:TYR:CD2	2.45	0.51
1:F:487:ILE:HG21	1:G:495:GLU:OE2	2.11	0.51
1:G:197:VAL:HG12	1:G:198:PHE:CD2	2.46	0.51
1:G:376:ASP:HB2	1:G:425:VAL:HG22	1.91	0.51
1:A:369:LEU:HD23	1:A:373:LEU:CD1	2.41	0.51
1:D:240:THR:CG2	1:D:246:LEU:HD11	2.40	0.51
1:D:393:LEU:HD22	1:D:398:PHE:CD1	2.45	0.51
1:F:136:THR:HA	1:F:139:GLN:HE22	1.76	0.51
1:H:473:LEU:HD13	1:H:478:VAL:HG22	1.92	0.51
1:D:103:LYS:CE	1:D:251:ASP:OD1	2.55	0.51
1:F:91:PHE:HE1	1:F:126:VAL:HB	1.74	0.51
1:G:407:GLU:OE2	1:G:429:ALA:HB3	2.10	0.51
1:C:193:ILE:HB	1:C:234:LEU:CD2	2.40	0.51
1:D:317:LEU:HD13	1:D:349:ARG:HA	1.93	0.51
1:G:124:TYR:CD1	1:G:188:VAL:HG13	2.45	0.51
1:C:235:THR:HB	1:C:237:LEU:HD22	1.93	0.50
1:E:193:ILE:O	1:E:193:ILE:HG22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:HG22	1:C:84:VAL:HG21	1.93	0.50
1:F:124:TYR:CD2	1:F:188:VAL:HG22	2.46	0.50
1:F:288:ASN:HD22	1:F:438:ASN:CG	2.15	0.50
1:A:140:VAL:HG11	1:A:158:ARG:NH2	2.27	0.50
1:A:340:THR:HG23	1:A:343:GLY:H	1.75	0.50
1:D:107:ALA:HB1	1:D:271:GLU:OE1	2.11	0.50
1:E:465:PHE:CD1	1:H:465:PHE:CD1	2.99	0.50
1:F:197:VAL:HG11	1:F:234:LEU:HD13	1.92	0.50
1:A:393:LEU:HD22	1:A:398:PHE:CE1	2.46	0.50
1:B:193:ILE:HB	1:B:234:LEU:CD2	2.41	0.50
1:F:354:LEU:CD2	1:F:439:VAL:HG22	2.41	0.50
1:D:407:GLU:OE2	1:D:429:ALA:HB3	2.10	0.50
1:F:203:LEU:HD12	1:F:208:TYR:CE2	2.46	0.50
1:H:479:LEU:HD12	1:H:480:PHE:N	2.26	0.50
1:A:119:CYS:SG	1:A:334:LEU:HD23	2.51	0.50
1:A:220:GLU:N	1:A:221:PRO:CD	2.75	0.50
1:E:157:ILE:HD12	1:E:208:TYR:CZ	2.46	0.50
1:E:487:ILE:HD11	1:H:491:SER:CB	2.37	0.50
1:F:99:PHE:CE2	1:F:123:LEU:HD22	2.43	0.50
1:F:297:MET:HE1	1:F:307:LYS:CB	2.42	0.50
1:B:486:ASP:CB	1:B:489:THR:HG23	2.42	0.50
1:F:471:SER:CB	1:G:471:SER:HG	2.24	0.50
1:E:193:ILE:HB	1:E:234:LEU:CD2	2.41	0.50
1:F:94:VAL:HG11	1:F:96:GLN:HE22	1.76	0.50
1:H:267:VAL:HG21	1:H:338:LEU:CD2	2.40	0.50
1:A:376:ASP:HB2	1:A:425:VAL:HG22	1.94	0.49
1:B:487:ILE:HD11	1:C:491:SER:CA	2.41	0.49
1:D:211:VAL:HG13	1:D:247:ASN:O	2.11	0.49
1:E:109:ILE:HG21	1:E:175:GLN:HG3	1.94	0.49
1:F:214:ILE:HG13	1:F:248:VAL:HG11	1.94	0.49
1:A:240:THR:HG23	1:A:246:LEU:HD11	1.92	0.49
1:C:163:HIS:CE1	1:F:404:GLU:OE2	2.66	0.49
1:D:286:MET:HE2	1:D:347:MET:SD	2.52	0.49
1:D:469:GLN:HE21	1:D:483:GLY:H	1.60	0.49
1:H:102:ILE:HD13	1:H:334:LEU:HD21	1.94	0.49
1:H:157:ILE:HD12	1:H:208:TYR:CZ	2.47	0.49
1:H:201:ASP:N	1:H:201:ASP:OD1	2.44	0.49
1:D:337:GLU:O	1:D:339:PHE:N	2.45	0.49
1:E:103:LYS:CE	1:E:251:ASP:OD1	2.58	0.49
1:E:491:SER:HA	1:H:487:ILE:HD11	1.93	0.49
1:F:201:ASP:OD1	1:F:201:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:407:GLU:HG3	1:H:427:SER:HB3	1.93	0.49
1:B:354:LEU:CD2	1:B:439:VAL:CG2	2.91	0.49
1:C:393:LEU:CD2	1:C:398:PHE:CD1	2.96	0.49
1:F:140:VAL:HG11	1:F:158:ARG:NH2	2.27	0.49
1:F:269:LEU:HD21	1:F:334:LEU:HD13	1.94	0.49
1:F:407:GLU:HG3	1:F:427:SER:HB3	1.95	0.49
1:G:379:ILE:HD11	1:G:423:LYS:HZ2	1.76	0.49
1:H:421:LEU:HD22	1:H:443:LEU:HD21	1.94	0.49
1:B:393:LEU:HD22	1:B:398:PHE:CE1	2.48	0.49
1:E:139:GLN:HE21	1:E:175:GLN:NE2	2.10	0.49
1:E:220:GLU:N	1:E:221:PRO:CD	2.76	0.49
1:E:330:ASN:ND2	1:E:332:GLN:HE21	2.11	0.49
1:F:473:LEU:HD12	1:F:474:LYS:N	2.26	0.49
1:F:486:ASP:HB3	1:F:489:THR:HG23	1.94	0.49
1:C:139:GLN:HE21	1:C:175:GLN:CD	2.16	0.49
1:E:424:PHE:HE1	1:E:439:VAL:HG11	1.76	0.49
1:F:424:PHE:HE1	1:F:439:VAL:HG11	1.77	0.49
1:A:275:ILE:HG21	1:A:284:ILE:HD12	1.95	0.49
1:C:393:LEU:HD21	1:C:398:PHE:CG	2.47	0.49
1:F:124:TYR:CD1	1:F:188:VAL:HG13	2.47	0.49
1:G:370:ARG:HG3	1:G:386:VAL:CG1	2.38	0.49
1:H:124:TYR:CD2	1:H:188:VAL:HG22	2.48	0.49
1:B:379:ILE:HD11	1:B:423:LYS:NZ	2.28	0.49
1:C:133:LEU:HD22	1:C:133:LEU:C	2.33	0.49
1:D:431:TRP:CE2	1:D:436:THR:HG21	2.48	0.49
1:E:407:GLU:HG3	1:E:427:SER:HB3	1.95	0.49
1:G:369:LEU:HD23	1:G:369:LEU:C	2.31	0.49
1:G:393:LEU:HD21	1:G:398:PHE:CG	2.48	0.49
1:G:407:GLU:HG3	1:G:427:SER:HB3	1.95	0.49
1:D:88:LEU:HD22	1:D:92:THR:CG2	2.42	0.49
1:E:354:LEU:CD2	1:E:439:VAL:CG2	2.91	0.49
1:F:266:ILE:HD13	1:F:316:LEU:HD21	1.94	0.49
1:B:364:PRO:HB3	1:H:407:GLU:CD	2.33	0.49
1:E:393:LEU:HD21	1:E:398:PHE:CG	2.47	0.49
1:H:220:GLU:N	1:H:221:PRO:CD	2.76	0.49
1:A:393:LEU:HD11	1:A:411:ILE:HD13	1.95	0.48
1:F:74:LEU:O	1:F:78:ILE:HD12	2.13	0.48
1:A:172:PHE:CE2	1:A:237:LEU:HD21	2.47	0.48
1:B:393:LEU:CD2	1:B:398:PHE:CD1	2.96	0.48
1:B:479:LEU:HD22	1:B:497:PHE:HB2	1.95	0.48
1:C:407:GLU:HG3	1:C:427:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ILE:HD13	1:E:222:ILE:HG21	1.94	0.48
1:E:198:PHE:CD1	1:E:214:ILE:HD13	2.47	0.48
1:H:400:SER:O	1:H:400:SER:OG	2.23	0.48
1:A:113:LEU:C	1:A:113:LEU:CD2	2.81	0.48
1:B:472:TYR:CD2	1:B:494:VAL:HG13	2.48	0.48
1:C:331:VAL:HG13	1:C:332:GLN:N	2.29	0.48
1:C:469:GLN:HE21	1:C:483:GLY:N	2.11	0.48
1:E:87:TYR:HB3	1:H:75:LEU:CD1	2.43	0.48
1:F:495:GLU:HG3	1:G:487:ILE:CD1	2.40	0.48
1:G:169:ARG:NE	1:G:245:MET:HE1	2.28	0.48
