Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 08:30 PM EST

PDB ID	:	3HRI
Title	:	Histidyl-tRNA synthetase (apo) from Trypanosoma brucei
Authors	:	Arakaki, T.L.; Merritt, E.A.; Larson, E.T.; Medical Structural Genomics of Pathogenic Protozoa (MSGPP)
Deposited on	:	2009-06-09
Resolution	:	2.85 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 ⓘ 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 ⓘ) were used in the production of this report:

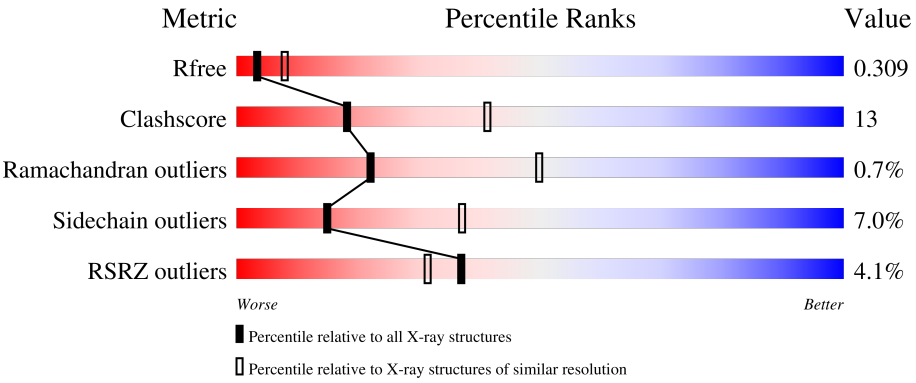
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	456	2% 61% 24% • 12%
1	B	456	3% 63% 22% • 13%
1	C	456	2% 63% 23% • 12%
1	D	456	6% 65% 21% • 13%
1	E	456	3% 63% 22% • 12%

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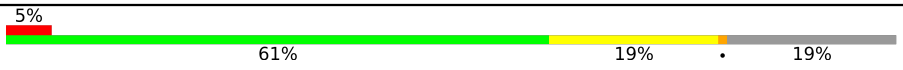
Mol	Chain	Length	Quality of chain
1	F	456	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18087 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 Histidyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	1	0
			3058	1958	518	565	17			
1	B	398	Total	C	N	O	S	0	1	0
			3036	1946	515	558	17			
1	C	400	Total	C	N	O	S	0	1	0
			3051	1953	517	564	17			
1	D	398	Total	C	N	O	S	0	1	0
			3036	1946	515	558	17			
1	E	401	Total	C	N	O	S	0	1	0
			3054	1956	518	563	17			
1	F	370	Total	C	N	O	S	0	1	0
			2852	1829	487	519	17			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q584V0
A	-21	ALA	-	expression tag	UNP Q584V0
A	-20	HIS	-	expression tag	UNP Q584V0
A	-19	HIS	-	expression tag	UNP Q584V0
A	-18	HIS	-	expression tag	UNP Q584V0
A	-17	HIS	-	expression tag	UNP Q584V0
A	-16	HIS	-	expression tag	UNP Q584V0
A	-15	HIS	-	expression tag	UNP Q584V0
A	-14	MET	-	expression tag	UNP Q584V0
A	-13	GLY	-	expression tag	UNP Q584V0
A	-12	THR	-	expression tag	UNP Q584V0
A	-11	LEU	-	expression tag	UNP Q584V0
A	-10	GLU	-	expression tag	UNP Q584V0
A	-9	ALA	-	expression tag	UNP Q584V0
A	-8	GLN	-	expression tag	UNP Q584V0
A	-7	THR	-	expression tag	UNP Q584V0
A	-6	GLN	-	expression tag	UNP Q584V0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q584V0
A	-4	PRO	-	expression tag	UNP Q584V0
A	-3	GLY	-	expression tag	UNP Q584V0
A	-2	SER	-	expression tag	UNP Q584V0
A	-1	MET	-	expression tag	UNP Q584V0
B	-22	MET	-	expression tag	UNP Q584V0
B	-21	ALA	-	expression tag	UNP Q584V0
B	-20	HIS	-	expression tag	UNP Q584V0
B	-19	HIS	-	expression tag	UNP Q584V0
B	-18	HIS	-	expression tag	UNP Q584V0
B	-17	HIS	-	expression tag	UNP Q584V0
B	-16	HIS	-	expression tag	UNP Q584V0
B	-15	HIS	-	expression tag	UNP Q584V0
B	-14	MET	-	expression tag	UNP Q584V0
B	-13	GLY	-	expression tag	UNP Q584V0
B	-12	THR	-	expression tag	UNP Q584V0
B	-11	LEU	-	expression tag	UNP Q584V0
B	-10	GLU	-	expression tag	UNP Q584V0
B	-9	ALA	-	expression tag	UNP Q584V0
B	-8	GLN	-	expression tag	UNP Q584V0
B	-7	THR	-	expression tag	UNP Q584V0
B	-6	GLN	-	expression tag	UNP Q584V0
B	-5	GLY	-	expression tag	UNP Q584V0
B	-4	PRO	-	expression tag	UNP Q584V0
B	-3	GLY	-	expression tag	UNP Q584V0
B	-2	SER	-	expression tag	UNP Q584V0
B	-1	MET	-	expression tag	UNP Q584V0
C	-22	MET	-	expression tag	UNP Q584V0
C	-21	ALA	-	expression tag	UNP Q584V0
C	-20	HIS	-	expression tag	UNP Q584V0
C	-19	HIS	-	expression tag	UNP Q584V0
C	-18	HIS	-	expression tag	UNP Q584V0
C	-17	HIS	-	expression tag	UNP Q584V0
C	-16	HIS	-	expression tag	UNP Q584V0
C	-15	HIS	-	expression tag	UNP Q584V0
C	-14	MET	-	expression tag	UNP Q584V0
C	-13	GLY	-	expression tag	UNP Q584V0
C	-12	THR	-	expression tag	UNP Q584V0
C	-11	LEU	-	expression tag	UNP Q584V0
C	-10	GLU	-	expression tag	UNP Q584V0
C	-9	ALA	-	expression tag	UNP Q584V0
C	-8	GLN	-	expression tag	UNP Q584V0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	THR	-	expression tag	UNP Q584V0
C	-6	GLN	-	expression tag	UNP Q584V0
C	-5	GLY	-	expression tag	UNP Q584V0
C	-4	PRO	-	expression tag	UNP Q584V0
C	-3	GLY	-	expression tag	UNP Q584V0
C	-2	SER	-	expression tag	UNP Q584V0
C	-1	MET	-	expression tag	UNP Q584V0
D	-22	MET	-	expression tag	UNP Q584V0
D	-21	ALA	-	expression tag	UNP Q584V0
D	-20	HIS	-	expression tag	UNP Q584V0
D	-19	HIS	-	expression tag	UNP Q584V0
D	-18	HIS	-	expression tag	UNP Q584V0
D	-17	HIS	-	expression tag	UNP Q584V0
D	-16	HIS	-	expression tag	UNP Q584V0
D	-15	HIS	-	expression tag	UNP Q584V0
D	-14	MET	-	expression tag	UNP Q584V0
D	-13	GLY	-	expression tag	UNP Q584V0
D	-12	THR	-	expression tag	UNP Q584V0
D	-11	LEU	-	expression tag	UNP Q584V0
D	-10	GLU	-	expression tag	UNP Q584V0
D	-9	ALA	-	expression tag	UNP Q584V0
D	-8	GLN	-	expression tag	UNP Q584V0
D	-7	THR	-	expression tag	UNP Q584V0
D	-6	GLN	-	expression tag	UNP Q584V0
D	-5	GLY	-	expression tag	UNP Q584V0
D	-4	PRO	-	expression tag	UNP Q584V0
D	-3	GLY	-	expression tag	UNP Q584V0
D	-2	SER	-	expression tag	UNP Q584V0
D	-1	MET	-	expression tag	UNP Q584V0
E	-22	MET	-	expression tag	UNP Q584V0
E	-21	ALA	-	expression tag	UNP Q584V0
E	-20	HIS	-	expression tag	UNP Q584V0
E	-19	HIS	-	expression tag	UNP Q584V0
E	-18	HIS	-	expression tag	UNP Q584V0
E	-17	HIS	-	expression tag	UNP Q584V0
E	-16	HIS	-	expression tag	UNP Q584V0
E	-15	HIS	-	expression tag	UNP Q584V0
E	-14	MET	-	expression tag	UNP Q584V0
E	-13	GLY	-	expression tag	UNP Q584V0
E	-12	THR	-	expression tag	UNP Q584V0
E	-11	LEU	-	expression tag	UNP Q584V0
E	-10	GLU	-	expression tag	UNP Q584V0

