



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:21 am BST

PDB ID : 5H4V
Title : Structure of glutamyl-tRNA synthetase (Xoo1504) from *Xanthomonas oryzae* pv. *oryzae*
Authors : Doan, T.-N.-T.; Ho, T.-H.; Kang, L.-W.
Deposited on : 2016-11-02
Resolution : 3.00 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 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	:	2.11
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)	:	2.11

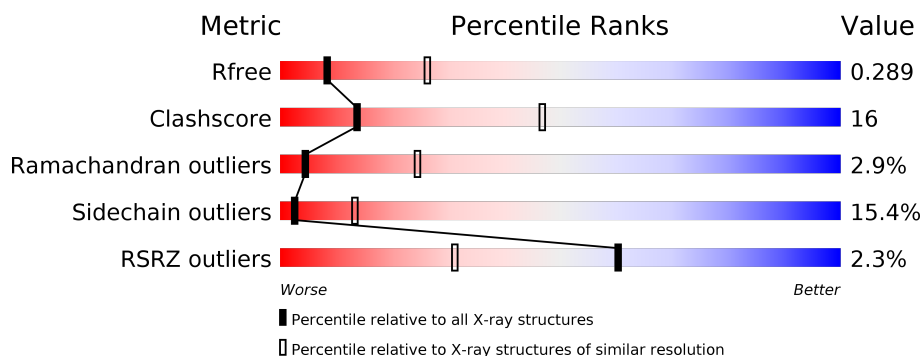
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	488	<div> <div>2%</div> <div> <div>67%</div> <div>24%</div> <div>• 5%</div> </div> </div>
1	B	488	<div> <div>%</div> <div> <div>68%</div> <div>22%</div> <div>• • 6%</div> </div> </div>
1	C	488	<div> <div>4%</div> <div> <div>66%</div> <div>22%</div> <div>5% • 7%</div> </div> </div>
1	D	488	<div> <div>3%</div> <div> <div>64%</div> <div>24%</div> <div>6% • 5%</div> </div> </div>
1	E	488	<div> <div>2%</div> <div> <div>67%</div> <div>24%</div> <div>5% 5%</div> </div> </div>
1	F	488	<div> <div>%</div> <div> <div>65%</div> <div>24%</div> <div>5% • 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glutamate–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3623	2290	640	679	14			
1	B	460	Total	C	N	O	S	0	0	0
			3586	2269	631	672	14			
1	C	455	Total	C	N	O	S	0	0	0
			3541	2242	622	663	14			
1	D	465	Total	C	N	O	S	0	0	0
			3623	2290	640	679	14			
1	E	465	Total	C	N	O	S	0	0	0
			3623	2290	640	679	14			
1	F	465	Total	C	N	O	S	0	0	0
			3620	2289	640	677	14			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q5H2R3
A	-19	GLY	-	expression tag	UNP Q5H2R3
A	-18	HIS	-	expression tag	UNP Q5H2R3
A	-17	HIS	-	expression tag	UNP Q5H2R3
A	-16	HIS	-	expression tag	UNP Q5H2R3
A	-15	HIS	-	expression tag	UNP Q5H2R3
A	-14	HIS	-	expression tag	UNP Q5H2R3
A	-13	HIS	-	expression tag	UNP Q5H2R3
A	-12	SER	-	expression tag	UNP Q5H2R3
A	-11	SER	-	expression tag	UNP Q5H2R3
A	-10	GLU	-	expression tag	UNP Q5H2R3
A	-9	ASN	-	expression tag	UNP Q5H2R3
A	-8	LEU	-	expression tag	UNP Q5H2R3
A	-7	TYR	-	expression tag	UNP Q5H2R3
A	-6	PHE	-	expression tag	UNP Q5H2R3
A	-5	GLN	-	expression tag	UNP Q5H2R3
A	-4	GLY	-	expression tag	UNP Q5H2R3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP Q5H2R3
A	-2	MET	-	expression tag	UNP Q5H2R3
A	-1	ALA	-	expression tag	UNP Q5H2R3
A	0	SER	-	expression tag	UNP Q5H2R3
B	-20	MET	-	expression tag	UNP Q5H2R3
B	-19	GLY	-	expression tag	UNP Q5H2R3
B	-18	HIS	-	expression tag	UNP Q5H2R3
B	-17	HIS	-	expression tag	UNP Q5H2R3
B	-16	HIS	-	expression tag	UNP Q5H2R3
B	-15	HIS	-	expression tag	UNP Q5H2R3
B	-14	HIS	-	expression tag	UNP Q5H2R3
B	-13	HIS	-	expression tag	UNP Q5H2R3
B	-12	SER	-	expression tag	UNP Q5H2R3
B	-11	SER	-	expression tag	UNP Q5H2R3
B	-10	GLU	-	expression tag	UNP Q5H2R3
B	-9	ASN	-	expression tag	UNP Q5H2R3
B	-8	LEU	-	expression tag	UNP Q5H2R3
B	-7	TYR	-	expression tag	UNP Q5H2R3
B	-6	PHE	-	expression tag	UNP Q5H2R3
B	-5	GLN	-	expression tag	UNP Q5H2R3
B	-4	GLY	-	expression tag	UNP Q5H2R3
B	-3	HIS	-	expression tag	UNP Q5H2R3
B	-2	MET	-	expression tag	UNP Q5H2R3
B	-1	ALA	-	expression tag	UNP Q5H2R3
B	0	SER	-	expression tag	UNP Q5H2R3
C	-20	MET	-	expression tag	UNP Q5H2R3