1:A:95:SER:CB	1:A:97:GLN:O	2.61	0.48
1:A:136:THR:HG22	1:A:172:PHE:CZ	2.48	0.48
1:A:473:LEU:HD13	1:A:478:VAL:CG2	2.43	0.48
1:A:486:ASP:O	1:A:487:ILE:C	2.50	0.48
1:B:330:ASN:OD1	1:B:331:VAL:N	2.47	0.48
1:B:354:LEU:CD2	1:B:439:VAL:HG22	2.43	0.48
1:D:180:VAL:HG13	1:D:190:ALA:HB3	1.95	0.48
1:G:208:TYR:O	1:G:211:VAL:HG23	2.13	0.48
1:G:418:VAL:HG21	1:G:493:LEU:CD1	2.33	0.48
1:B:386:VAL:HG12	1:B:390:LEU:HD22	1.96	0.48
1:B:408:ALA:HB1	1:B:426:CYS:SG	2.53	0.48
1:B:491:SER:CA	1:C:487:ILE:HD11	2.43	0.48
1:C:275:ILE:HG21	1:C:284:ILE:HD12	1.96	0.48
1:C:386:VAL:HG13	1:C:390:LEU:HD13	1.95	0.48
1:E:136:THR:HG22	1:E:172:PHE:CZ	2.49	0.48
1:E:484:ILE:CD1	1:E:493:LEU:HD22	2.43	0.48
1:G:189:ARG:HG2	1:H:189:ARG:NH1	2.28	0.48
1:A:262:GLU:HA	1:A:320:LEU:CD2	2.43	0.48
1:B:84:VAL:HG12	1:B:85:GLU:N	2.29	0.48
1:B:407:GLU:OE2	1:B:429:ALA:HB3	2.13	0.48
1:E:210:LEU:N	1:E:210:LEU:HD12	2.29	0.48
1:E:473:LEU:HD13	1:E:478:VAL:HG22	1.96	0.48
1:G:222:ILE:CD1	1:G:234:LEU:HD21	2.43	0.48
1:D:82:ARG:HG2	1:D:86:GLN:HE21	1.77	0.48
1:H:473:LEU:HD12	1:H:477:LYS:O	2.14	0.48
1:C:417:ASN:O	1:C:418:VAL:HG22	2.14	0.48
1:D:113:LEU:HD23	1:D:113:LEU:O	2.13	0.48
1:D:486:ASP:HB3	1:D:489:THR:HG23	1.96	0.48
1:E:393:LEU:HD22	1:E:398:PHE:CD1	2.49	0.48
1:H:393:LEU:CD2	1:H:398:PHE:CG	2.97	0.48
1:A:77:ASN:ND2	1:A:335:GLN:HE21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLU:HG3	1:B:427:SER:HB3	1.95	0.48
1:D:456:GLU:OE2	1:D:473:LEU:HD21	2.13	0.48
1:E:334:LEU:CD1	1:E:338:LEU:HD22	2.44	0.48
1:G:116:LEU:HD13	1:G:179:LEU:HD11	1.95	0.48
1:G:244:GLN:HE21	1:G:245:MET:N	2.11	0.48
1:G:431:TRP:CE2	1:G:436:THR:HG21	2.49	0.48
1:B:173:LEU:HD22	1:B:194:THR:HG21	1.96	0.48
1:C:201:ASP:N	1:C:201:ASP:OD1	2.47	0.48
1:C:244:GLN:HE21	1:C:245:MET:N	2.12	0.48
1:E:262:GLU:HA	1:E:320:LEU:HD22	1.94	0.48
1:F:121:ALA:HA	1:F:188:VAL:HG21	1.95	0.48
1:H:84:VAL:HG12	1:H:85:GLU:N	2.28	0.48
1:A:331:VAL:HG13	1:A:332:GLN:N	2.29	0.47
1:D:99:PHE:CZ	1:D:338:LEU:HD22	2.48	0.47
1:D:486:ASP:O	1:D:487:ILE:C	2.52	0.47
1:F:453:VAL:HG12	1:F:454:VAL:N	2.29	0.47
1:H:97:GLN:HB3	1:H:264:LEU:HD22	1.96	0.47
1:H:266:ILE:CD1	1:H:316:LEU:HD21	2.43	0.47
1:H:276:ILE:HG23	1:H:281:GLY:O	2.14	0.47
1:A:88:LEU:HD22	1:A:92:THR:CG2	2.43	0.47
1:A:95:SER:HB2	1:A:97:GLN:O	2.14	0.47
1:G:449:ALA:HB1	1:G:484:ILE:HG22	1.97	0.47
1:A:275:ILE:CG2	1:A:284:ILE:HD12	2.44	0.47
1:A:431:TRP:CE2	1:A:436:THR:HG21	2.49	0.47
1:C:340:THR:HG23	1:C:343:GLY:H	1.79	0.47
1:D:121:ALA:HA	1:D:188:VAL:HG21	1.97	0.47
1:E:431:TRP:CE2	1:E:436:THR:HG21	2.48	0.47
1:E:442:VAL:HG22	1:E:445:ARG:HH12	1.79	0.47
1:G:393:LEU:HD22	1:G:398:PHE:CD1	2.49	0.47
1:E:340:THR:HG23	1:E:343:GLY:H	1.79	0.47
1:G:327:ALA:CB	1:G:347:MET:HE3	2.44	0.47
1:C:140:VAL:HG13	1:C:144:LEU:HD23	1.97	0.47
1:C:456:GLU:OE2	1:C:473:LEU:HD21	2.14	0.47
1:D:329:ILE:HD13	1:D:337:GLU:HB2	1.96	0.47
1:A:330:ASN:OD1	1:A:331:VAL:N	2.47	0.47
1:B:449:ALA:HB1	1:B:484:ILE:HG22	1.97	0.47
1:B:471:SER:HG	1:C:471:SER:CB	2.27	0.47
1:G:133:LEU:HD23	1:G:254:ALA:HA	1.96	0.47
1:A:201:ASP:OD1	1:A:201:ASP:N	2.48	0.47
1:A:318:ASP:O	1:A:319:TYR:HD1	1.98	0.47
1:D:303:LYS:O	1:D:306:THR:OG1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ILE:CG2	1:H:84:VAL:CG2	2.92	0.47
1:E:454:VAL:HG12	1:E:455:SER:N	2.29	0.47
1:H:363:PHE:CE1	1:H:369:LEU:CD1	2.97	0.47
1:H:457:ASN:H	1:H:457:ASN:ND2	2.12	0.47
1:H:473:LEU:HD12	1:H:474:LYS:O	2.14	0.47
1:B:126:VAL:O	1:C:68:ARG:HG2	2.15	0.47
1:C:220:GLU:N	1:C:221:PRO:CD	2.78	0.47
1:E:121:ALA:HA	1:E:188:VAL:HG21	1.97	0.47
1:G:68:ARG:O	1:G:69:SER:C	2.52	0.47
1:A:140:VAL:CG1	1:A:141:ASN:N	2.77	0.47
1:A:354:LEU:HD21	1:A:439:VAL:HG23	1.95	0.47
1:A:369:LEU:HD21	1:A:373:LEU:HD11	1.95	0.47
1:B:266:ILE:HD11	1:B:320:LEU:CD1	2.45	0.47
1:C:139:GLN:HB2	1:F:96:GLN:HG3	1.97	0.47
1:C:197:VAL:HG12	1:C:198:PHE:CG	2.49	0.47
1:D:472:TYR:CD2	1:D:494:VAL:HG13	2.50	0.47
1:F:426:CYS:SG	1:F:436:THR:HG22	2.55	0.47
1:G:372:ALA:O	1:G:375:ARG:HG2	2.15	0.47
1:C:372:ALA:O	1:C:375:ARG:HG2	2.15	0.47
1:D:407:GLU:HG3	1:D:427:SER:HB3	1.97	0.47
1:D:479:LEU:HD22	1:D:497:PHE:HB2	1.96	0.47
1:E:147:GLN:OE1	1:E:167:VAL:HG21	2.14	0.47
1:E:327:ALA:HB2	1:E:347:MET:CE	2.45	0.47
1:F:473:LEU:HD12	1:F:477:LYS:O	2.15	0.47
1:F:486:ASP:O	1:F:487:ILE:C	2.52	0.47
1:G:201:ASP:OD1	1:G:201:ASP:N	2.46	0.47
1:B:363:PHE:CD2	1:B:369:LEU:HD12	2.49	0.46
1:D:334:LEU:HD12	1:D:334:LEU:O	2.15	0.46
1:E:68:ARG:O	1:E:72:ILE:CD1	2.63	0.46
1:F:401:TYR:CE2	1:F:443:LEU:CD1	2.98	0.46
1:B:193:ILE:CB	1:B:234:LEU:HD22	2.45	0.46
1:C:473:LEU:HD12	1:C:477:LYS:O	2.16	0.46
1:G:197:VAL:HG12	1:G:198:PHE:CG	2.50	0.46
1:G:376:ASP:HB2	1:G:425:VAL:CG2	2.45	0.46
1:H:421:LEU:HD22	1:H:443:LEU:CD2	2.45	0.46
1:C:82:ARG:HG2	1:C:86:GLN:HE21	1.80	0.46
1:D:140:VAL:CG1	1:D:141:ASN:N	2.77	0.46
1:E:147:GLN:OE1	1:E:167:VAL:CG2	2.63	0.46