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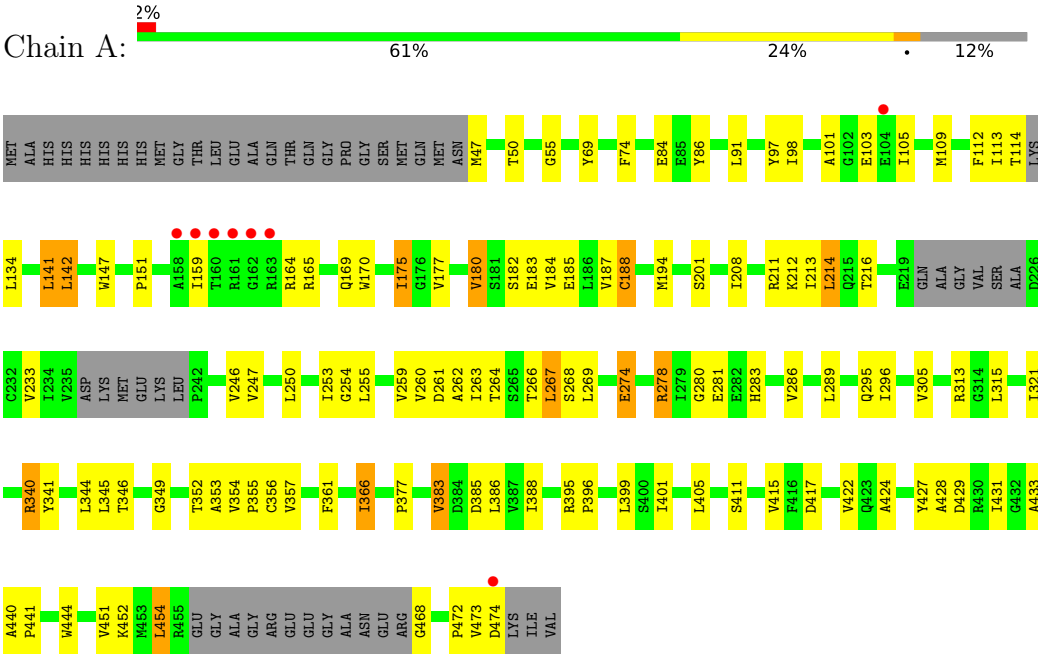
Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	ALA	-	expression tag	UNP Q584V0
E	-8	GLN	-	expression tag	UNP Q584V0
E	-7	THR	-	expression tag	UNP Q584V0
E	-6	GLN	-	expression tag	UNP Q584V0
E	-5	GLY	-	expression tag	UNP Q584V0
E	-4	PRO	-	expression tag	UNP Q584V0
E	-3	GLY	-	expression tag	UNP Q584V0
E	-2	SER	-	expression tag	UNP Q584V0
E	-1	MET	-	expression tag	UNP Q584V0
F	-22	MET	-	expression tag	UNP Q584V0
F	-21	ALA	-	expression tag	UNP Q584V0
F	-20	HIS	-	expression tag	UNP Q584V0
F	-19	HIS	-	expression tag	UNP Q584V0
F	-18	HIS	-	expression tag	UNP Q584V0
F	-17	HIS	-	expression tag	UNP Q584V0
F	-16	HIS	-	expression tag	UNP Q584V0
F	-15	HIS	-	expression tag	UNP Q584V0
F	-14	MET	-	expression tag	UNP Q584V0
F	-13	GLY	-	expression tag	UNP Q584V0
F	-12	THR	-	expression tag	UNP Q584V0
F	-11	LEU	-	expression tag	UNP Q584V0
F	-10	GLU	-	expression tag	UNP Q584V0
F	-9	ALA	-	expression tag	UNP Q584V0
F	-8	GLN	-	expression tag	UNP Q584V0
F	-7	THR	-	expression tag	UNP Q584V0
F	-6	GLN	-	expression tag	UNP Q584V0
F	-5	GLY	-	expression tag	UNP Q584V0
F	-4	PRO	-	expression tag	UNP Q584V0
F	-3	GLY	-	expression tag	UNP Q584V0
F	-2	SER	-	expression tag	UNP Q584V0
F	-1	MET	-	expression tag	UNP Q584V0

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.

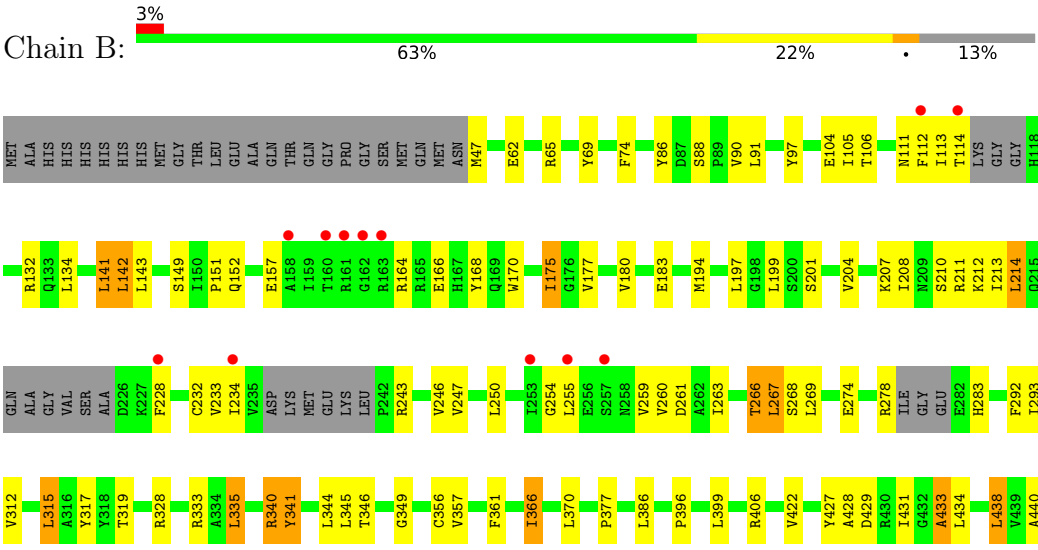
• Molecule 1: Histidyl-tRNA synthetase

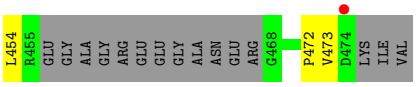
Chain A:



• Molecule 1: Histidyl-tRNA synthetase

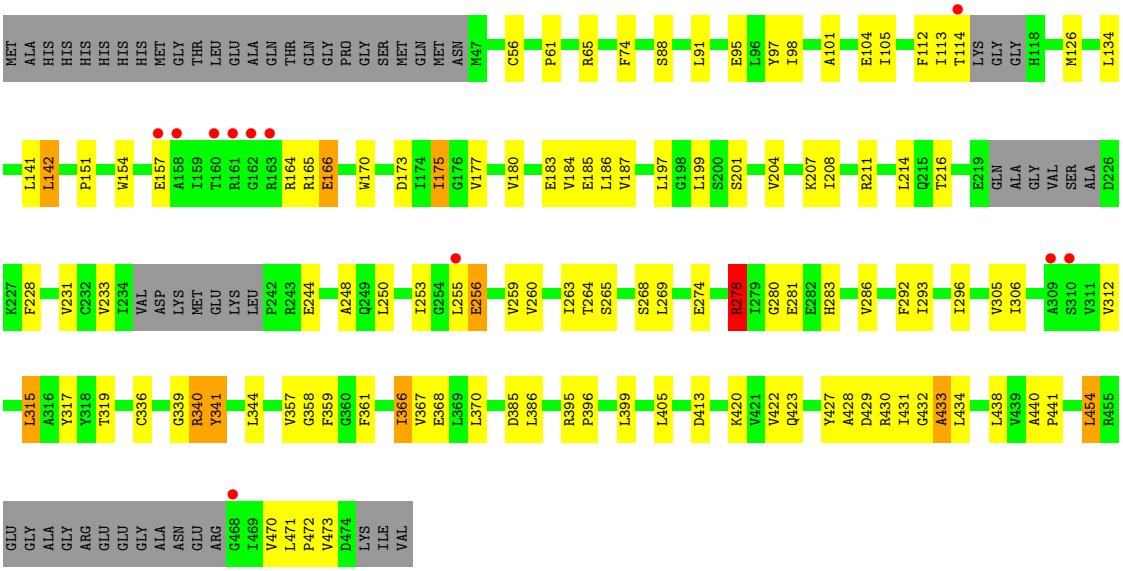
Chain B:





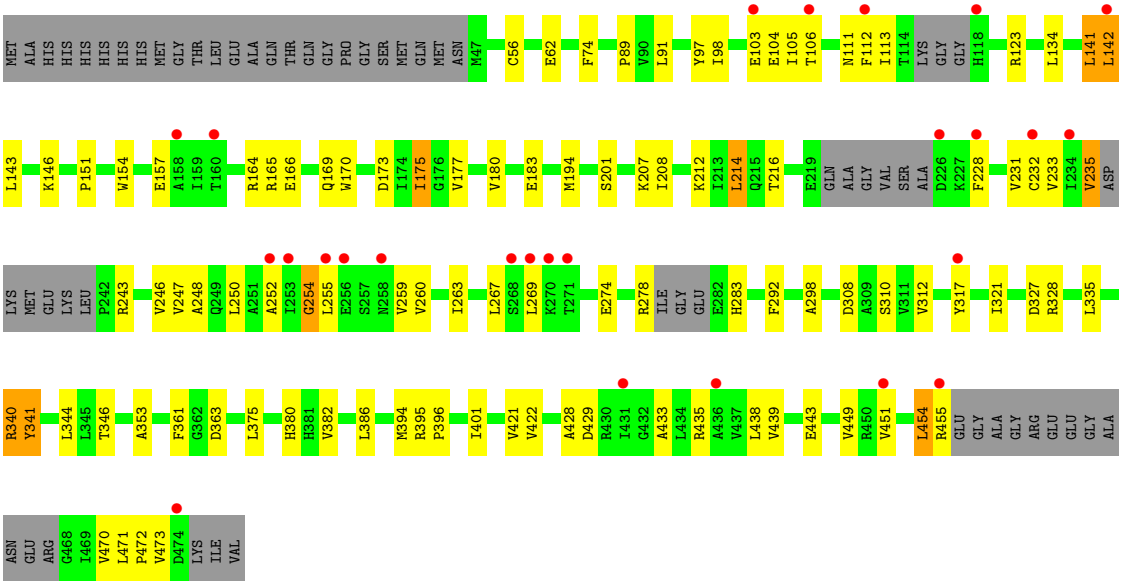
• Molecule 1: Histidyl-tRNA synthetase

Chain C:



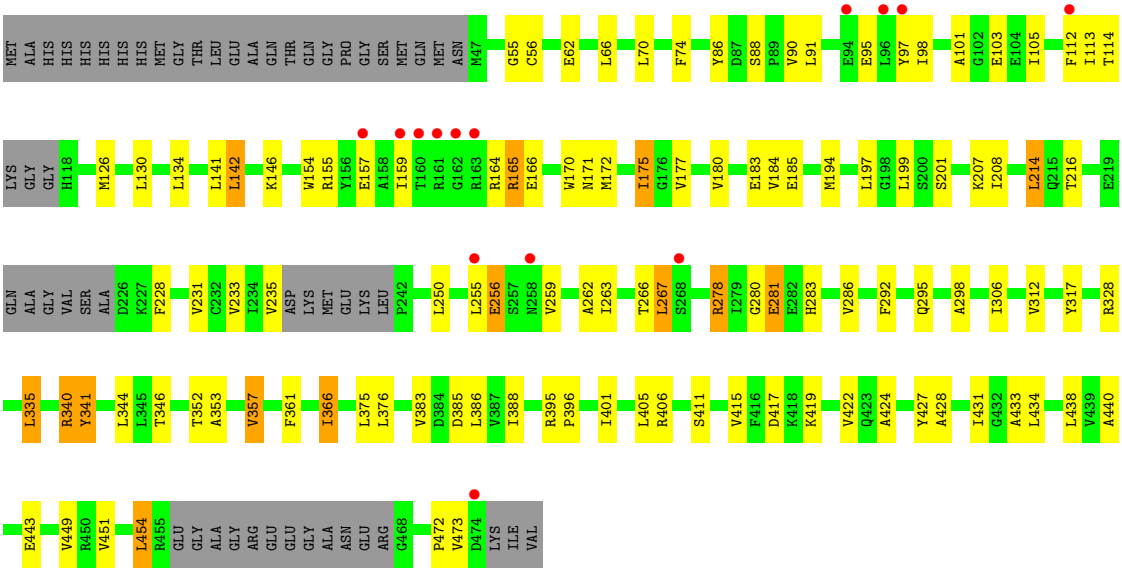
• Molecule 1: Histidyl-tRNA synthetase

Chain D:

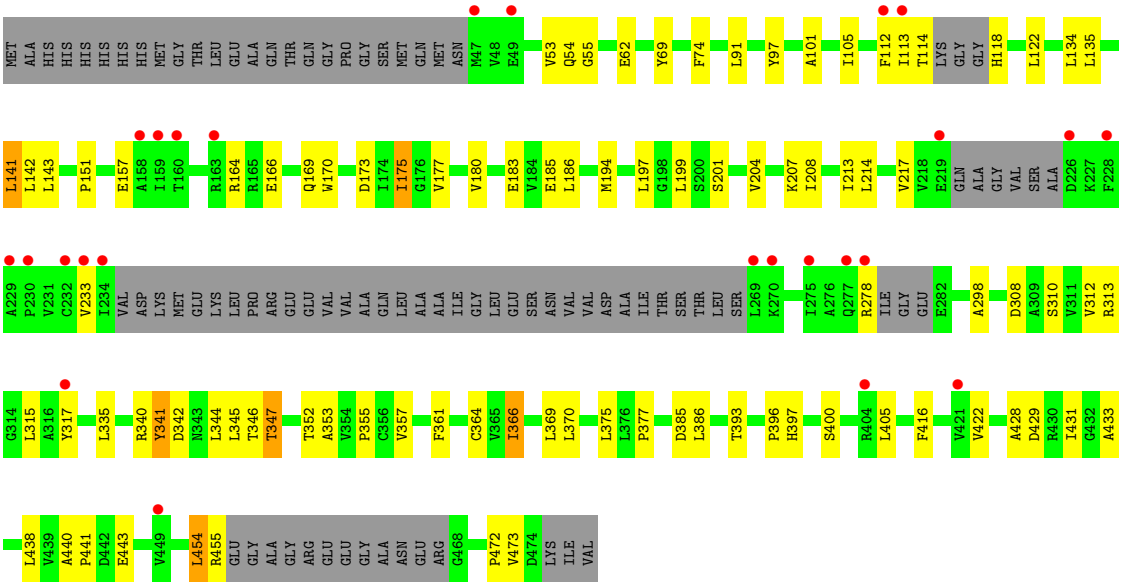


• Molecule 1: Histidyl-tRNA synthetase

Chain E:



• Molecule 1: Histidyl-tRNA synthetase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.61Å 98.38Å 251.97Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	35.00 – 2.85 63.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.00-2.85) 98.3 (63.88-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.272 , 0.313 0.270 , 0.309	Depositor DCC
R_{free} test set	4998 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	18087	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% 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

5.1 Standard geometry

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	0.54	1/3121 (0.0%)	0.64	0/4241
1	B	0.50	0/3098	0.61	0/4209
1	C	0.50	0/3114	0.63	0/4231
1	D	0.47	0/3098	0.59	0/4209
1	E	0.49	0/3117	0.62	0/4236
1	F	0.52	2/2913 (0.1%)	0.61	0/3953
All	All	0.50	3/18461 (0.0%)	0.62	0/25079

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	CYS	CB-SG	5.69	1.92	1.82
1	F	364[A]	CYS	CB-SG	5.55	1.91	1.82
1	F	364[B]	CYS	CB-SG	5.55	1.91	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3058	0	2959	95	0
1	B	3036	0	2943	82	0
1	C	3051	0	2950	85	0
1	D	3036	0	2943	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3054	0	2955	81	0
1	F	2852	0	2759	77	0
All	All	18087	0	17509	477	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 13.