C	-19	GLY	-	expression tag	UNP Q5H2R3
C	-18	HIS	-	expression tag	UNP Q5H2R3
C	-17	HIS	-	expression tag	UNP Q5H2R3
C	-16	HIS	-	expression tag	UNP Q5H2R3
C	-15	HIS	-	expression tag	UNP Q5H2R3
C	-14	HIS	-	expression tag	UNP Q5H2R3
C	-13	HIS	-	expression tag	UNP Q5H2R3
C	-12	SER	-	expression tag	UNP Q5H2R3
C	-11	SER	-	expression tag	UNP Q5H2R3
C	-10	GLU	-	expression tag	UNP Q5H2R3
C	-9	ASN	-	expression tag	UNP Q5H2R3
C	-8	LEU	-	expression tag	UNP Q5H2R3
C	-7	TYR	-	expression tag	UNP Q5H2R3
C	-6	PHE	-	expression tag	UNP Q5H2R3
C	-5	GLN	-	expression tag	UNP Q5H2R3
C	-4	GLY	-	expression tag	UNP Q5H2R3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP Q5H2R3
C	-2	MET	-	expression tag	UNP Q5H2R3
C	-1	ALA	-	expression tag	UNP Q5H2R3
C	0	SER	-	expression tag	UNP Q5H2R3
D	-20	MET	-	expression tag	UNP Q5H2R3
D	-19	GLY	-	expression tag	UNP Q5H2R3
D	-18	HIS	-	expression tag	UNP Q5H2R3
D	-17	HIS	-	expression tag	UNP Q5H2R3
D	-16	HIS	-	expression tag	UNP Q5H2R3
D	-15	HIS	-	expression tag	UNP Q5H2R3
D	-14	HIS	-	expression tag	UNP Q5H2R3
D	-13	HIS	-	expression tag	UNP Q5H2R3
D	-12	SER	-	expression tag	UNP Q5H2R3
D	-11	SER	-	expression tag	UNP Q5H2R3
D	-10	GLU	-	expression tag	UNP Q5H2R3
D	-9	ASN	-	expression tag	UNP Q5H2R3
D	-8	LEU	-	expression tag	UNP Q5H2R3
D	-7	TYR	-	expression tag	UNP Q5H2R3
D	-6	PHE	-	expression tag	UNP Q5H2R3
D	-5	GLN	-	expression tag	UNP Q5H2R3
D	-4	GLY	-	expression tag	UNP Q5H2R3
D	-3	HIS	-	expression tag	UNP Q5H2R3
D	-2	MET	-	expression tag	UNP Q5H2R3
D	-1	ALA	-	expression tag	UNP Q5H2R3
D	0	SER	-	expression tag	UNP Q5H2R3
E	-20	MET	-	expression tag	UNP Q5H2R3
E	-19	GLY	-	expression tag	UNP Q5H2R3
E	-18	HIS	-	expression tag	UNP Q5H2R3
E	-17	HIS	-	expression tag	UNP Q5H2R3
E	-16	HIS	-	expression tag	UNP Q5H2R3
E	-15	HIS	-	expression tag	UNP Q5H2R3
E	-14	HIS	-	expression tag	UNP Q5H2R3
E	-13	HIS	-	expression tag	UNP Q5H2R3
E	-12	SER	-	expression tag	UNP Q5H2R3
E	-11	SER	-	expression tag	UNP Q5H2R3
E	-10	GLU	-	expression tag	UNP Q5H2R3
E	-9	ASN	-	expression tag	UNP Q5H2R3
E	-8	LEU	-	expression tag	UNP Q5H2R3
E	-7	TYR	-	expression tag	UNP Q5H2R3
E	-6	PHE	-	expression tag	UNP Q5H2R3
E	-5	GLN	-	expression tag	UNP Q5H2R3
E	-4	GLY	-	expression tag	UNP Q5H2R3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	HIS	-	expression tag	UNP Q5H2R3
E	-2	MET	-	expression tag	UNP Q5H2R3
E	-1	ALA	-	expression tag	UNP Q5H2R3
E	0	SER	-	expression tag	UNP Q5H2R3
F	-20	MET	-	expression tag	UNP Q5H2R3
F	-19	GLY	-	expression tag	UNP Q5H2R3
F	-18	HIS	-	expression tag	UNP Q5H2R3
F	-17	HIS	-	expression tag	UNP Q5H2R3
F	-16	HIS	-	expression tag	UNP Q5H2R3
F	-15	HIS	-	expression tag	UNP Q5H2R3
F	-14	HIS	-	expression tag	UNP Q5H2R3
F	-13	HIS	-	expression tag	UNP Q5H2R3
F	-12	SER	-	expression tag	UNP Q5H2R3
F	-11	SER	-	expression tag	UNP Q5H2R3
F	-10	GLU	-	expression tag	UNP Q5H2R3
F	-9	ASN	-	expression tag	UNP Q5H2R3
F	-8	LEU	-	expression tag	UNP Q5H2R3
F	-7	TYR	-	expression tag	UNP Q5H2R3
F	-6	PHE	-	expression tag	UNP Q5H2R3
F	-5	GLN	-	expression tag	UNP Q5H2R3
F	-4	GLY	-	expression tag	UNP Q5H2R3
F	-3	HIS	-	expression tag	UNP Q5H2R3
F	-2	MET	-	expression tag	UNP Q5H2R3
F	-1	ALA	-	expression tag	UNP Q5H2R3
F	0	SER	-	expression tag	UNP Q5H2R3