1:E:486:ASP:HB3	1:E:489:THR:HG23	1.96	0.46
1:A:472:TYR:CD2	1:A:494:VAL:HG13	2.51	0.46
1:E:77:ASN:HD21	1:E:335:GLN:NE2	2.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:GLN:NE2	1:F:245:MET:N	2.60	0.46
1:G:197:VAL:HG21	1:G:222:ILE:HD11	1.95	0.46
1:B:393:LEU:HD21	1:B:398:PHE:CG	2.50	0.46
1:D:379:ILE:CG2	1:D:386:VAL:HG23	2.40	0.46
1:F:73:GLN:HG2	1:F:335:GLN:OE1	2.15	0.46
1:H:193:ILE:HG22	1:H:193:ILE:O	2.15	0.46
1:C:240:THR:HG22	1:C:246:LEU:HD11	1.98	0.46
1:C:393:LEU:HD22	1:C:398:PHE:CE1	2.51	0.46
1:F:97:GLN:HB3	1:F:264:LEU:HD23	1.97	0.46
1:F:425:VAL:O	1:F:425:VAL:HG12	2.16	0.46
1:H:372:ALA:O	1:H:375:ARG:HG2	2.16	0.46
1:B:104:VAL:HG21	1:B:116:LEU:HD21	1.98	0.46
1:B:198:PHE:CD1	1:B:214:ILE:HD13	2.50	0.46
1:B:465:PHE:CD1	1:C:465:PHE:CD1	3.04	0.46
1:C:133:LEU:C	1:C:133:LEU:CD2	2.84	0.46
1:C:147:GLN:HG3	1:F:322:ARG:CB	2.40	0.46
1:C:379:ILE:HG21	1:C:386:VAL:CG2	2.40	0.46
1:D:372:ALA:O	1:D:375:ARG:HG2	2.16	0.46
1:F:417:ASN:N	1:F:417:ASN:OD1	2.49	0.46
1:G:266:ILE:HD13	1:G:316:LEU:CD2	2.43	0.46
1:G:340:THR:HG23	1:G:343:GLY:H	1.81	0.46
1:G:488:ASN:HD22	1:G:489:THR:N	2.13	0.46
1:B:402:ALA:HB2	1:B:409:VAL:HG22	1.98	0.46
1:B:431:TRP:CE2	1:B:436:THR:HG21	2.51	0.46
1:C:417:ASN:O	1:C:418:VAL:HG23	2.16	0.46
1:D:498:VAL:CG1	1:D:499:LYS:N	2.79	0.46
1:G:486:ASP:O	1:G:487:ILE:C	2.54	0.46
1:H:140:VAL:HG12	1:H:141:ASN:H	1.77	0.46
1:A:372:ALA:O	1:A:375:ARG:HG2	2.16	0.46
1:E:352:TYR:CD1	1:E:352:TYR:N	2.83	0.46
1:F:197:VAL:HG11	1:F:234:LEU:CD1	2.46	0.46
1:H:340:THR:CG2	1:H:342:SER:HB3	2.46	0.46
1:A:140:VAL:HG13	1:A:144:LEU:HD12	1.98	0.46
1:A:474:LYS:CE	1:A:501:CYS:SG	3.04	0.46
1:B:234:LEU:N	1:B:234:LEU:HD23	2.30	0.46
1:B:379:ILE:HD11	1:B:423:LYS:HZ3	1.79	0.46
1:F:267:VAL:HG21	1:F:338:LEU:CD1	2.46	0.46
1:E:240:THR:CG2	1:E:246:LEU:HD11	2.47	0.45
1:E:469:GLN:HE21	1:E:483:GLY:H	1.62	0.45
1:E:471:SER:CB	1:H:471:SER:HG	2.29	0.45
1:F:379:ILE:HD13	1:F:386:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:GLN:HB2	1:H:302:VAL:HG23	1.97	0.45
1:A:121:ALA:HA	1:A:188:VAL:HG21	1.98	0.45
1:C:188:VAL:HG11	1:C:231:LEU:HD12	1.98	0.45
1:C:421:LEU:HD13	1:C:443:LEU:HD21	1.98	0.45
1:F:372:ALA:O	1:F:375:ARG:HG2	2.16	0.45
1:G:417:ASN:OD1	1:G:417:ASN:N	2.50	0.45
1:B:116:LEU:HD12	1:B:116:LEU:O	2.16	0.45
1:B:329:ILE:HG22	1:B:330:ASN:N	2.31	0.45
1:D:257:LEU:HA	1:D:257:LEU:HD23	1.62	0.45
1:E:336:LYS:HG2	1:E:340:THR:HG21	1.99	0.45
1:E:372:ALA:O	1:E:375:ARG:HG2	2.16	0.45
1:G:147:GLN:OE1	1:G:167:VAL:HG21	2.16	0.45
1:G:197:VAL:HG12	1:G:198:PHE:N	2.30	0.45
1:C:197:VAL:HG12	1:C:198:PHE:CD2	2.52	0.45
1:F:73:GLN:OE1	1:F:118:SER:O	2.34	0.45
1:F:193:ILE:HG21	1:F:234:LEU:HD22	1.99	0.45
1:F:485:ASP:HB3	1:G:472:TYR:OH	2.17	0.45
1:A:68:ARG:O	1:A:72:ILE:CD1	2.65	0.45
1:A:160:THR:O	1:A:160:THR:HG22	2.16	0.45
1:A:234:LEU:N	1:A:234:LEU:CD1	2.80	0.45
1:A:491:SER:CA	1:D:487:ILE:HD11	2.44	0.45
1:G:88:LEU:HA	1:G:88:LEU:HD23	1.67	0.45
1:D:240:THR:HG22	1:D:246:LEU:HD11	1.98	0.45
1:D:277:ASN:OD1	1:D:301:TRP:CE2	2.70	0.45
1:D:417:ASN:OD1	1:D:417:ASN:N	2.49	0.45
1:F:203:LEU:HD13	1:F:203:LEU:O	2.17	0.45
1:F:456:GLU:OE2	1:F:473:LEU:HD21	2.17	0.45
1:G:173:LEU:N	1:G:173:LEU:CD2	2.79	0.45
1:H:88:LEU:HD12	1:H:88:LEU:HA	1.67	0.45
1:H:386:VAL:HG12	1:H:390:LEU:HD22	1.98	0.45
1:B:484:ILE:HD11	1:B:493:LEU:HD22	1.99	0.45
1:D:120:LEU:HA	1:D:123:LEU:HD12	1.97	0.45
1:E:88:LEU:CD2	1:E:92:THR:HG23	2.46	0.45
1:E:338:LEU:HD12	1:E:338:LEU:HA	1.76	0.45
1:E:354:LEU:CD2	1:E:439:VAL:HG23	2.46	0.45
1:E:365:SER:OG	1:E:368:ALA:HB3	2.17	0.45
1:E:412:VAL:HG13	1:E:420:THR:O	2.17	0.45
1:E:454:VAL:HG21	1:E:464:HIS:CD2	2.51	0.45
1:F:103:LYS:CE	1:F:251:ASP:OD1	2.60	0.45
1:H:303:LYS:O	1:H:306:THR:OG1	2.33	0.45
1:H:330:ASN:OD1	1:H:331:VAL:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HG2	1:A:86:GLN:HE21	1.82	0.45
1:A:84:VAL:HG21	1:D:78:ILE:CG2	2.47	0.45
1:D:201:ASP:OD1	1:D:201:ASP:N	2.49	0.45
1:H:417:ASN:O	1:H:418:VAL:HG23	2.15	0.45
1:H:486:ASP:CB	1:H:489:THR:HG23	2.46	0.45
1:A:473:LEU:HD13	1:A:478:VAL:HG22	1.97	0.45
1:B:410:ALA:HB1	1:B:421:LEU:HD11	1.98	0.45
1:B:474:LYS:CE	1:B:501:CYS:SG	3.05	0.45
1:G:74:LEU:HD11	1:G:87:TYR:CE2	2.51	0.45
1:G:240:THR:HG22	1:G:246:LEU:HD11	1.98	0.45
1:H:369:LEU:HD23	1:H:373:LEU:CD1	2.47	0.45
1:B:367:ASP:CG	1:H:323:SER:HB2	2.32	0.45
1:B:479:LEU:HD12	1:B:480:PHE:H	1.82	0.45
1:C:144:LEU:HD22	1:C:167:VAL:CG1	2.46	0.45
1:C:330:ASN:OD1	1:C:331:VAL:N	2.50	0.45
1:D:270:ASN:ND2	1:D:272:LYS:HG2	2.31	0.45
1:F:193:ILE:HB	1:F:234:LEU:HD22	1.98	0.45
1:H:180:VAL:HG13	1:H:190:ALA:CB	2.41	0.45
1:E:140:VAL:HG23	1:E:171:CYS:SG	2.56	0.44
1:E:267:VAL:CG2	1:E:338:LEU:CD1	2.79	0.44
1:H:425:VAL:O	1:H:425:VAL:HG12	2.17	0.44
1:B:354:LEU:HD13	1:B:442:VAL:HG21	1.99	0.44
1:B:426:CYS:SG	1:B:436:THR:HG22	2.57	0.44
1:B:488:ASN:HD22	1:B:489:THR:N	2.16	0.44