All (477) 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:194:MET:HE2	1:F:335:LEU:HD23	1.36	1.06
1:A:386:LEU:HD23	1:A:428:ALA:HB2	1.49	0.93
1:F:194:MET:CE	1:F:335:LEU:HD23	1.97	0.93
1:B:433:ALA:HB1	1:B:454:LEU:HD22	1.58	0.86
1:D:141:LEU:CD1	1:D:175:ILE:HD11	2.06	0.86
1:B:250:LEU:HD12	1:B:260:VAL:HG13	1.61	0.83
1:C:433:ALA:HB1	1:C:454:LEU:HD22	1.62	0.82
1:D:228:PHE:CZ	1:D:263:ILE:HD13	2.16	0.81
1:F:207:LYS:C	1:F:208:ILE:HD12	2.00	0.81
1:B:134:LEU:HD22	1:B:175:ILE:HD13	1.62	0.81
1:C:134:LEU:HD22	1:C:175:ILE:HD13	1.64	0.80
1:C:256:GLU:O	1:C:260:VAL:HG23	1.80	0.79
1:A:247:VAL:HG22	1:A:260:VAL:HG11	1.63	0.79
1:C:265:SER:OG	1:C:278:ARG:NH2	2.16	0.79
1:A:262:ALA:O	1:A:266:THR:HG23	1.83	0.78
1:E:126:MET:HB3	1:E:171:ASN:OD1	1.82	0.78
1:C:197:LEU:HD13	1:C:370:LEU:HD11	1.66	0.77
1:C:386:LEU:HD23	1:C:428:ALA:HB2	1.66	0.77
1:E:228:PHE:CE1	1:E:250:LEU:HD22	2.20	0.77
1:D:386:LEU:HD23	1:D:428:ALA:HB2	1.66	0.76
1:F:431:ILE:HD12	1:F:431:ILE:O	1.85	0.76
1:F:177:VAL:O	1:F:340:ARG:NH2	2.17	0.76
1:B:91:LEU:HD11	1:B:112:PHE:HZ	1.50	0.76
1:A:177:VAL:O	1:A:340:ARG:NH2	2.19	0.75
1:D:177:VAL:O	1:D:340:ARG:NH2	2.19	0.74
1:A:142:LEU:HD23	1:A:142:LEU:H	1.53	0.73
1:B:177:VAL:O	1:B:340:ARG:NH2	2.22	0.73
1:E:281:GLU:HA	1:E:286:VAL:HG21	1.71	0.73
1:E:91:LEU:HD11	1:E:112:PHE:CZ	2.24	0.73
1:B:207:LYS:C	1:B:208:ILE:HD12	2.10	0.72
1:A:228:PHE:CE1	1:A:250:LEU:HD22	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:ILE:HD13	1:E:366:ILE:N	2.05	0.71
1:D:231:VAL:HG11	1:D:250:LEU:HD23	1.72	0.71
1:E:233:VAL:HG22	1:E:312:VAL:O	1.90	0.70
1:D:433:ALA:HB1	1:D:454:LEU:HD22	1.73	0.70
1:A:433:ALA:HB1	1:A:454:LEU:HD22	1.74	0.70
1:B:91:LEU:HD11	1:B:112:PHE:CZ	2.27	0.70
1:A:91:LEU:HD11	1:A:112:PHE:CZ	2.27	0.69
1:A:141:LEU:HD11	1:A:175:ILE:HD11	1.73	0.69
1:B:344:LEU:HG	1:B:345:LEU:HD23	1.74	0.69
1:C:228:PHE:CZ	1:C:263:ILE:HD13	2.28	0.69
1:F:440:ALA:HB3	1:F:443:GLU:OE1	1.93	0.69
1:F:134:LEU:HD22	1:F:175:ILE:HD13	1.75	0.69
1:B:233:VAL:HG22	1:B:312:VAL:O	1.94	0.68
1:D:214:LEU:HD21	1:D:267:LEU:HD11	1.74	0.68
1:D:134:LEU:HD13	1:D:175:ILE:HD12	1.75	0.68
1:D:248:ALA:O	1:D:252:ALA:HB2	1.94	0.67
1:F:386:LEU:HD23	1:F:428:ALA:HB2	1.77	0.67
1:E:177:VAL:O	1:E:340:ARG:NH2	2.28	0.66
1:B:386:LEU:HD23	1:B:428:ALA:HB2	1.77	0.66
1:A:141:LEU:CD1	1:A:175:ILE:HD11	2.24	0.66
1:C:422:VAL:CG2	1:F:375:LEU:HD23	2.25	0.66
1:E:386:LEU:HD23	1:E:428:ALA:HB2	1.77	0.66
1:F:386:LEU:CD2	1:F:428:ALA:HB2	2.25	0.66
1:D:134:LEU:HD22	1:D:141:LEU:HD11	1.76	0.66
1:C:253:ILE:O	1:C:253:ILE:HG22	1.94	0.66
1:E:146:LYS:HZ3	1:F:416:PHE:HZ	1.44	0.65
1:D:141:LEU:HD11	1:D:175:ILE:HD11	1.77	0.65
1:C:386:LEU:CD2	1:C:428:ALA:HB2	2.27	0.65
1:D:142:LEU:HD23	1:D:142:LEU:H	1.60	0.65
1:D:194:MET:CE	1:D:335:LEU:HD23	2.27	0.65
1:E:180:VAL:O	1:E:184:VAL:HG23	1.97	0.65
1:A:228:PHE:CZ	1:A:263:ILE:HD13	2.33	0.64
1:E:262:ALA:O	1:E:266:THR:HG23	1.98	0.64
1:F:433:ALA:HB1	1:F:454:LEU:HD23	1.79	0.64
1:E:101:ALA:HB3	1:E:105:ILE:HD13	1.80	0.63
1:A:134:LEU:HD13	1:A:175:ILE:HD12	1.81	0.63
1:B:212:LYS:O	1:B:216:THR:HG23	1.99	0.63
1:B:199:LEU:HD13	1:B:204:VAL:HG11	1.81	0.62
1:B:234:ILE:HG22	1:B:234:ILE:O	1.99	0.62
1:A:228:PHE:HZ	1:A:263:ILE:HG21	1.65	0.62
1:A:383:VAL:HG12	1:A:411:SER:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:ALA:HB1	1:C:454:LEU:CD2	2.28	0.62
1:C:134:LEU:HD22	1:C:175:ILE:CD1	2.29	0.61
1:A:280:GLY:O	1:A:286:VAL:HG21	2.00	0.61
1:B:134:LEU:HD22	1:B:175:ILE:CD1	2.29	0.61
1:C:470:VAL:O	1:C:471:LEU:HD23	2.00	0.61
1:D:235:VAL:CG2	1:D:246:VAL:HG21	2.31	0.61
1:E:134:LEU:HD22	1:E:175:ILE:HD13	1.82	0.61
1:A:216:THR:HG21	1:A:283:HIS:CE1	2.36	0.61
1:D:134:LEU:HD22	1:D:141:LEU:CD1	2.30	0.61
1:A:134:LEU:HD22	1:A:175:ILE:CD1	2.29	0.61
1:B:194:MET:CE	1:B:335:LEU:HD23	2.30	0.61
1:E:91:LEU:HD11	1:E:112:PHE:HZ	1.66	0.61
1:E:386:LEU:CD2	1:E:428:ALA:HB2	2.31	0.61
1:B:366:ILE:HD13	1:B:366:ILE:N	2.15	0.60
1:E:341:TYR:CE1	1:E:344:LEU:HD22	2.36	0.60
1:D:164:ARG:O	1:D:166:GLU:N	2.30	0.60
1:E:183:GLU:OE2	1:E:340:ARG:NH1	2.33	0.60
1:B:216:THR:HG21	1:B:283:HIS:CE1	2.35	0.60
1:D:170:TRP:HB3	1:D:361:PHE:HB3	1.83	0.60
1:C:280:GLY:O	1:C:286:VAL:HG21	2.01	0.60
1:C:170:TRP:HB3	1:C:361:PHE:HB3	1.84	0.60
1:C:255:LEU:HD23	1:C:259:VAL:HG13	1.84	0.59
1:D:207:LYS:C	1:D:208:ILE:HD12	2.23	0.59
1:B:194:MET:HE1	1:B:335:LEU:HD23	1.83	0.59
1:A:183:GLU:O	1:A:187:VAL:HG23	2.02	0.59
1:F:170:TRP:HB3	1:F:361:PHE:HB3	1.85	0.59
1:B:134:LEU:CD2	1:B:175:ILE:HD13	2.31	0.59
1:B:183:GLU:OE1	1:B:340:ARG:NH1	2.31	0.59
1:D:228:PHE:CE1	1:D:250:LEU:HD22	2.38	0.59
1:F:199:LEU:HD23	1:F:375:LEU:CD1	2.33	0.59
1:F:233:VAL:HG22	1:F:312:VAL:O	2.02	0.59
1:F:344:LEU:O	1:F:347:THR:HB	2.02	0.59
1:A:91:LEU:HD11	1:A:112:PHE:HZ	1.65	0.59
1:C:211:ARG:HB2	1:C:315:LEU:HD21	1.85	0.58
1:A:170:TRP:HB3	1:A:361:PHE:HB3	1.84	0.58
1:B:386:LEU:HD22	1:B:428:ALA:HA	1.85	0.58
1:E:142:LEU:H	1:E:142:LEU:HD23	1.69	0.58
1:D:91:LEU:HD11	1:D:112:PHE:CZ	2.39	0.58
1:A:366:ILE:N	1:A:366:ILE:HD13	2.19	0.57
1:E:170:TRP:CZ2	1:E:172:MET:SD	2.97	0.57
1:B:228:PHE:CZ	1:B:263:ILE:HD13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLY:O	1:B:255:LEU:HD12	2.03	0.57
1:E:183:GLU:HG3	1:E:357:VAL:HG11	1.87	0.57
1:E:298:ALA:HB1	1:F:396:PRO:O	2.04	0.57
1:E:366:ILE:HD13	1:E:366:ILE:H	1.68	0.56
1:F:91:LEU:HD11	1:F:112:PHE:CZ	2.39	0.56
1:F:194:MET:CE	1:F:335:LEU:CD2	2.78	0.56
1:E:97:TYR:C	1:E:105:ILE:HD11	2.26	0.56
1:F:69:TYR:CE1	1:F:377:PRO:HG3	2.40	0.56
1:A:101:ALA:HB3	1:A:105:ILE:HD13	1.88	0.56
1:A:134:LEU:HD22	1:A:175:ILE:HD13	1.88	0.56
1:D:386:LEU:CD2	1:D:428:ALA:HB2	2.34	0.56
1:B:293:ILE:HD12	1:B:294:THR:N	2.20	0.56
1:F:433:ALA:HB1	1:F:454:LEU:CD2	2.35	0.56
1:B:142:LEU:HD23	1:B:142:LEU:H	1.70	0.56
1:E:228:PHE:CD1	1:E:250:LEU:HD22	2.40	0.56
1:A:55:GLY:O	1:A:164:ARG:O	2.23	0.55
1:B:268:SER:O	1:B:269:LEU:HD23	2.06	0.55
1:A:214:LEU:CD2	1:A:267:LEU:HD11	2.36	0.55
1:F:134:LEU:HD13	1:F:175:ILE:HD13	1.88	0.55
1:A:246:VAL:O	1:A:250:LEU:HG	2.07	0.55
1:C:101:ALA:HB3	1:C:105:ILE:HD13	1.89	0.55
1:A:233:VAL:HG12	1:A:313:ARG:HH21	1.72	0.55
1:D:451:VAL:HG12	1:D:451:VAL:O	2.06	0.55
1:A:434:LEU:HD11	1:D:455:ARG:O	2.07	0.55
1:D:89:PRO:O	1:D:123:ARG:NH1	2.40	0.55
1:C:269:LEU:HD22	1:C:274:GLU:HG2	1.89	0.55
1:A:388:ILE:HD13	1:A:424:ALA:CB	2.37	0.55
1:A:395:ARG:HB3	1:A:396:PRO:HD3	1.89	0.54
1:C:233:VAL:HG22	1:C:312:VAL:O	2.07	0.54
1:A:159:ILE:HD11	1:A:165:ARG:HG3	1.89	0.54
1:D:98:ILE:HD11	1:D:103:GLU:HG2	1.88	0.54
1:F:91:LEU:HD12	1:F:122:LEU:HD23	1.88	0.54
1:D:233:VAL:HG22	1:D:312:VAL:O	2.07	0.54
1:E:216:THR:HG21	1:E:283:HIS:CE1	2.43	0.54
1:B:228:PHE:CE1	1:B:263:ILE:HD13	2.43	0.54
1:F:208:ILE:HD12	1:F:208:ILE:N	2.23	0.54
1:E:55:GLY:O	1:E:164:ARG:O	2.25	0.54
1:C:422:VAL:HG21	1:F:375:LEU:CD2	2.38	0.53
1:F:312:VAL:HG12	1:F:315:LEU:HD13	1.89	0.53
1:C:134:LEU:CD2	1:C:175:ILE:HD13	2.37	0.53
1:F:397:HIS:O	1:F:400:SER:OG	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:LEU:HD11	1:F:112:PHE:HZ	1.73	0.53
1:F:344:LEU:HG	1:F:345:LEU:HD23	1.89	0.53
1:C:126:MET:HG2	1:C:151:PRO:HG3	1.90	0.53
1:C:427:TYR:O	1:C:431:ILE:HG23	2.08	0.53
1:D:433:ALA:HB1	1:D:454:LEU:CD2	2.37	0.53