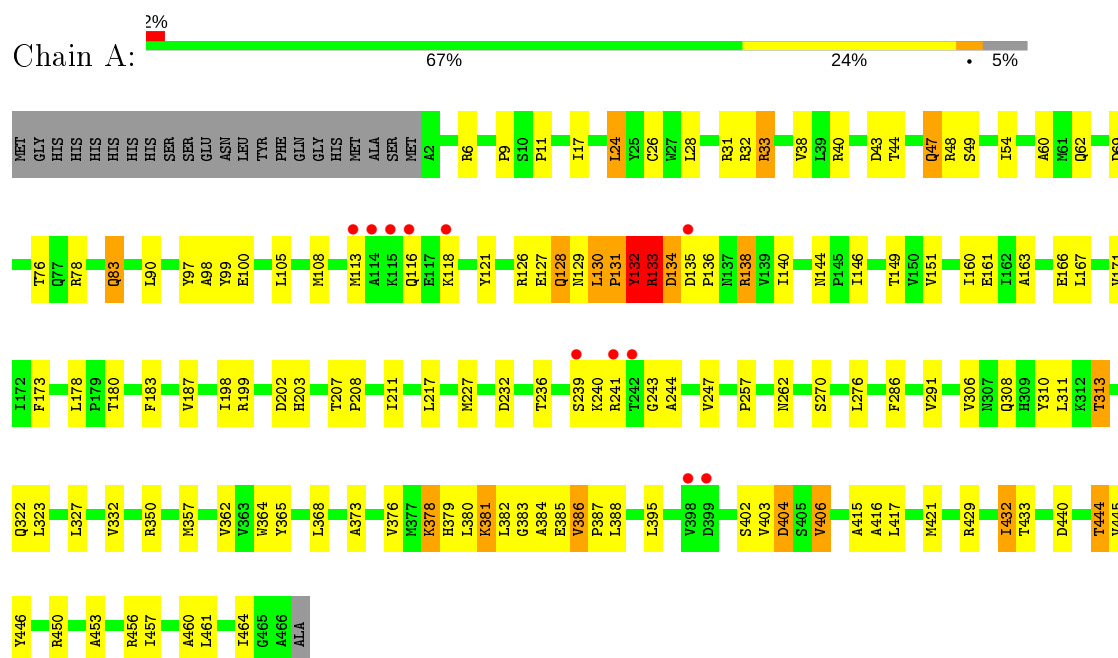
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0
2	B	9	Total O 9 9	0	0
2	C	4	Total O 4 4	0	0
2	D	8	Total O 8 8	0	0
2	E	13	Total O 13 13	0	0
2	F	10	Total O 10 10	0	0