1:B:491:SER:HB3	1:C:487:ILE:HD11	1.99	0.44
1:D:88:LEU:HD22	1:D:92:THR:HG23	2.00	0.44
1:D:286:MET:CE	1:D:347:MET:HB3	2.47	0.44
1:F:266:ILE:HB	1:F:326:VAL:HG22	1.98	0.44
1:H:411:ILE:O	1:H:421:LEU:HD12	2.17	0.44
1:B:374:GLN:CD	1:H:97:GLN:HB2	2.37	0.44
1:C:124:TYR:CD2	1:C:188:VAL:HG22	2.52	0.44
1:C:469:GLN:NE2	1:C:483:GLY:H	2.13	0.44
1:E:417:ASN:OD1	1:E:417:ASN:N	2.50	0.44
1:F:133:LEU:HD11	1:F:253:ALA:HB3	1.99	0.44
1:F:275:ILE:CG2	1:F:284:ILE:HD12	2.48	0.44
1:A:86:GLN:OE1	1:A:432:LEU:HD13	2.17	0.44
1:B:337:GLU:HG2	1:B:340:THR:O	2.18	0.44
1:D:140:VAL:HG13	1:D:144:LEU:HD12	2.00	0.44
1:E:201:ASP:N	1:E:201:ASP:OD1	2.50	0.44
1:F:373:LEU:HA	1:F:373:LEU:HD23	1.75	0.44
1:G:369:LEU:C	1:G:369:LEU:CD2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:VAL:O	1:H:101:VAL:HG12	2.15	0.44
1:H:486:ASP:O	1:H:487:ILE:C	2.55	0.44
1:B:417:ASN:OD1	1:B:417:ASN:N	2.50	0.44
1:D:199:THR:HG22	1:D:215:LYS:HB3	1.99	0.44
1:D:337:GLU:C	1:D:339:PHE:N	2.71	0.44
1:E:113:LEU:O	1:E:113:LEU:HD23	2.17	0.44
1:G:266:ILE:HB	1:G:326:VAL:HG22	1.99	0.44
1:F:419:PRO:O	1:F:450:LEU:HD12	2.17	0.44
1:H:363:PHE:CD2	1:H:369:LEU:HD12	2.53	0.44
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.70	0.44
1:G:489:THR:O	1:G:493:LEU:HD13	2.18	0.44
1:A:474:LYS:O	1:A:475:GLY:C	2.56	0.44
1:B:387:ALA:CB	1:H:262:GLU:OE1	2.66	0.44
1:B:486:ASP:HB3	1:B:489:THR:HG23	2.00	0.44
1:E:91:PHE:CB	1:H:72:ILE:HD13	2.41	0.44
1:E:359:SER:OG	1:E:362:GLU:HB2	2.17	0.44
1:F:74:LEU:HD21	1:G:75:LEU:HD11	1.99	0.44
1:G:189:ARG:HE	1:G:189:ARG:HB3	1.64	0.44
1:A:386:VAL:HG13	1:A:390:LEU:HD22	1.98	0.44
1:A:393:LEU:CD2	1:A:398:PHE:CD1	3.00	0.44
1:B:139:GLN:OE1	1:B:139:GLN:N	2.49	0.44
1:E:275:ILE:HG21	1:E:284:ILE:HD12	2.00	0.44
1:F:244:GLN:NE2	1:F:245:MET:H	2.16	0.44
1:G:408:ALA:HB1	1:G:426:CYS:SG	2.57	0.44
1:B:124:TYR:CG	1:B:188:VAL:HG13	2.52	0.43
1:B:359:SER:OG	1:B:362:GLU:HB2	2.18	0.43
1:D:295:ASP:HA	1:D:298:LYS:HG2	2.00	0.43
1:A:327:ALA:HB2	1:A:347:MET:CE	2.48	0.43
1:A:418:VAL:HG21	1:A:493:LEU:CD1	2.45	0.43
1:B:479:LEU:HD12	1:B:480:PHE:N	2.33	0.43
1:C:193:ILE:HB	1:C:234:LEU:HD23	2.00	0.43
1:C:258:ALA:O	1:C:320:LEU:HD21	2.18	0.43
1:E:486:ASP:O	1:E:487:ILE:C	2.55	0.43
1:G:203:LEU:HD22	1:G:208:TYR:CE2	2.53	0.43
1:G:369:LEU:HD21	1:G:373:LEU:HD11	1.99	0.43
1:A:68:ARG:O	1:A:72:ILE:HD12	2.18	0.43
1:A:417:ASN:N	1:A:417:ASN:OD1	2.51	0.43
1:C:104:VAL:HG11	1:C:116:LEU:CD2	2.48	0.43
1:C:352:TYR:CE2	1:C:405:PRO:HG3	2.53	0.43
1:C:359:SER:OG	1:C:362:GLU:HB2	2.19	0.43
1:D:474:LYS:CE	1:D:501:CYS:SG	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:ASN:HA	1:D:491:SER:OG	2.19	0.43
1:F:359:SER:OG	1:F:362:GLU:HB2	2.17	0.43
1:G:74:LEU:CD1	1:G:87:TYR:CE2	3.02	0.43
1:G:456:GLU:OE2	1:G:473:LEU:HD21	2.19	0.43
1:G:488:ASN:HA	1:G:491:SER:OG	2.19	0.43
1:C:270:ASN:ND2	1:C:272:LYS:HB2	2.34	0.43
1:D:286:MET:HE3	1:D:347:MET:CB	2.48	0.43
1:D:365:SER:O	1:D:365:SER:OG	2.36	0.43
1:D:418:VAL:HG11	1:D:484:ILE:HD13	1.99	0.43
1:F:474:LYS:HD2	1:F:501:CYS:SG	2.58	0.43
1:H:73:GLN:OE1	1:H:118:SER:O	2.36	0.43
1:C:486:ASP:O	1:C:487:ILE:C	2.55	0.43
1:E:406:LEU:HD12	1:E:409:VAL:CG2	2.49	0.43
1:G:365:SER:O	1:G:365:SER:OG	2.36	0.43
1:H:73:GLN:CG	1:H:335:GLN:OE1	2.60	0.43
1:A:363:PHE:CE1	1:A:369:LEU:HD12	2.52	0.43
1:B:275:ILE:HG21	1:B:284:ILE:HD12	2.00	0.43
1:E:330:ASN:HD21	1:E:332:GLN:HE21	1.65	0.43
1:F:97:GLN:OE1	1:F:264:LEU:HD23	2.12	0.43
1:F:275:ILE:HG21	1:F:284:ILE:HD12	2.01	0.43
1:F:277:ASN:ND2	1:F:280:THR:OG1	2.52	0.43
1:F:338:LEU:HD12	1:F:338:LEU:HA	1.73	0.43
1:G:393:LEU:HD11	1:G:411:ILE:HD13	2.00	0.43
1:H:408:ALA:HB3	1:H:435:VAL:HG11	1.99	0.43
1:B:308:LEU:HD23	1:B:308:LEU:O	2.18	0.43
1:D:193:ILE:HG21	1:D:234:LEU:CD1	2.47	0.43
1:D:376:ASP:HB2	1:D:425:VAL:HG22	2.00	0.43
1:D:474:LYS:HD2	1:D:501:CYS:SG	2.58	0.43
1:F:401:TYR:CD2	1:F:443:LEU:CD1	3.01	0.43
1:H:474:LYS:CE	1:H:501:CYS:SG	3.06	0.43
1:B:393:LEU:CD2	1:B:398:PHE:CG	3.01	0.43
1:C:417:ASN:OD1	1:C:417:ASN:N	2.52	0.43
1:D:133:LEU:HD23	1:D:254:ALA:HA	2.01	0.43
1:D:279:SER:HB2	1:D:301:TRP:CD1	2.54	0.43
1:E:329:ILE:HG21	1:E:329:ILE:HD13	1.75	0.43
1:F:180:VAL:HG13	1:F:190:ALA:HB3	2.00	0.43
1:G:220:GLU:N	1:G:221:PRO:CD	2.82	0.43
1:H:97:GLN:HB3	1:H:264:LEU:CD2	2.48	0.43
1:A:359:SER:OG	1:A:362:GLU:HB2	2.18	0.43
1:C:139:GLN:CA	1:F:96:GLN:HE21	2.31	0.43
1:C:140:VAL:HG12	1:C:141:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ILE:HB	1:E:326:VAL:HG22	2.01	0.43
1:G:133:LEU:CD2	1:G:254:ALA:HA	2.49	0.43
1:G:338:LEU:HD12	1:G:338:LEU:HA	1.75	0.43
1:G:359:SER:OG	1:G:362:GLU:HB2	2.19	0.43
1:G:370:ARG:CG	1:G:386:VAL:HG11	2.43	0.43
1:H:139:GLN:OE1	1:H:139:GLN:N	2.52	0.43
1:A:363:PHE:CE1	1:A:369:LEU:CD1	3.01	0.43
1:A:474:LYS:HD2	1:A:501:CYS:SG	2.59	0.43
1:A:486:ASP:CB	1:A:489:THR:HG23	2.48	0.43
1:D:180:VAL:HG13	1:D:190:ALA:HB1	2.01	0.43