1:A:385:ASP:OD2	1:A:405:LEU:HD22	2.09	0.53
1:B:90:VAL:HG12	1:B:123:ARG:NH2	2.23	0.53
1:B:141:LEU:HD13	1:B:143:LEU:CD2	2.39	0.53
1:D:346:THR:HG23	1:D:353:ALA:HA	1.91	0.53
1:E:396:PRO:O	1:F:298:ALA:HB1	2.09	0.53
1:E:401:ILE:CD1	1:E:449:VAL:HG11	2.38	0.53
1:B:126:MET:HG2	1:B:151:PRO:HG3	1.89	0.53
1:A:98:ILE:HD11	1:A:103:GLU:HG2	1.89	0.53
1:D:134:LEU:HD13	1:D:175:ILE:CD1	2.38	0.53
1:E:383:VAL:HG12	1:E:411:SER:O	2.09	0.53
1:A:296:ILE:HG21	1:A:305:VAL:HG11	1.91	0.52
1:B:74:PHE:CD1	1:B:170:TRP:CE3	2.98	0.52
1:E:56:CYS:HG	1:E:154:TRP:HZ3	1.57	0.52
1:E:98:ILE:HD11	1:E:103:GLU:HG2	1.92	0.52
1:E:228:PHE:HZ	1:E:263:ILE:HG21	1.73	0.52
1:F:346:THR:HG23	1:F:353:ALA:HA	1.92	0.52
1:A:113:ILE:HG22	1:A:114:THR:N	2.24	0.52
1:D:56:CYS:HG	1:D:154:TRP:HZ3	1.58	0.52
1:E:231:VAL:HG21	1:E:250:LEU:HD23	1.90	0.52
1:A:296:ILE:HG21	1:A:305:VAL:CG1	2.39	0.52
1:A:182:SER:OG	1:A:357:VAL:HG21	2.09	0.52
1:A:194:MET:CE	1:A:335:LEU:HD23	2.40	0.52
1:D:113:ILE:N	1:D:113:ILE:HD12	2.25	0.52
1:F:386:LEU:HD22	1:F:428:ALA:CA	2.39	0.52
1:A:151:PRO:HD2	1:A:169:GLN:O	2.10	0.52
1:B:214:LEU:HD21	1:B:267:LEU:HD13	1.91	0.52
1:C:180:VAL:O	1:C:184:VAL:HG23	2.09	0.52
1:D:401:ILE:HD13	1:D:449:VAL:HG11	1.92	0.52
1:C:228:PHE:HE1	1:C:250:LEU:HD22	1.75	0.52
1:F:194:MET:HE1	1:F:335:LEU:CD2	2.40	0.51
1:D:216:THR:HG21	1:D:283:HIS:CE1	2.45	0.51
1:B:152:GLN:HB2	1:B:168:TYR:CE1	2.45	0.51
1:E:199:LEU:HD23	1:E:375:LEU:CD1	2.41	0.51
1:C:207:LYS:C	1:C:208:ILE:HD12	2.30	0.51
1:C:228:PHE:CE1	1:C:250:LEU:HD22	2.46	0.51
1:C:422:VAL:HG21	1:F:375:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:TYR:CE1	1:F:344:LEU:HD22	2.45	0.51
1:B:106:THR:O	1:B:111:ASN:ND2	2.39	0.51
1:A:211:ARG:HB2	1:A:315:LEU:HD21	1.93	0.51
1:E:214:LEU:HD21	1:E:267:LEU:CD1	2.40	0.51
1:B:97:TYR:C	1:B:105:ILE:HD11	2.31	0.51
1:E:184:VAL:HG11	1:E:295:GLN:HB3	1.93	0.51
1:A:228:PHE:HE1	1:A:250:LEU:HD22	1.74	0.50
1:D:401:ILE:CD1	1:D:449:VAL:HG11	2.41	0.50
1:F:101:ALA:HB3	1:F:105:ILE:HD13	1.93	0.50
1:B:366:ILE:HD13	1:B:366:ILE:H	1.75	0.50
1:C:250:LEU:HD12	1:C:260:VAL:HG13	1.94	0.50
1:F:141:LEU:HD13	1:F:143:LEU:HD23	1.92	0.50
1:E:97:TYR:O	1:E:105:ILE:HD11	2.11	0.50
1:A:214:LEU:HD21	1:A:267:LEU:HD11	1.93	0.50
1:C:231:VAL:HG11	1:C:250:LEU:HD23	1.93	0.50
1:F:180:VAL:HA	1:F:183:GLU:OE2	2.11	0.50
1:F:308:ASP:OD1	1:F:310:SER:OG	2.20	0.50
1:E:113:ILE:HD12	1:E:113:ILE:N	2.26	0.50
1:E:170:TRP:HB3	1:E:361:PHE:HB3	1.93	0.50
1:F:113:ILE:HG22	1:F:114:THR:N	2.27	0.50
1:A:454:LEU:CD1	1:A:454:LEU:N	2.74	0.50
1:B:255:LEU:HG	1:B:259:VAL:HG11	1.94	0.50
1:C:142:LEU:H	1:C:142:LEU:HD23	1.76	0.49
1:F:113:ILE:N	1:F:113:ILE:HD12	2.26	0.49
1:B:113:ILE:HD12	1:B:113:ILE:N	2.27	0.49
1:A:415:VAL:HG12	1:A:417:ASP:O	2.12	0.49
1:E:171:ASN:N	1:E:171:ASN:HD22	2.11	0.49
1:A:440:ALA:HB1	1:A:441:PRO:HD2	1.93	0.49
1:B:440:ALA:HB1	1:B:441:PRO:HD2	1.94	0.49
1:D:247:VAL:HG12	1:D:247:VAL:O	2.12	0.49
1:B:69:TYR:CE1	1:B:377:PRO:HG3	2.48	0.49
1:C:95:GLU:HA	1:C:98:ILE:HG22	1.94	0.49
1:F:207:LYS:O	1:F:208:ILE:HD12	2.13	0.49
1:A:433:ALA:HB1	1:A:454:LEU:CD2	2.40	0.49
1:D:454:LEU:CD1	1:D:454:LEU:N	2.76	0.49
1:A:74:PHE:CD1	1:A:170:TRP:CE3	3.01	0.49
1:A:183:GLU:HG2	1:A:321:ILE:HB	1.95	0.49
1:A:266:THR:HA	1:A:269:LEU:HG	1.95	0.49
1:C:97:TYR:O	1:C:105:ILE:HD11	2.13	0.49
1:C:341:TYR:CE1	1:C:344:LEU:HD22	2.48	0.48
1:A:134:LEU:CD2	1:A:175:ILE:HD13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:VAL:O	1:C:340:ARG:NH2	2.45	0.48
1:C:454:LEU:N	1:C:454:LEU:CD1	2.77	0.48
1:A:352:THR:O	1:A:354:VAL:HG23	2.14	0.48
1:C:340:ARG:HB2	1:C:357:VAL:HG22	1.95	0.48
1:F:197:LEU:HD13	1:F:370:LEU:HD11	1.95	0.48
1:A:212:LYS:O	1:A:216:THR:HG23	2.13	0.48
1:E:66:LEU:HD11	1:E:376:LEU:HD22	1.95	0.48
1:C:74:PHE:CD1	1:C:170:TRP:CE3	3.02	0.48
1:D:141:LEU:HD13	1:D:175:ILE:HD11	1.93	0.48
1:A:266:THR:HG22	1:A:278:ARG:CZ	2.43	0.48
1:C:427:TYR:CE1	1:C:431:ILE:HG21	2.48	0.48
1:C:472:PRO:N	1:C:473:VAL:HA	2.29	0.48
1:E:440:ALA:HB3	1:E:443:GLU:OE1	2.13	0.48
1:A:228:PHE:CD1	1:A:250:LEU:HD22	2.49	0.48
1:A:366:ILE:HD13	1:A:366:ILE:H	1.78	0.48
1:B:243:ARG:O	1:B:247:VAL:HG23	2.13	0.48
1:C:113:ILE:HG22	1:C:114:THR:N	2.28	0.48
1:F:385:ASP:OD2	1:F:405:LEU:HD13	2.14	0.48
1:A:388:ILE:HD13	1:A:424:ALA:HB3	1.96	0.48
1:C:396:PRO:O	1:D:298:ALA:HB1	2.13	0.48
1:D:243:ARG:O	1:D:247:VAL:HG23	2.13	0.48
1:A:47:MET:HA	1:B:349:GLY:HA3	1.95	0.47
1:B:197:LEU:HD13	1:B:370:LEU:HD11	1.96	0.47
1:D:134:LEU:HD22	1:D:175:ILE:CD1	2.43	0.47
1:E:207:LYS:HA	1:E:306:ILE:O	2.14	0.47
1:D:97:TYR:C	1:D:105:ILE:HD11	2.34	0.47
1:F:213:ILE:O	1:F:217:VAL:HG23	2.15	0.47
1:A:429:ASP:HA	1:A:433:ALA:HB2	1.96	0.47
1:B:217:VAL:HG21	1:B:266:THR:HG21	1.97	0.47
1:B:234:ILE:O	1:B:234:ILE:CG2	2.63	0.47
1:D:194:MET:SD	1:D:335:LEU:HD23	2.55	0.47
1:A:427:TYR:CE1	1:A:431:ILE:HG21	2.50	0.47
1:B:126:MET:CG	1:B:151:PRO:HG3	2.45	0.47
1:E:366:ILE:N	1:E:366:ILE:CD1	2.75	0.47
1:F:151:PRO:HD2	1:F:169:GLN:O	2.15	0.47
1:F:204:VAL:HG12	1:F:369:LEU:HD21	1.97	0.47
1:A:344:LEU:HG	1:A:345:LEU:HD23	1.97	0.46
1:F:97:TYR:C	1:F:105:ILE:HD11	2.35	0.46
1:F:186:LEU:HD12	1:F:357:VAL:HG12	1.96	0.46
1:C:187:VAL:HG21	1:C:292:PHE:HZ	1.80	0.46
1:E:395:ARG:HB3	1:E:396:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:ALA:HB1	1:E:454:LEU:CD2	2.45	0.46
1:F:164:ARG:O	1:F:166:GLU:N	2.41	0.46
1:A:422:VAL:CG2	1:D:375:LEU:HA	2.45	0.46
1:B:208:ILE:HD12	1:B:208:ILE:N	2.31	0.46
1:B:345:LEU:HD23	1:B:345:LEU:N	2.30	0.46
1:C:173:ASP:OD2	1:C:358:GLY:HA3	2.15	0.46
1:D:470:VAL:O	1:D:471:LEU:HD23	2.15	0.46
1:F:386:LEU:HD22	1:F:428:ALA:HB2	1.97	0.46
1:E:164:ARG:O	1:E:166:GLU:N	2.45	0.46
1:C:91:LEU:HD11	1:C:112:PHE:CZ	2.50	0.46
1:C:422:VAL:CG2	1:F:375:LEU:CD2	2.93	0.46
1:D:235:VAL:HG23	1:D:246:VAL:HG21	1.98	0.46
1:F:114:THR:OG1	1:F:118:HIS:HB3	2.16	0.46
1:A:142:LEU:H	1:A:142:LEU:CD2	2.26	0.46
1:A:452:LYS:HE2	1:A:468:GLY:N	2.31	0.46
1:C:126:MET:CG	1:C:151:PRO:HG3	2.46	0.46
1:E:113:ILE:HG22	1:E:114:THR:N	2.31	0.46
1:F:141:LEU:HD13	1:F:143:LEU:CD2	2.46	0.46
1:C:395:ARG:HB3	1:C:396:PRO:HD3	1.97	0.45
1:D:106:THR:O	1:D:111:ASN:ND2	2.47	0.45
1:E:352:THR:HG23	1:E:352:THR:O	2.16	0.45
1:F:74:PHE:CD1	1:F:170:TRP:CE3	3.04	0.45
1:A:231:VAL:HG11	1:A:250:LEU:CD2	2.47	0.45
1:C:199:LEU:HD22	1:C:204:VAL:HG13	1.98	0.45
1:E:228:PHE:CZ	1:E:263:ILE:HD13	2.52	0.45
1:E:280:GLY:O	1:E:286:VAL:HG21	2.16	0.45
1:B:250:LEU:CD1	1:B:260:VAL:HG13	2.40	0.45
1:C:183:GLU:OE2	1:C:340:ARG:NH1	2.49	0.45
1:C:187:VAL:HG21	1:C:292:PHE:CZ	2.51	0.45
1:C:253:ILE:O	1:C:253:ILE:CG2	2.63	0.45
1:D:454:LEU:N	1:D:454:LEU:HD12	2.31	0.45
1:E:415:VAL:HG13	1:E:419:LYS:HG3	1.97	0.45
1:F:204:VAL:CG1	1:F:369:LEU:HD21	2.47	0.45
1:B:396:PRO:HA	1:B:399:LEU:HD12	1.98	0.45
1:C:183:GLU:O	1:C:187:VAL:HG23	2.16	0.45
1:E:281:GLU:CA	1:E:286:VAL:HG21	2.44	0.45
1:C:164:ARG:O	1:C:166:GLU:N	2.44	0.45
1:E:194:MET:CE	1:E:335:LEU:HD23	2.46	0.45
1:E:255:LEU:HG	1:E:259:VAL:HG11	1.97	0.45
1:F:134:LEU:HD13	1:F:175:ILE:CD1	2.45	0.45
1:F:55:GLY:O	1:F:164:ARG:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PHE:HZ	1:B:263:ILE:HG21	1.82	0.45
1:B:433:ALA:CB	1:B:454:LEU:HD22	2.37	0.45
1:E:159:ILE:HD11	1:E:165:ARG:NE	2.32	0.45
1:E:415:VAL:HG12	1:E:417:ASP:O	2.16	0.45