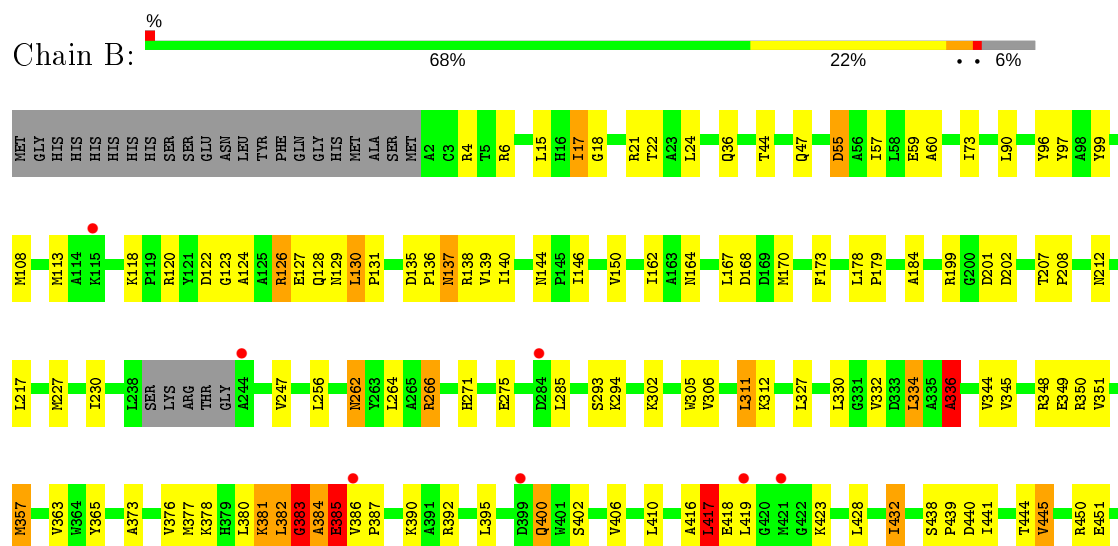
3 Residue-property plots [i](#)