1:D:259:ARG:HG3	1:D:316:LEU:CD1	2.49	0.43
1:D:452:TRP:O	1:D:479:LEU:HD12	2.19	0.43
1:E:337:GLU:HG2	1:E:340:THR:O	2.19	0.43
1:G:474:LYS:CE	1:G:501:CYS:SG	3.07	0.43
1:G:474:LYS:HD2	1:G:501:CYS:SG	2.59	0.43
1:H:432:LEU:C	1:H:432:LEU:HD12	2.38	0.43
1:B:193:ILE:CG2	1:B:234:LEU:HD22	2.49	0.42
1:D:359:SER:OG	1:D:362:GLU:HB2	2.19	0.42
1:E:491:SER:HB3	1:H:487:ILE:HD11	2.00	0.42
1:F:136:THR:HG22	1:F:172:PHE:CZ	2.53	0.42
1:F:184:GLU:HA	1:F:188:VAL:O	2.19	0.42
1:F:297:MET:CE	1:F:307:LYS:HG2	2.48	0.42
1:G:418:VAL:CG2	1:G:493:LEU:HD11	2.37	0.42
1:H:173:LEU:N	1:H:173:LEU:HD23	2.33	0.42
1:A:354:LEU:HD12	1:A:438:ASN:ND2	2.34	0.42
1:B:372:ALA:O	1:B:375:ARG:HG2	2.18	0.42
1:B:474:LYS:HD2	1:B:501:CYS:SG	2.59	0.42
1:B:487:ILE:HD11	1:C:491:SER:HA	2.01	0.42
1:C:113:LEU:CD2	1:C:113:LEU:C	2.88	0.42
1:D:109:ILE:HG21	1:D:175:GLN:HG3	2.01	0.42
1:D:276:ILE:HG23	1:D:281:GLY:O	2.18	0.42
1:E:124:TYR:CG	1:E:188:VAL:HG13	2.54	0.42
1:E:275:ILE:CG2	1:E:284:ILE:HD12	2.49	0.42
1:E:365:SER:OG	1:E:365:SER:O	2.36	0.42
1:F:488:ASN:HD22	1:F:489:THR:N	2.17	0.42
1:G:203:LEU:HD22	1:G:208:TYR:CD2	2.54	0.42
1:H:365:SER:O	1:H:365:SER:OG	2.37	0.42
1:H:417:ASN:N	1:H:417:ASN:OD1	2.52	0.42
1:A:210:LEU:N	1:A:210:LEU:HD12	2.34	0.42
1:A:308:LEU:HA	1:A:308:LEU:HD12	1.78	0.42
1:B:365:SER:O	1:B:365:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:SER:O	1:C:365:SER:OG	2.36	0.42
1:F:390:LEU:HD12	1:F:390:LEU:HA	1.69	0.42
1:A:91:PHE:HE1	1:A:126:VAL:O	2.02	0.42
1:A:454:VAL:HG12	1:A:455:SER:N	2.34	0.42
1:E:390:LEU:HD12	1:E:390:LEU:HA	1.89	0.42
1:E:474:LYS:O	1:E:475:GLY:C	2.58	0.42
1:F:70:THR:HG23	1:F:122:PHE:CD1	2.53	0.42
1:F:123:LEU:HD21	1:F:338:LEU:HD23	2.00	0.42
1:H:431:TRP:CE2	1:H:436:THR:HG21	2.54	0.42
1:A:403:ASP:OD1	1:A:403:ASP:N	2.52	0.42
1:C:474:LYS:CE	1:C:501:CYS:SG	3.08	0.42
1:D:337:GLU:C	1:D:339:PHE:H	2.23	0.42
1:E:91:PHE:HB3	1:H:72:ILE:HD11	1.95	0.42
1:E:197:VAL:HG21	1:E:234:LEU:CD1	2.49	0.42
1:E:206:ASP:N	1:E:206:ASP:OD1	2.53	0.42
1:E:318:ASP:O	1:E:319:TYR:HD1	2.02	0.42
1:F:84:VAL:HG21	1:G:78:ILE:HG22	2.02	0.42
1:H:376:ASP:HB2	1:H:425:VAL:HG22	2.00	0.42
1:H:474:LYS:O	1:H:475:GLY:C	2.58	0.42
1:A:401:TYR:CE1	1:A:442:VAL:HG11	2.55	0.42
1:B:470:GLY:HA3	1:B:481:TRP:CZ2	2.54	0.42
1:E:100:ALA:HA	1:E:265:LYS:O	2.19	0.42
1:E:474:LYS:CE	1:E:501:CYS:SG	3.07	0.42
1:F:119:CYS:HG	1:F:335:GLN:HB3	1.84	0.42
1:F:386:VAL:CG1	1:F:390:LEU:CD2	2.95	0.42
1:F:431:TRP:CE2	1:F:436:THR:HG21	2.54	0.42
1:H:342:SER:O	1:H:343:GLY:C	2.58	0.42
1:H:457:ASN:ND2	1:H:457:ASN:N	2.66	0.42
1:B:220:GLU:N	1:B:221:PRO:CD	2.83	0.42
1:C:104:VAL:HG11	1:C:116:LEU:HD21	2.02	0.42
1:C:234:LEU:HD12	1:C:257:LEU:HD11	2.02	0.42
1:G:184:GLU:HA	1:G:188:VAL:O	2.20	0.42
1:A:484:ILE:HG21	1:A:484:ILE:HD13	1.78	0.42
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.88	0.42
1:C:269:LEU:HD23	1:C:269:LEU:HA	1.81	0.42
1:C:337:GLU:HG2	1:C:340:THR:O	2.20	0.42
1:D:189:ARG:HE	1:D:189:ARG:HB3	1.67	0.42
1:D:330:ASN:OD1	1:D:331:VAL:N	2.52	0.42
1:E:386:VAL:CG1	1:E:390:LEU:HD22	2.49	0.42
1:F:140:VAL:HG12	1:F:141:ASN:H	1.79	0.42
1:G:208:TYR:HB3	1:G:211:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LEU:HB3	1:C:452:TRP:HB3	2.02	0.42
1:E:207:LYS:HB3	1:E:208:TYR:CD2	2.55	0.42
1:H:474:LYS:HD2	1:H:501:CYS:SG	2.59	0.42
1:H:479:LEU:HD22	1:H:497:PHE:HB2	2.02	0.42
1:A:406:LEU:HD12	1:A:409:VAL:CG2	2.50	0.42
1:B:316:LEU:HA	1:B:316:LEU:HD12	1.76	0.42
1:C:150:GLU:N	1:F:407:GLU:OE2	2.48	0.42
1:C:373:LEU:HD23	1:C:373:LEU:HA	1.83	0.42
1:C:458:ASP:O	1:C:459:ALA:C	2.57	0.42
1:C:474:LYS:HD2	1:C:501:CYS:SG	2.60	0.42
1:E:234:LEU:HD12	1:E:257:LEU:HD11	2.02	0.42
1:E:454:VAL:HG21	1:E:464:HIS:CG	2.54	0.42
1:F:139:GLN:HG3	1:F:175:GLN:HE22	1.85	0.42
1:F:393:LEU:HD21	1:F:398:PHE:CG	2.55	0.42
1:H:197:VAL:HG12	1:H:198:PHE:CD2	2.55	0.42
1:D:86:GLN:O	1:D:89:LYS:HB2	2.20	0.41
1:E:354:LEU:CD2	1:E:439:VAL:HG22	2.50	0.41
1:G:113:LEU:O	1:G:113:LEU:HD23	2.20	0.41
1:H:252:VAL:HG22	1:H:312:GLU:CD	2.40	0.41
1:H:354:LEU:HD21	1:H:439:VAL:HG22	2.02	0.41
1:H:486:ASP:HB3	1:H:489:THR:HG23	2.02	0.41
1:C:431:TRP:CE2	1:C:436:THR:HG21	2.55	0.41
1:E:184:GLU:HA	1:E:188:VAL:O	2.19	0.41
1:F:474:LYS:CE	1:F:501:CYS:SG	3.08	0.41
1:A:469:GLN:NE2	1:A:483:GLY:H	2.17	0.41
1:B:130:PRO:HG2	1:B:231:LEU:HD22	2.02	0.41
1:D:474:LYS:O	1:D:475:GLY:C	2.59	0.41
1:F:203:LEU:C	1:F:203:LEU:CD1	2.89	0.41
1:G:116:LEU:CD1	1:G:179:LEU:HD11	2.49	0.41
1:H:386:VAL:HG13	1:H:390:LEU:HD22	2.00	0.41
1:B:211:VAL:HG13	1:B:247:ASN:O	2.20	0.41
1:C:379:ILE:HD11	1:C:423:LYS:NZ	2.35	0.41
1:E:133:LEU:HD23	1:E:254:ALA:HA	2.02	0.41
1:F:421:LEU:HB3	1:F:452:TRP:HB3	2.02	0.41
1:G:337:GLU:HG2	1:G:340:THR:O	2.20	0.41
1:H:488:ASN:HD22	1:H:489:THR:N	2.18	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.70	0.41
1:B:443:LEU:HA	1:B:443:LEU:HD12	1.66	0.41