1:C:432:GLY:O	1:C:433:ALA:HB3	2.17	0.45
1:D:212:LYS:O	1:D:216:THR:HG23	2.17	0.45
1:E:385:ASP:OD2	1:E:405:LEU:HD22	2.16	0.45
1:F:472:PRO:N	1:F:473:VAL:HA	2.31	0.45
1:B:211:ARG:HB2	1:B:315:LEU:HD21	1.98	0.45
1:B:141:LEU:HD13	1:B:143:LEU:HD23	1.97	0.44
1:B:214:LEU:HD21	1:B:267:LEU:CD1	2.47	0.44
1:A:185:GLU:OE1	1:B:406:ARG:NH2	2.44	0.44
1:B:255:LEU:CG	1:B:259:VAL:HG11	2.47	0.44
1:E:433:ALA:HB1	1:E:454:LEU:HD23	1.99	0.44
1:A:388:ILE:HD13	1:A:424:ALA:HB1	2.00	0.44
1:A:473:VAL:O	1:A:474:ASP:CB	2.65	0.44
1:B:340:ARG:HB2	1:B:357:VAL:HG22	1.98	0.44
1:C:61:PRO:O	1:C:65:ARG:HB2	2.18	0.44
1:A:86:TYR:CD2	1:A:147:TRP:HB3	2.52	0.44
1:A:422:VAL:HG21	1:D:375:LEU:HA	2.00	0.44
1:A:451:VAL:HG12	1:A:451:VAL:O	2.16	0.44
1:E:388:ILE:HD13	1:E:424:ALA:CB	2.48	0.44
1:B:386:LEU:HD22	1:B:428:ALA:CA	2.46	0.44
1:D:228:PHE:HZ	1:D:263:ILE:HG21	1.81	0.44
1:D:254:GLY:C	1:D:255:LEU:HD12	2.38	0.44
1:A:184:VAL:HG21	1:A:295:GLN:HB2	1.99	0.44
1:A:386:LEU:CD2	1:A:428:ALA:HB2	2.34	0.44
1:E:112:PHE:CD2	1:F:112:PHE:CD2	3.05	0.44
1:E:208:ILE:HG12	1:E:292:PHE:CE1	2.52	0.44
1:F:199:LEU:HD23	1:F:375:LEU:HD12	2.00	0.44
1:C:244:GLU:O	1:C:248:ALA:HB2	2.17	0.44
1:F:69:TYR:CZ	1:F:377:PRO:HG3	2.52	0.44
1:C:296:ILE:HG21	1:C:305:VAL:HG11	1.99	0.44
1:E:201:SER:O	1:E:328:ARG:HD2	2.17	0.44
1:A:97:TYR:C	1:A:105:ILE:HD11	2.38	0.43
1:C:386:LEU:HD22	1:C:428:ALA:CA	2.48	0.43
1:D:255:LEU:HB3	1:D:260:VAL:HG23	2.00	0.43
1:A:105:ILE:HG13	1:A:109:MET:HE3	2.00	0.43
1:B:141:LEU:HD12	1:B:175:ILE:HD11	2.00	0.43
1:B:210:SER:HB3	1:B:213:ILE:HG13	2.00	0.43
1:C:366:ILE:HD13	1:C:366:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.93	0.43
1:D:74:PHE:CD1	1:D:170:TRP:CE3	3.07	0.43
1:D:472:PRO:N	1:D:473:VAL:HA	2.33	0.43
1:E:346:THR:HG21	1:E:353:ALA:HB2	2.01	0.43
1:B:429:ASP:HA	1:B:433:ALA:HB2	2.01	0.43
1:C:180:VAL:O	1:C:180:VAL:HG22	2.19	0.43
1:D:429:ASP:HA	1:D:433:ALA:HB2	1.99	0.43
1:C:386:LEU:HD22	1:C:428:ALA:HA	1.99	0.43
1:E:406:ARG:NH2	1:F:185:GLU:OE1	2.41	0.43
1:A:188:CYS:SG	1:A:296:ILE:HD13	2.59	0.43
1:A:213:ILE:HD11	1:A:289:LEU:HD11	2.00	0.43
1:A:349:GLY:HA3	1:B:47:MET:HA	2.00	0.43
1:C:367:VAL:O	1:C:368:GLU:C	2.56	0.43
1:E:256:GLU:O	1:E:259:VAL:HG12	2.19	0.43
1:E:159:ILE:HD11	1:E:165:ARG:CD	2.48	0.43
1:A:250:LEU:HD12	1:A:260:VAL:HG13	2.00	0.43
1:C:336:CYS:HB3	1:C:361:PHE:CD1	2.54	0.43
1:D:269:LEU:HD22	1:D:274:GLU:HG2	2.01	0.43
1:E:427:TYR:O	1:E:431:ILE:HG23	2.19	0.43
1:F:135:LEU:HD21	1:F:345:LEU:HB3	2.01	0.43
1:B:113:ILE:HG22	1:B:114:THR:N	2.34	0.42
1:B:164:ARG:O	1:B:166:GLU:N	2.50	0.42
1:F:429:ASP:HA	1:F:433:ALA:HB2	2.01	0.42
1:E:70:LEU:HD12	1:E:197:LEU:HD21	2.00	0.42
1:F:366:ILE:N	1:F:366:ILE:HD13	2.34	0.42
1:D:380:HIS:O	1:D:382:VAL:HG23	2.18	0.42
1:B:170:TRP:HB3	1:B:361:PHE:HB3	2.00	0.42
1:D:183:GLU:HG2	1:D:321:ILE:HB	2.01	0.42
1:E:401:ILE:HD11	1:E:449:VAL:HG11	2.01	0.42
1:A:454:LEU:N	1:A:454:LEU:HD12	2.33	0.42
1:C:434:LEU:HD11	1:F:455:ARG:O	2.20	0.42
1:C:440:ALA:HB1	1:C:441:PRO:HD2	2.00	0.42
1:C:420:LYS:O	1:C:423:GLN:HB3	2.20	0.42
1:E:194:MET:HE2	1:E:335:LEU:HD23	2.01	0.42
1:A:180:VAL:O	1:A:180:VAL:HG13	2.20	0.42
1:A:208:ILE:CG2	1:A:289:LEU:CD2	2.98	0.42
1:C:186:LEU:HD22	1:C:359:PHE:CD2	2.54	0.42
1:D:228:PHE:CE1	1:D:263:ILE:HD13	2.54	0.42
1:E:401:ILE:HD13	1:E:449:VAL:HG11	2.00	0.42
1:F:342:ASP:OD1	1:F:355:PRO:HA	2.19	0.42
1:A:208:ILE:N	1:A:208:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:CZ	1:A:263:ILE:HG21	2.49	0.42
1:A:50:THR:HA	1:B:132:ARG:HG3	2.02	0.42
1:A:231:VAL:HG11	1:A:250:LEU:HD23	2.01	0.42
1:B:246:VAL:HG12	1:B:250:LEU:HG	2.01	0.42
1:A:346:THR:HG23	1:A:353:ALA:HA	2.02	0.42
1:A:472:PRO:N	1:A:473:VAL:HA	2.35	0.42
1:C:207:LYS:HA	1:C:306:ILE:O	2.20	0.42
1:C:340:ARG:NH1	1:C:357:VAL:CG2	2.82	0.42
1:D:255:LEU:HD23	1:D:259:VAL:HG22	2.01	0.42
1:D:394:MET:HE2	1:D:439:VAL:HG12	2.01	0.42
1:E:388:ILE:HD13	1:E:424:ALA:HB1	2.02	0.42
1:F:233:VAL:HG12	1:F:313:ARG:HH21	1.85	0.42
1:B:152:GLN:HE21	1:B:166:GLU:CG	2.33	0.41
1:B:194:MET:HE2	1:B:335:LEU:HD23	2.02	0.41
1:D:395:ARG:HB3	1:D:396:PRO:HD3	2.02	0.41
1:B:341:TYR:O	1:B:356:CYS:HB2	2.20	0.41
1:F:134:LEU:CD2	1:F:175:ILE:HD13	2.46	0.41
1:F:386:LEU:HD22	1:F:428:ALA:HA	2.01	0.41
1:B:86:TYR:O	1:B:149:SER:HB3	2.20	0.41
1:B:361:PHE:HE2	1:B:366:ILE:HG13	1.86	0.41
1:D:141:LEU:HD13	1:D:143:LEU:HD21	2.02	0.41
1:E:74:PHE:CD1	1:E:170:TRP:CE3	3.08	0.41
1:E:86:TYR:CZ	1:E:130:LEU:HD13	2.56	0.41
1:E:155:ARG:O	1:E:165:ARG:HA	2.20	0.41
1:C:56:CYS:HG	1:C:154:TRP:HZ3	1.65	0.41
1:C:340:ARG:NH1	1:C:357:VAL:HG21	2.35	0.41
1:A:269:LEU:HD22	1:A:274:GLU:HG2	2.01	0.41
1:B:427:TYR:CE1	1:B:431:ILE:HG21	2.56	0.41
1:C:339:GLY:C	1:C:357:VAL:HG13	2.40	0.41
1:C:399:LEU:HD23	1:C:399:LEU:HA	1.93	0.41
1:C:454:LEU:N	1:C:454:LEU:HD12	2.35	0.41
1:D:443:GLU:OE1	1:D:443:GLU:N	2.53	0.41
1:A:355:PRO:O	1:A:356:CYS:SG	2.76	0.41
1:D:173:ASP:OD2	1:D:341:TYR:OH	2.36	0.41
1:B:141:LEU:HD13	1:B:143:LEU:HD21	2.03	0.41
1:B:228:PHE:CE2	1:B:232:CYS:SG	3.14	0.41
1:D:142:LEU:H	1:D:142:LEU:CD2	2.32	0.41
1:D:341:TYR:CE1	1:D:344:LEU:HD22	2.56	0.41
1:D:363:ASP:OD1	1:D:363:ASP:C	2.57	0.41
1:D:386:LEU:HD22	1:D:428:ALA:HA	2.02	0.41
1:D:435:ARG:HD2	1:D:451:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LEU:HB3	1:B:450:ARG:HB3	2.03	0.41
1:C:95:GLU:O	1:C:98:ILE:HG22	2.21	0.41
1:C:112:PHE:CD2	1:D:112:PHE:CD2	3.09	0.41
1:C:429:ASP:HA	1:C:433:ALA:HB2	2.03	0.41
1:D:151:PRO:HD2	1:D:169:GLN:O	2.20	0.41
1:D:228:PHE:HE1	1:D:250:LEU:HD22	1.81	0.41
1:D:308:ASP:OD1	1:D:310:SER:OG	2.37	0.41
1:E:95:GLU:HA	1:E:98:ILE:HG22	2.03	0.41
1:E:177:VAL:O	1:E:177:VAL:HG12	2.19	0.41
1:E:216:THR:HG21	1:E:283:HIS:HE1	1.86	0.41
1:E:451:VAL:O	1:E:451:VAL:HG12	2.20	0.41
1:F:173:ASP:OD2	1:F:341:TYR:OH	2.35	0.41
1:F:208:ILE:N	1:F:208:ILE:CD1	2.84	0.41
1:F:440:ALA:HB1	1:F:441:PRO:HD2	2.03	0.41
1:C:216:THR:HG21	1:C:283:HIS:CE1	2.56	0.41
1:C:385:ASP:OD2	1:C:405:LEU:HD22	2.21	0.41
1:F:53:VAL:O	1:F:54:GLN:C	2.60	0.41
1:B:366:ILE:H	1:B:366:ILE:CD1	2.31	0.40
1:C:228:PHE:CE1	1:C:263:ILE:HD13	2.56	0.40
1:E:472:PRO:N	1:E:473:VAL:HA	2.36	0.40
1:F:135:LEU:CD2	1:F:345:LEU:HD13	2.50	0.40
1:A:401:ILE:HD11	1:A:444:TRP:HZ3	1.86	0.40
1:B:292:PHE:CE1	1:B:296:ILE:HG13	2.57	0.40
1:B:454:LEU:N	1:B:454:LEU:HD12	2.37	0.40
1:B:472:PRO:N	1:B:473:VAL:HA	2.36	0.40
1:C:97:TYR:C	1:C:105:ILE:HD11	2.41	0.40
1:D:250:LEU:HB3	1:D:260:VAL:HG22	2.03	0.40
1:A:69:TYR:CE1	1:A:377:PRO:HG3	2.56	0.40
1:A:253:ILE:HB	1:A:255:LEU:HD13	2.03	0.40
1:A:255:LEU:HB3	1:A:259:VAL:HG13	2.04	0.40
1:C:413:ASP:OD1	1:D:146:LYS:NZ	2.50	0.40
1:D:228:PHE:CE2	1:D:232:CYS:SG	3.14	0.40
1:F:366:ILE:HD13	1:F:366:ILE:H	1.86	0.40
1:A:84:GLU:OE2	1:B:65:ARG:NH1	2.54	0.40
1:C:98:ILE:HA	1:C:105:ILE:HD11	2.03	0.40
1:D:208:ILE:HG12	1:D:292:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/456 (86%)	361 (92%)	28 (7%)	3 (1%)	19	46
1	B	387/456 (85%)	349 (90%)	35 (9%)	3 (1%)	19	46
1	C	391/456 (86%)	351 (90%)	35 (9%)	5 (1%)	12	33
1	D	387/456 (85%)	351 (91%)	34 (9%)	2 (0%)	29	57
1	E	392/456 (86%)	363 (93%)	26 (7%)	3 (1%)	19	46
1	F	359/456 (79%)	334 (93%)	25 (7%)	0	100	100
All	All	2308/2736 (84%)	2109 (91%)	183 (8%)	16 (1%)	22	50