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

• Molecule 1: Glutamate-tRNA ligase

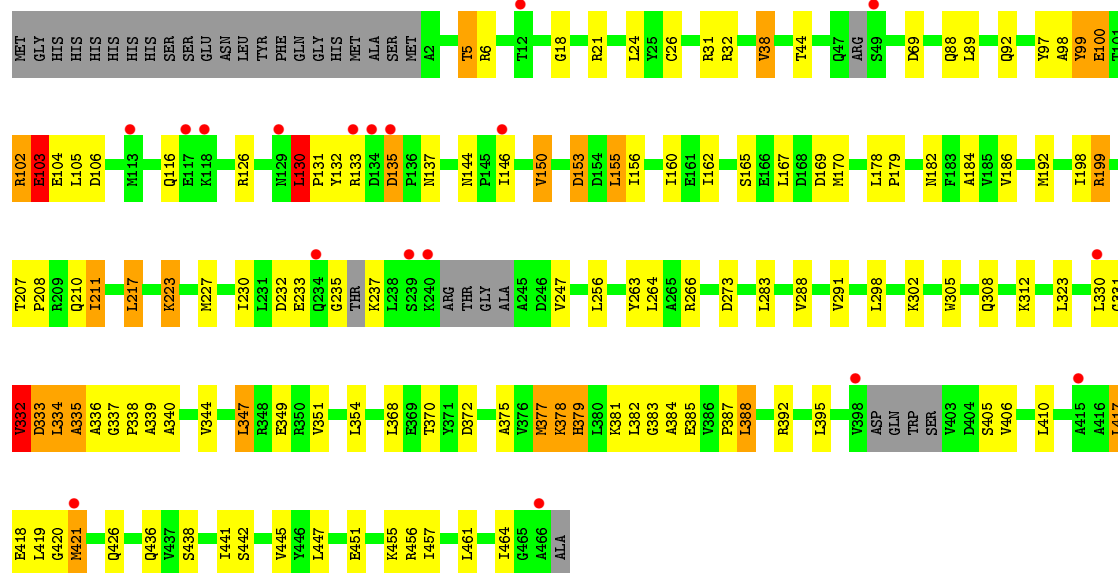


• Molecule 1: Glutamate-tRNA ligase

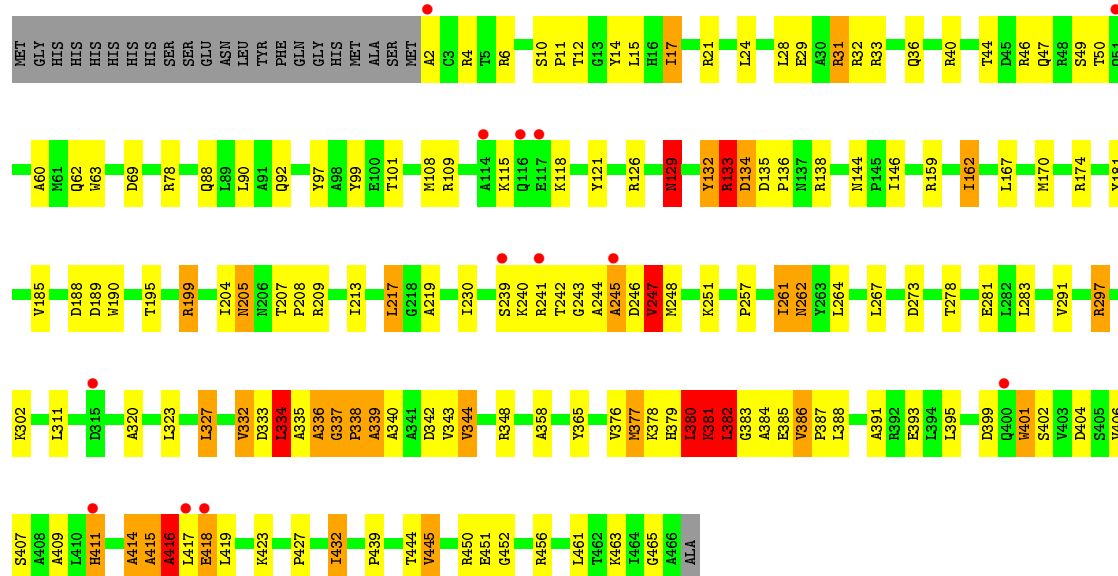




• Molecule 1: Glutamate-tRNA ligase

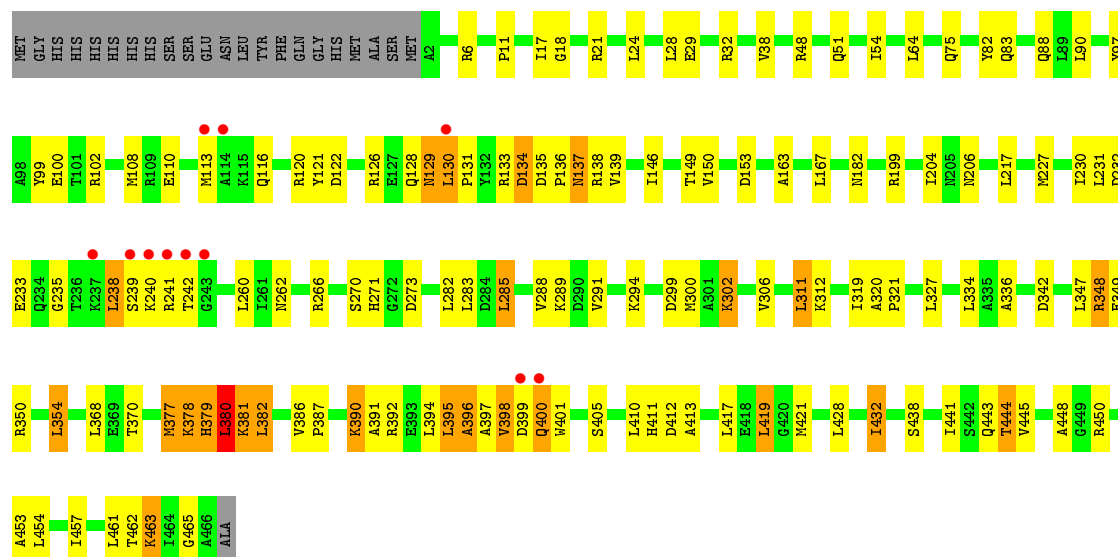


• Molecule 1: Glutamate-tRNA ligase

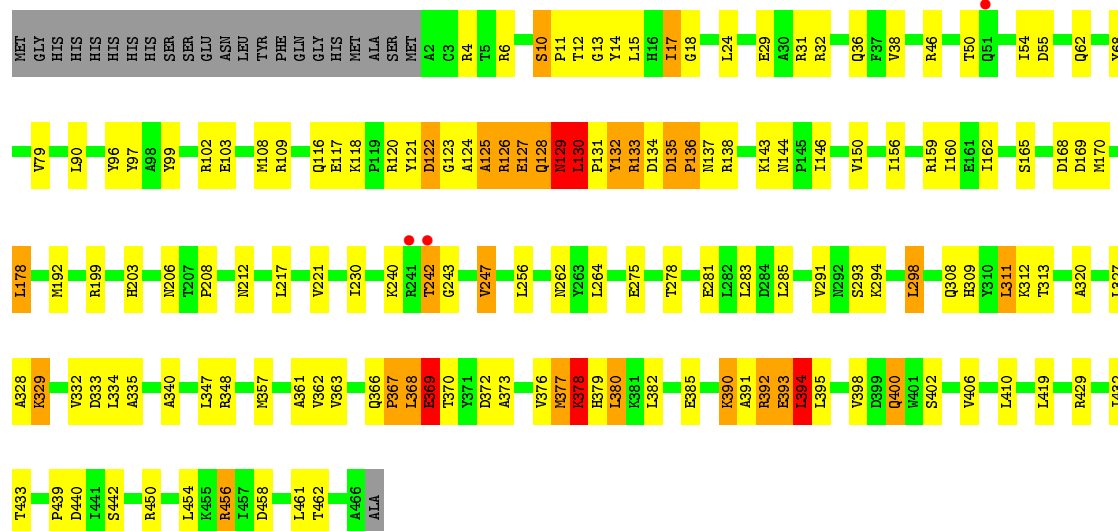


• Molecule 1: Glutamate-tRNA ligase





• Molecule 1: Glutamate-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.35Å 107.94Å 165.90Å 90.00° 96.24° 90.00°	Depositor
Resolution (Å)	29.44 – 3.00 29.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.44-3.00) 90.4 (29.44-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.200 , 0.291 0.206 , 0.289	Depositor DCC
R_{free} test set	3046 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21668	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0/3696	0.79	2/5018 (0.0%)
1	B	0.55	0/3658	0.80	5/4967 (0.1%)
1	C	0.49	0/3608	0.78	4/4892 (0.1%)
1	D	0.57	1/3696 (0.0%)	0.86	5/5018 (0.1%)
1	E	0.52	0/3696	0.81	2/5018 (0.0%)
1	F	0.55	0/3693	0.81	4/5014 (0.1%)
All	All	0.54	1/22047 (0.0%)	0.81	22/29927 (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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	273	ASP	CB-CG	5.50	1.63	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	LEU	CA-CB-CG	7.72	133.06	115.30
1	F	456	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	E	380	LEU	CA-CB-CG	6.66	130.62	115.30
1	B	383	GLY	N-CA-C	-6.27	97.43	113.10
1	D	416	ALA	N-CA-C	-6.05	94.67	111.00
1	D	199	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	F	122	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	199	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	337	GLY	C-N-CD	5.48	139.90	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	415	ALA	N-CA-C	-5.47	96.24	111.00
1	B	135	ASP	C-N-CD	5.45	139.84	128.40
1	D	297	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	E	350	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	417	LEU	CA-CB-CG	5.42	127.75	115.30
1	A	350	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	388	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	78	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	F	456	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	C	336	ALA	N-CA-C	-5.12	97.19	111.00
1	C	103	GLU	N-CA-C	-5.11	97.21	111.00
1	F	378	LYS	N-CA-C	-5.09	97.25	111.00
1	B	266	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	336	ALA	Peptide
1	B	383	GLY	Peptide