1:C:121:ALA:HA	1:C:188:VAL:HG21	2.01	0.41
1:D:393:LEU:HA	1:D:393:LEU:HD23	1.67	0.41
1:F:113:LEU:HD23	1:F:113:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:THR:HG22	1:G:172:PHE:CZ	2.56	0.41
1:G:470:GLY:HA3	1:G:481:TRP:CZ2	2.56	0.41
1:H:403:ASP:OD1	1:H:403:ASP:N	2.53	0.41
1:H:456:GLU:OE2	1:H:473:LEU:HD21	2.20	0.41
1:B:86:GLN:O	1:B:89:LYS:HB2	2.20	0.41
1:B:370:ARG:NH1	1:H:323:SER:OG	2.52	0.41
1:E:375:ARG:HA	1:E:375:ARG:HD2	1.96	0.41
1:G:372:ALA:O	1:G:425:VAL:HG11	2.20	0.41
1:H:379:ILE:HD11	1:H:423:LYS:NZ	2.36	0.41
1:A:354:LEU:HD21	1:A:439:VAL:CG2	2.50	0.41
1:B:474:LYS:O	1:B:475:GLY:C	2.59	0.41
1:D:244:GLN:HE21	1:D:245:MET:N	2.18	0.41
1:F:144:LEU:CD2	1:F:167:VAL:HG11	2.49	0.41
1:F:189:ARG:HE	1:F:189:ARG:HB3	1.65	0.41
1:G:100:ALA:HA	1:G:265:LYS:O	2.21	0.41
1:A:337:GLU:HG2	1:A:340:THR:O	2.20	0.41
1:A:386:VAL:CG1	1:A:390:LEU:HD22	2.51	0.41
1:B:488:ASN:HA	1:B:491:SER:OG	2.21	0.41
1:E:369:LEU:HD21	1:E:373:LEU:HD11	2.00	0.41
1:E:401:TYR:CD1	1:E:442:VAL:HG11	2.56	0.41
1:F:70:THR:HG23	1:F:122:PHE:HD1	1.86	0.41
1:F:407:GLU:HG3	1:F:430:ALA:HB2	2.03	0.41
1:F:443:LEU:HA	1:F:443:LEU:HD12	1.80	0.41
1:A:91:PHE:O	1:D:68:ARG:NH1	2.53	0.41
1:A:458:ASP:O	1:A:459:ALA:C	2.58	0.41
1:B:124:TYR:CD1	1:B:188:VAL:HG13	2.56	0.41
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.90	0.41
1:B:404:GLU:N	1:B:405:PRO:CD	2.84	0.41
1:B:473:LEU:HD13	1:B:478:VAL:HG23	2.03	0.41
1:C:322:ARG:HD3	1:C:352:TYR:CZ	2.56	0.41
1:D:120:LEU:HD23	1:D:120:LEU:HA	1.66	0.41
1:D:289:LEU:HD23	1:D:289:LEU:HA	1.94	0.41
1:D:404:GLU:N	1:D:405:PRO:CD	2.83	0.41
1:E:84:VAL:CG2	1:H:78:ILE:HG21	2.47	0.41
1:F:329:ILE:HG22	1:F:330:ASN:N	2.36	0.41
1:F:365:SER:O	1:F:365:SER:OG	2.35	0.41
1:F:472:TYR:CD2	1:F:494:VAL:HG13	2.56	0.41
1:G:330:ASN:OD1	1:G:331:VAL:N	2.54	0.41
1:G:393:LEU:CD2	1:G:398:PHE:CG	3.04	0.41
1:H:99:PHE:CE2	1:H:123:LEU:HD22	2.56	0.41
1:H:121:ALA:HA	1:H:188:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:369:LEU:CD2	1:H:373:LEU:CD1	2.97	0.41
1:A:183:LEU:HD13	1:A:190:ALA:HB2	2.03	0.41
1:A:379:ILE:HD13	1:A:379:ILE:HG21	1.85	0.41
1:B:214:ILE:HG13	1:B:248:VAL:HG11	2.01	0.41
1:E:470:GLY:HA3	1:E:481:TRP:CZ2	2.56	0.41
1:H:133:LEU:HD12	1:H:254:ALA:HA	2.02	0.41
1:B:144:LEU:HD12	1:B:149:ILE:CG2	2.51	0.40
1:E:71:VAL:HG13	1:H:74:LEU:CD2	2.52	0.40
1:E:102:ILE:HG21	1:E:102:ILE:HD13	1.76	0.40
1:E:184:GLU:OE1	1:F:228:ALA:HB1	2.21	0.40
1:E:257:LEU:HD23	1:E:257:LEU:HA	1.79	0.40
1:E:316:LEU:HD12	1:E:316:LEU:HA	1.66	0.40
1:H:404:GLU:N	1:H:405:PRO:CD	2.83	0.40
1:B:313:ILE:CD1	1:B:326:VAL:HG11	2.49	0.40
1:B:379:ILE:O	1:B:379:ILE:HG22	2.21	0.40
1:C:286:MET:HA	1:C:347:MET:O	2.21	0.40
1:C:360:ILE:HD11	1:C:393:LEU:HD13	2.03	0.40
1:C:474:LYS:O	1:C:475:GLY:C	2.58	0.40
1:D:286:MET:HG3	1:D:347:MET:HB3	2.03	0.40
1:E:191:ARG:HD2	1:E:225:SER:HB2	2.03	0.40
1:E:289:LEU:HD13	1:E:314:LYS:HA	2.02	0.40
1:E:328:ILE:HG21	1:E:328:ILE:HD13	1.64	0.40
1:E:374:GLN:HE21	1:E:374:GLN:HB3	1.76	0.40
1:F:193:ILE:HB	1:F:234:LEU:CD2	2.51	0.40
1:H:408:ALA:HB1	1:H:426:CYS:SG	2.61	0.40
1:A:172:PHE:CD2	1:A:237:LEU:HD21	2.56	0.40
1:B:403:ASP:OD1	1:B:403:ASP:N	2.54	0.40
1:D:104:VAL:HG22	1:D:269:LEU:HD12	2.03	0.40
1:D:303:LYS:HA	1:D:303:LYS:HD2	1.93	0.40
1:D:334:LEU:HD12	1:D:334:LEU:C	2.41	0.40
1:E:474:LYS:HD2	1:E:501:CYS:SG	2.61	0.40
1:F:379:ILE:HG21	1:F:386:VAL:CG2	2.37	0.40
1:F:418:VAL:HG21	1:F:493:LEU:CD1	2.49	0.40
1:H:359:SER:OG	1:H:362:GLU:HB2	2.21	0.40
1:A:113:LEU:HD23	1:A:113:LEU:C	2.39	0.40
1:B:165:MET:CE	1:B:245:MET:O	2.70	0.40
1:C:473:LEU:HD13	1:C:478:VAL:HG23	2.01	0.40
1:C:479:LEU:HD22	1:C:497:PHE:HB2	2.03	0.40
1:D:206:ASP:OD1	1:D:206:ASP:N	2.54	0.40
1:E:180:VAL:HG13	1:E:190:ALA:CB	2.47	0.40
1:G:375:ARG:HA	1:G:375:ARG:HD2	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:VAL:CG1	1:H:96:GLN:NE2	2.85	0.40
1:H:131:ILE:HD13	1:H:222:ILE:HG21	2.04	0.40
1:D:175:GLN:HE21	1:D:175:GLN:HB2	1.67	0.40
1:D:288:ASN:OD1	1:D:438:ASN:ND2	2.55	0.40
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.73	0.40
1:E:352:TYR:HE1	1:E:433:ASN:HD22	1.69	0.40
1:E:403:ASP:OD1	1:E:403:ASP:N	2.54	0.40
1:E:488:ASN:HA	1:E:491:SER:OG	2.21	0.40
1:F:288:ASN:ND2	1:F:438:ASN:ND2	2.55	0.40
1:G:72:ILE:HD12	1:G:72:ILE:N	2.35	0.40
1:G:206:ASP:OD1	1:G:206:ASP:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TYR:OH	1:G:495:GLU:OE2[1_546]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/464 (94%)	386 (89%)	44 (10%)	4 (1%)	17	54
1	B	434/464 (94%)	386 (89%)	44 (10%)	4 (1%)	17	54
1	C	434/464 (94%)	385 (89%)	45 (10%)	4 (1%)	17	54
1	D	434/464 (94%)	386 (89%)	44 (10%)	4 (1%)	17	54
1	E	434/464 (94%)	387 (89%)	43 (10%)	4 (1%)	17	54
1	F	434/464 (94%)	387 (89%)	43 (10%)	4 (1%)	17	54
1	G	434/464 (94%)	388 (89%)	42 (10%)	4 (1%)	17	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	434/464 (94%)	381 (88%)	46 (11%)	7 (2%)	9 44