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	433	ALA
1	A	434	LEU
1	C	278	ARG
1	D	165	ARG
1	D	254	GLY
1	E	278	ARG
1	A	278	ARG
1	B	333	ARG
1	B	434	LEU
1	C	264	THR
1	B	433	ALA
1	C	165	ARG
1	E	165	ARG
1	E	434	LEU
1	C	430	ARG
1	A	254	GLY

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	314/383 (82%)	294 (94%)	20 (6%)	17	41
1	B	312/383 (82%)	286 (92%)	26 (8%)	11	29
1	C	313/383 (82%)	290 (93%)	23 (7%)	14	35
1	D	312/383 (82%)	292 (94%)	20 (6%)	17	41
1	E	313/383 (82%)	290 (93%)	23 (7%)	14	35
1	F	293/383 (76%)	276 (94%)	17 (6%)	20	46
All	All	1857/2298 (81%)	1728 (93%)	129 (7%)	15	38

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	142	LEU
1	A	175	ILE
1	A	180	VAL
1	A	201	SER
1	A	214	LEU
1	A	261	ASP
1	A	264	THR
1	A	267	LEU
1	A	268	SER
1	A	274	GLU
1	A	281	GLU
1	A	328	ARG
1	A	335	LEU
1	A	340	ARG
1	A	341	TYR
1	A	366	ILE
1	A	383	VAL
1	A	438	LEU
1	A	454	LEU
1	B	62	GLU
1	B	88	SER