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	3623	0	3607	104	0
1	B	3586	0	3565	103	0
1	C	3541	0	3528	125	0
1	D	3623	0	3606	144	0
1	E	3623	0	3607	65	0
1	F	3620	0	3605	157	0
2	A	8	0	0	1	0
2	B	9	0	0	0	0
2	C	4	0	0	0	0
2	D	8	0	0	0	0
2	E	13	0	0	0	0
2	F	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21668	0	21518	685	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 16.

All (685) 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:C:99:TYR:HE2	1:C:131:PRO:CG	1.02	1.59
1:F:97:TYR:H	1:F:130:LEU:CD2	1.16	1.58
1:F:96:TYR:CA	1:F:130:LEU:HD21	1.35	1.54
1:C:382:LEU:HD12	1:C:385:GLU:CB	1.34	1.52
1:C:99:TYR:CE2	1:C:131:PRO:CG	1.93	1.51
1:C:382:LEU:CD1	1:C:385:GLU:CB	1.85	1.50
1:C:99:TYR:CE2	1:C:131:PRO:HG3	1.49	1.44
1:F:97:TYR:N	1:F:130:LEU:CD2	1.88	1.33
1:C:382:LEU:CD1	1:C:385:GLU:HB2	1.45	1.32
1:D:15:LEU:O	1:D:247:VAL:HG12	1.33	1.29
1:C:382:LEU:O	1:C:385:GLU:N	1.66	1.28
1:F:129:ASN:OD1	1:F:130:LEU:N	1.71	1.23
1:C:99:TYR:CE2	1:C:131:PRO:HG2	1.64	1.21
1:B:383:GLY:O	1:B:385:GLU:N	1.70	1.21
1:A:131:PRO:O	1:A:132:TYR:CB	1.84	1.20
1:F:132:TYR:CD1	1:F:133:ARG:O	1.95	1.19
1:A:9:PRO:O	1:A:11:PRO:HD3	1.45	1.17
1:D:411:HIS:HA	1:D:414:ALA:HB2	1.25	1.15
1:F:129:ASN:OD1	1:F:131:PRO:HD2	1.46	1.14
1:D:239:SER:O	1:D:242:THR:OG1	1.64	1.14
1:C:382:LEU:CD1	1:C:385:GLU:HB3	1.59	1.13
1:A:99:TYR:HE2	1:A:131:PRO:CB	1.61	1.13
1:D:15:LEU:O	1:D:247:VAL:CG1	1.98	1.11
1:F:97:TYR:H	1:F:130:LEU:HD23	1.02	1.11
1:A:99:TYR:CE2	1:A:131:PRO:HB2	1.85	1.11
1:C:382:LEU:HD11	1:C:385:GLU:HB3	1.20	1.11
1:C:102:ARG:H	1:C:105:LEU:CD1	1.64	1.11
1:A:97:TYR:HB2	1:A:131:PRO:HG3	1.21	1.10
1:F:99:TYR:OH	1:F:132:TYR:O	1.69	1.10
1:D:415:ALA:O	1:D:416:ALA:C	1.90	1.09
1:F:96:TYR:CA	1:F:130:LEU:CD2	2.30	1.09
1:F:97:TYR:H	1:F:130:LEU:HD22	1.16	1.09
1:F:96:TYR:HA	1:F:130:LEU:CD2	1.84	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ASN:O	1:F:130:LEU:HB2	1.43	1.06
1:B:386:VAL:HG22	1:B:417:LEU:CD1	1.84	1.06
1:B:386:VAL:HG22	1:B:417:LEU:HD11	1.09	1.06
1:B:386:VAL:CG1	1:B:387:PRO:HD3	1.84	1.06
1:B:386:VAL:HG13	1:B:387:PRO:HD3	1.10	1.06
1:F:366:GLN:HG3	1:F:368:LEU:HB3	1.38	1.05
1:F:96:TYR:CB	1:F:130:LEU:HD21	1.87	1.04