All	All	3472/3712 (94%)	3086 (89%)	351 (10%)	35 (1%)	15 52

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	343	GLY
1	H	343	GLY
1	C	434	ASN
1	D	434	ASN
1	E	434	ASN
1	F	434	ASN
1	F	501	CYS
1	G	434	ASN
1	H	434	ASN
1	A	501	CYS
1	B	501	CYS
1	C	321	PRO
1	C	501	CYS
1	D	501	CYS
1	G	69	SER
1	H	98	GLN
1	H	501	CYS
1	B	98	GLN
1	B	475	GLY
1	E	501	CYS
1	H	69	SER
1	H	475	GLY
1	A	443	LEU
1	A	475	GLY
1	C	475	GLY
1	E	443	LEU
1	F	475	GLY
1	B	321	PRO
1	D	475	GLY
1	E	475	GLY
1	G	475	GLY
1	H	443	LEU
1	F	321	PRO
1	G	321	PRO
1	A	321	PRO

5.3.2 Protein sidechains (i)

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	372/397 (94%)	322 (87%)	50 (13%)	4	22
1	B	372/397 (94%)	322 (87%)	50 (13%)	4	22
1	C	373/397 (94%)	322 (86%)	51 (14%)	3	22
1	D	372/397 (94%)	316 (85%)	56 (15%)	3	18
1	E	373/397 (94%)	324 (87%)	49 (13%)	4	23
1	F	373/397 (94%)	323 (87%)	50 (13%)	4	22
1	G	373/397 (94%)	321 (86%)	52 (14%)	3	21
1	H	373/397 (94%)	316 (85%)	57 (15%)	2	17
All	All	2981/3176 (94%)	2566 (86%)	415 (14%)	3	21

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	68	ARG
1	A	78	ILE
1	A	113	LEU
1	A	116	LEU
1	A	140	VAL
1	A	157	ILE
1	A	171	CYS
1	A	172	PHE
1	A	174	GLU
1	A	175	GLN
1	A	195	SER
1	A	210	LEU
1	A	213	ASN
1	A	218	THR
1	A	220	GLU
1	A	239	GLU
1	A	246	LEU
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	286	MET
1	A	290	ASP
1	A	296	LEU
1	A	322	ARG
1	A	337	GLU
1	A	338	LEU
1	A	341	ASP
1	A	347	MET
1	A	349	ARG
1	A	365	SER
1	A	374	GLN
1	A	375	ARG
1	A	383	LYS
1	A	390	LEU
1	A	393	LEU
1	A	400	SER
1	A	432	LEU
1	A	434	ASN
1	A	440	PHE
1	A	445	ARG
1	A	453	VAL
1	A	455	SER
1	A	457	ASN
1	A	460	ASN
1	A	469	GLN
1	A	484	ILE
1	A	485	ASP
1	A	486	ASP
1	A	488	ASN
1	A	491	SER
1	A	498	VAL
1	B	67	THR
1	B	68	ARG
1	B	78	ILE
1	B	82	ARG
1	B	84	VAL
1	B	133	LEU
1	B	157	ILE
1	B	165	MET
1	B	171	CYS
1	B	172	PHE
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	195	SER
1	B	203	LEU
1	B	210	LEU
1	B	213	ASN
1	B	218	THR
1	B	220	GLU
1	B	239	GLU
1	B	248	VAL
1	B	264	LEU
1	B	286	MET
1	B	290	ASP
1	B	295	ASP
1	B	322	ARG
1	B	337	GLU
1	B	338	LEU
1	B	341	ASP
1	B	349	ARG
1	B	365	SER
1	B	375	ARG
1	B	383	LYS
1	B	390	LEU
1	B	393	LEU
1	B	400	SER
1	B	434	ASN
1	B	440	PHE
1	B	443	LEU
1	B	445	ARG
1	B	453	VAL
1	B	455	SER
1	B	457	ASN
1	B	460	ASN
1	B	469	GLN
1	B	484	ILE
1	B	485	ASP
1	B	486	ASP
1	B	487	ILE
1	B	488	ASN
1	B	491	SER
1	B	498	VAL
1	C	67	THR
1	C	68	ARG
1	C	82	ARG

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Mol	Chain	Res	Type
1	C	113	LEU
1	C	118	SER
1	C	133	LEU
1	C	140	VAL
1	C	157	ILE
1	C	171	CYS
1	C	172	PHE
1	C	174	GLU
1	C	175	GLN
1	C	195	SER
1	C	197	VAL
1	C	203	LEU
1	C	213	ASN
1	C	218	THR
1	C	220	GLU
1	C	239	GLU
1	C	264	LEU
1	C	286	MET
1	C	290	ASP
1	C	295	ASP
1	C	308	LEU
1	C	322	ARG
1	C	337	GLU
1	C	338	LEU
1	C	341	ASP
1	C	349	ARG
1	C	365	SER
1	C	375	ARG
1	C	383	LYS
1	C	391	ARG
1	C	393	LEU
1	C	400	SER
1	C	418	VAL
1	C	432	LEU
1	C	434	ASN
1	C	440	PHE
1	C	445	ARG
1	C	453	VAL
1	C	455	SER
1	C	457	ASN
1	C	460	ASN
1	C	469	GLN

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Mol	Chain	Res	Type
1	C	484	ILE
1	C	485	ASP
1	C	486	ASP
1	C	488	ASN
1	C	491	SER
1	C	498	VAL
1	D	67	THR
1	D	68	ARG
1	D	78	ILE
1	D	116	LEU
1	D	118	SER
1	D	140	VAL
1	D	157	ILE
1	D	167	VAL
1	D	171	CYS
1	D	172	PHE
1	D	175	GLN
1	D	195	SER
1	D	213	ASN
1	D	218	THR
1	D	220	GLU
1	D	246	LEU
1	D	260	VAL
1	D	264	LEU
1	D	282	GLU
1	D	283	LYS
1	D	286	MET
1	D	288	ASN
1	D	290	ASP
1	D	296	LEU
1	D	297	MET
1	D	299	GLN
1	D	308	LEU
1	D	322	ARG
1	D	323	SER
1	D	324	SER
1	D	337	GLU
1	D	338	LEU
1	D	347	MET
1	D	349	ARG
1	D	365	SER
1	D	375	ARG

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Mol	Chain	Res	Type
1	D	383	LYS
1	D	391	ARG
1	D	393	LEU
1	D	400	SER
1	D	417	ASN
1	D	434	ASN
1	D	440	PHE
1	D	443	LEU
1	D	445	ARG
1	D	453	VAL
1	D	455	SER
1	D	457	ASN
1	D	460	ASN
1	D	469	GLN
1	D	484	ILE
1	D	485	ASP
1	D	486	ASP
1	D	488	ASN
1	D	491	SER
1	D	498	VAL
1	E	67	THR
1	E	68	ARG
1	E	78	ILE
1	E	113	LEU
1	E	116	LEU
1	E	140	VAL
1	E	144	LEU
1	E	157	ILE
1	E	171	CYS
1	E	175	GLN
1	E	195	SER
1	E	213	ASN
1	E	218	THR
1	E	220	GLU
1	E	239	GLU
1	E	264	LEU
1	E	286	MET
1	E	290	ASP
1	E	295	ASP
1	E	322	ARG
1	E	331	VAL
1	E	337	GLU

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Mol	Chain	Res	Type
1	E	338	LEU
1	E	341	ASP
1	E	347	MET
1	E	349	ARG
1	E	355	VAL
1	E	365	SER
1	E	375	ARG
1	E	383	LYS
1	E	390	LEU
1	E	393	LEU
1	E	400	SER
1	E	417	ASN
1	E	434	ASN
1	E	440	PHE
1	E	443	LEU
1	E	445	ARG
1	E	453	VAL
1	E	455	SER
1	E	457	ASN
1	E	460	ASN
1	E	469	GLN
1	E	484	ILE
1	E	485	ASP
1	E	486	ASP
1	E	488	ASN
1	E	491	SER
1	E	498	VAL
1	F	67	THR
1	F	68	ARG
1	F	72	ILE
1	F	78	ILE
1	F	83	GLU
1	F	95	SER
1	F	98	GLN
1	F	113	LEU
1	F	118	SER
1	F	123	LEU
1	F	133	LEU