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Mol	Chain	Res	Type
1	B	104	GLU
1	B	141	LEU
1	B	142	LEU
1	B	157	GLU
1	B	175	ILE
1	B	180	VAL
1	B	201	SER
1	B	214	LEU
1	B	261	ASP
1	B	266	THR
1	B	267	LEU
1	B	274	GLU
1	B	278	ARG
1	B	315	LEU
1	B	317	TYR
1	B	319	THR
1	B	328	ARG
1	B	335	LEU
1	B	340	ARG
1	B	341	TYR
1	B	346	THR
1	B	366	ILE
1	B	422	VAL
1	B	438	LEU
1	C	88	SER
1	C	104	GLU
1	C	141	LEU
1	C	142	LEU
1	C	157	GLU
1	C	166	GLU
1	C	175	ILE
1	C	185	GLU
1	C	201	SER
1	C	214	LEU
1	C	256	GLU
1	C	268	SER
1	C	278	ARG
1	C	281	GLU
1	C	293	ILE
1	C	315	LEU
1	C	317	TYR
1	C	319	THR

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Mol	Chain	Res	Type
1	C	340	ARG
1	C	341	TYR
1	C	366	ILE
1	C	438	LEU
1	C	454	LEU
1	D	62	GLU
1	D	104	GLU
1	D	141	LEU
1	D	142	LEU
1	D	157	GLU
1	D	175	ILE
1	D	180	VAL
1	D	201	SER
1	D	214	LEU
1	D	235	VAL
1	D	278	ARG
1	D	317	TYR
1	D	327	ASP
1	D	328	ARG
1	D	340	ARG
1	D	341	TYR
1	D	421	VAL
1	D	422	VAL
1	D	438	LEU
1	D	454	LEU
1	E	62	GLU
1	E	88	SER
1	E	90	VAL
1	E	141	LEU
1	E	142	LEU
1	E	157	GLU
1	E	175	ILE
1	E	185	GLU
1	E	214	LEU
1	E	235	VAL
1	E	256	GLU
1	E	267	LEU
1	E	278	ARG
1	E	281	GLU
1	E	317	TYR
1	E	335	LEU
1	E	340	ARG

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Mol	Chain	Res	Type
1	E	341	TYR
1	E	357	VAL
1	E	366	ILE
1	E	422	VAL
1	E	438	LEU
1	E	454	LEU
1	F	62	GLU
1	F	141	LEU
1	F	142	LEU
1	F	157	GLU
1	F	175	ILE
1	F	201	SER
1	F	214	LEU
1	F	278	ARG
1	F	317	TYR
1	F	341	TYR
1	F	347	THR
1	F	352	THR
1	F	366	ILE
1	F	393	THR
1	F	422	VAL
1	F	438	LEU
1	F	454	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	GLN
1	E	171	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	401/456 (87%)	0.03	8 (1%)	65	62	20, 20, 20, 20	0
1	B	398/456 (87%)	0.12	13 (3%)	46	41	20, 20, 20, 20	0
1	C	400/456 (87%)	0.06	11 (2%)	53	48	20, 20, 20, 20	0
1	D	398/456 (87%)	0.30	26 (6%)	18	14	20, 20, 20, 20	0
1	E	401/456 (87%)	0.20	14 (3%)	44	38	20, 20, 20, 20	0
1	F	370/456 (81%)	0.28	25 (6%)	17	13	20, 20, 20, 20	0
All	All	2368/2736 (86%)	0.16	97 (4%)	37	31	20, 20, 20, 20	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	THR	10.6
1	F	229	ALA	7.7
1	F	234	ILE	7.6
1	E	160	THR	7.1
1	B	158	ALA	7.1
1	C	160	THR	7.0
1	E	162	GLY	6.4
1	A	161	ARG	5.8
1	D	253	ILE	5.6
1	C	161	ARG	5.3
1	D	474	ASP	5.3
1	F	158	ALA	4.7
1	D	158	ALA	4.4
1	C	158	ALA	4.3
1	F	226	ASP	4.3
1	D	258	ASN	4.2
1	E	94	GLU	4.2
1	F	230	PRO	4.1
1	E	161	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	255	LEU	4.0
1	F	269	LEU	4.0
1	D	270	LYS	4.0
1	F	270	LYS	4.0
1	E	255	LEU	3.9
1	F	219	GLU	3.9
1	D	160	THR	3.9
1	D	142	LEU	3.7
1	E	157	GLU	3.7
1	B	163	ARG	3.7
1	F	275	ILE	3.6
1	E	96	LEU	3.5
1	B	160	THR	3.4
1	F	233	VAL	3.4
1	A	162	GLY	3.4
1	B	112	PHE	3.4
1	F	317	TYR	3.4
1	F	112	PHE	3.3
1	F	159	ILE	3.3
1	D	228	PHE	3.2
1	A	159	ILE	3.2
1	D	103	GLU	3.1
1	A	474	ASP	3.1
1	A	104	GLU	3.1
1	C	163	ARG	3.1
1	C	157	GLU	3.0
1	B	255	LEU	3.0
1	D	234	ILE	3.0
1	E	268	SER	3.0
1	F	278	ARG	2.9
1	F	163	ARG	2.9
1	B	161	ARG	2.8
1	B	253	ILE	2.8
1	B	474	ASP	2.7
1	F	277	GLN	2.7
1	B	234	ILE	2.7
1	F	113	ILE	2.7
1	C	310	SER	2.6
1	F	160	THR	2.6
1	F	404	ARG	2.6
1	D	118	HIS	2.5
1	C	162	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	268	SER	2.4
1	F	228	PHE	2.4
1	D	271	THR	2.4
1	F	49	GLU	2.4
1	E	97	TYR	2.4
1	D	106	THR	2.4
1	E	163	ARG	2.4
1	E	258	ASN	2.3
1	A	163	ARG	2.3
1	B	228	PHE	2.3
1	E	159	ILE	2.3
1	D	112	PHE	2.3
1	D	436	ALA	2.2
1	B	257	SER	2.2
1	D	455	ARG	2.2
1	D	317	TYR	2.2
1	D	256	GLU	2.2
1	C	114	THR	2.2
1	F	421	VAL	2.2
1	D	226	ASP	2.2
1	B	162	GLY	2.2
1	C	309	ALA	2.2
1	C	255	LEU	2.1
1	F	232	CYS	2.1
1	C	468	GLY	2.1
1	F	47	MET	2.1
1	B	114	THR	2.1
1	D	269	LEU	2.1
1	E	474	ASP	2.1
1	A	158	ALA	2.1
1	D	451	VAL	2.1
1	E	112	PHE	2.0
1	D	431	ILE	2.0
1	D	252	ALA	2.0
1	D	232	CYS	2.0
1	F	449	VAL	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.