1	F	140	VAL
1	F	167	VAL
1	F	171	CYS
1	F	174	GLU

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Mol	Chain	Res	Type
1	F	175	GLN
1	F	195	SER
1	F	218	THR
1	F	220	GLU
1	F	239	GLU
1	F	264	LEU
1	F	290	ASP
1	F	295	ASP
1	F	296	LEU
1	F	308	LEU
1	F	322	ARG
1	F	337	GLU
1	F	338	LEU
1	F	341	ASP
1	F	349	ARG
1	F	365	SER
1	F	375	ARG
1	F	383	LYS
1	F	390	LEU
1	F	393	LEU
1	F	400	SER
1	F	434	ASN
1	F	440	PHE
1	F	443	LEU
1	F	445	ARG
1	F	455	SER
1	F	457	ASN
1	F	460	ASN
1	F	469	GLN
1	F	484	ILE
1	F	485	ASP
1	F	486	ASP
1	F	488	ASN
1	F	491	SER
1	F	498	VAL
1	G	67	THR
1	G	68	ARG
1	G	78	ILE
1	G	113	LEU
1	G	116	LEU
1	G	140	VAL
1	G	157	ILE

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Mol	Chain	Res	Type
1	G	171	CYS
1	G	172	PHE
1	G	173	LEU
1	G	175	GLN
1	G	195	SER
1	G	197	VAL
1	G	210	LEU
1	G	213	ASN
1	G	218	THR
1	G	220	GLU
1	G	239	GLU
1	G	264	LEU
1	G	286	MET
1	G	290	ASP
1	G	295	ASP
1	G	322	ARG
1	G	337	GLU
1	G	338	LEU
1	G	341	ASP
1	G	349	ARG
1	G	365	SER
1	G	375	ARG
1	G	383	LYS
1	G	390	LEU
1	G	391	ARG
1	G	393	LEU
1	G	400	SER
1	G	406	LEU
1	G	417	ASN
1	G	432	LEU
1	G	434	ASN
1	G	439	VAL
1	G	440	PHE
1	G	445	ARG
1	G	453	VAL
1	G	455	SER
1	G	457	ASN
1	G	460	ASN
1	G	469	GLN
1	G	484	ILE
1	G	485	ASP
1	G	486	ASP

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Mol	Chain	Res	Type
1	G	487	ILE
1	G	488	ASN
1	G	491	SER
1	H	67	THR
1	H	68	ARG
1	H	72	ILE
1	H	78	ILE
1	H	88	LEU
1	H	95	SER
1	H	98	GLN
1	H	113	LEU
1	H	118	SER
1	H	133	LEU
1	H	140	VAL
1	H	157	ILE
1	H	171	CYS
1	H	172	PHE
1	H	175	GLN
1	H	195	SER
1	H	203	LEU
1	H	213	ASN
1	H	218	THR
1	H	220	GLU
1	H	248	VAL
1	H	264	LEU
1	H	283	LYS
1	H	286	MET
1	H	288	ASN
1	H	290	ASP
1	H	299	GLN
1	H	308	LEU
1	H	322	ARG
1	H	323	SER
1	H	324	SER
1	H	337	GLU
1	H	338	LEU
1	H	347	MET
1	H	349	ARG
1	H	350	ARG
1	H	365	SER
1	H	375	ARG
1	H	383	LYS

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Mol	Chain	Res	Type
1	H	390	LEU
1	H	391	ARG
1	H	393	LEU
1	H	400	SER
1	H	432	LEU
1	H	434	ASN
1	H	440	PHE
1	H	445	ARG
1	H	453	VAL
1	H	455	SER
1	H	457	ASN
1	H	460	ASN
1	H	469	GLN
1	H	484	ILE
1	H	485	ASP
1	H	486	ASP
1	H	488	ASN
1	H	491	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	114	HIS
1	A	175	GLN
1	A	213	ASN
1	A	335	GLN
1	A	374	GLN
1	A	438	ASN
1	A	457	ASN
1	A	469	GLN
1	A	488	ASN
1	B	96	GLN
1	B	114	HIS
1	B	175	GLN
1	B	213	ASN
1	B	244	GLN
1	B	438	ASN
1	B	457	ASN
1	B	469	GLN
1	B	488	ASN
1	C	86	GLN

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Mol	Chain	Res	Type
1	C	114	HIS
1	C	175	GLN
1	C	213	ASN
1	C	244	GLN
1	C	374	GLN
1	C	457	ASN
1	C	469	GLN
1	C	488	ASN
1	D	86	GLN
1	D	114	HIS
1	D	175	GLN
1	D	213	ASN
1	D	244	GLN
1	D	247	ASN
1	D	299	GLN
1	D	374	GLN
1	D	438	ASN
1	D	469	GLN
1	D	488	ASN
1	E	77	ASN
1	E	97	GLN
1	E	114	HIS
1	E	175	GLN
1	E	213	ASN
1	E	332	GLN
1	E	374	GLN
1	E	433	ASN
1	E	438	ASN
1	E	457	ASN
1	E	469	GLN
1	E	488	ASN
1	F	96	GLN
1	F	114	HIS
1	F	175	GLN
1	F	213	ASN
1	F	244	GLN
1	F	277	ASN
1	F	288	ASN
1	F	374	GLN
1	F	438	ASN
1	F	488	ASN
1	G	86	GLN

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Mol	Chain	Res	Type
1	G	114	HIS
1	G	175	GLN
1	G	213	ASN
1	G	244	GLN
1	G	374	GLN
1	G	469	GLN
1	G	488	ASN
1	H	96	GLN
1	H	114	HIS
1	H	175	GLN
1	H	213	ASN
1	H	299	GLN
1	H	374	GLN
1	H	457	ASN
1	H	469	GLN
1	H	488	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	436/464 (93%)	-0.23	1 (0%)	95	94	52, 102, 194, 258	0
1	B	436/464 (93%)	-0.19	2 (0%)	91	87	63, 107, 191, 268	0
1	C	436/464 (93%)	-0.11	11 (2%)	57	49	76, 126, 279, 425	0
1	D	436/464 (93%)	-0.15	5 (1%)	80	74	72, 124, 202, 273	0
1	E	436/464 (93%)	-0.20	6 (1%)	75	68	49, 101, 184, 260	0
1	F	436/464 (93%)	-0.18	4 (0%)	84	79	54, 117, 194, 296	0
1	G	436/464 (93%)	-0.03	15 (3%)	45	37	74, 139, 214, 274	0
1	H	436/464 (93%)	-0.16	4 (0%)	84	79	70, 134, 211, 284	0
All	All	3488/3712 (93%)	-0.16	48 (1%)	75	68	49, 118, 210, 425	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	383	LYS	5.7
1	G	384	GLU	5.5
1	H	379	ILE	5.4
1	G	382	GLY	4.3
1	G	376	ASP	4.2
1	H	380	SER	3.8
1	G	379	ILE	3.7
1	C	373	LEU	3.7
1	B	147	GLN	3.4
1	F	376	ASP	3.3
1	G	380	SER	3.3
1	G	403	ASP	3.1
1	G	339	PHE	2.9
1	H	378	GLY	2.8
1	C	379	ILE	2.8
1	C	401	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	282	GLU	2.7
1	G	335	GLN	2.7
1	E	337	GLU	2.7
1	E	339	PHE	2.7
1	C	281	GLY	2.6
1	F	379	ILE	2.6
1	G	381	SER	2.5
1	C	279	SER	2.4
1	E	341	ASP	2.4
1	F	341	ASP	2.4
1	G	386	VAL	2.4
1	D	379	ILE	2.3
1	G	413	LYS	2.3
1	G	214	ILE	2.2
1	G	96	GLN	2.2
1	G	360	ILE	2.2
1	F	384	GLU	2.2
1	C	277	ASN	2.2
1	E	97	GLN	2.2
1	B	67	THR	2.2
1	A	338	LEU	2.1
1	C	369	LEU	2.1
1	D	152	ASP	2.1
1	E	91	PHE	2.1
1	H	352	TYR	2.1
1	D	502	ASP	2.0
1	D	300	SER	2.0
1	C	306	THR	2.0
1	C	424	PHE	2.0
1	D	154	ILE	2.0
1	E	502	ASP	2.0
1	C	356	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.