1:F:390:LYS:NZ	1:F:393:GLU:OE2	1.89	1.04
1:B:385:GLU:CG	1:B:464:ILE:HD13	1.88	1.04
1:D:415:ALA:HB1	1:D:419:LEU:H	1.20	1.04
1:C:99:TYR:HE2	1:C:131:PRO:HG2	0.87	1.03
1:A:379:HIS:O	1:A:381:LYS:O	1.76	1.02
1:A:380:LEU:HD23	1:A:381:LYS:H	1.22	1.01
1:F:96:TYR:HA	1:F:130:LEU:HD21	1.02	1.01
1:C:99:TYR:OH	1:C:133:ARG:HB3	1.59	0.99
1:B:128:GLN:O	1:B:129:ASN:HB3	1.58	0.99
1:D:377:MET:HA	1:D:380:LEU:CD2	1.92	0.99
1:A:97:TYR:CB	1:A:131:PRO:HG3	1.92	0.99
1:F:129:ASN:OD1	1:F:131:PRO:CD	2.10	0.99
1:B:137:ASN:OD1	1:D:302:LYS:HE2	1.63	0.99
1:C:102:ARG:HA	1:C:105:LEU:HD13	1.45	0.98
1:D:415:ALA:HB1	1:D:419:LEU:N	1.78	0.98
1:B:385:GLU:CD	1:B:464:ILE:HD13	1.84	0.98
1:D:411:HIS:CA	1:D:414:ALA:HB2	1.94	0.98
1:B:384:ALA:O	1:B:385:GLU:HB2	1.61	0.97
1:D:415:ALA:CB	1:D:419:LEU:H	1.77	0.97
1:C:100:GLU:N	1:C:100:GLU:OE2	1.98	0.97
1:F:394:LEU:H	1:F:394:LEU:HD22	1.27	0.97
1:C:102:ARG:N	1:C:105:LEU:HD13	1.79	0.96
1:C:102:ARG:NH1	1:C:102:ARG:HB2	1.81	0.95
1:F:129:ASN:CG	1:F:130:LEU:H	1.67	0.95
1:D:415:ALA:O	1:D:417:LEU:N	1.88	0.95
1:D:383:GLY:O	1:D:387:PRO:HD2	1.66	0.95
1:A:382:LEU:O	1:A:384:ALA:N	1.99	0.95
1:F:96:TYR:C	1:F:130:LEU:HD21	1.87	0.94
1:F:132:TYR:CE1	1:F:133:ARG:O	2.21	0.94
1:F:366:GLN:O	1:F:368:LEU:N	2.02	0.93
1:C:102:ARG:CA	1:C:105:LEU:HD13	1.99	0.92
1:F:11:PRO:HA	1:F:12:THR:OG1	1.70	0.92
1:F:125:ALA:O	1:F:126:ARG:O	1.87	0.92
1:F:132:TYR:HD1	1:F:133:ARG:O	1.45	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:LEU:HD23	1:D:380:LEU:H	1.35	0.91
1:D:134:ASP:HB2	1:D:138:ARG:HH12	1.34	0.91
1:F:398:VAL:O	1:F:450:ARG:NH2	2.03	0.91
1:B:386:VAL:HG13	1:B:387:PRO:CD	1.99	0.91
1:E:238:LEU:HA	1:E:242:THR:HG21	1.52	0.91
1:F:130:LEU:N	1:F:131:PRO:CD	2.35	0.90
1:C:102:ARG:O	1:C:106:ASP:N	2.04	0.90
1:A:99:TYR:OH	1:A:132:TYR:N	2.05	0.89
1:C:383:GLY:O	1:C:387:PRO:HD3	1.71	0.89
1:F:97:TYR:N	1:F:130:LEU:HD23	1.67	0.89
1:F:393:GLU:HB3	1:F:394:LEU:HD22	1.53	0.89
1:D:244:ALA:C	1:D:246:ASP:H	1.76	0.89
1:A:130:LEU:HD23	1:A:130:LEU:H	1.37	0.89
1:D:415:ALA:C	1:D:417:LEU:N	2.14	0.89
1:A:99:TYR:CE2	1:A:131:PRO:CB	2.48	0.88
1:F:363:VAL:O	1:F:368:LEU:CD2	2.21	0.88
1:F:133:ARG:HG3	1:F:134:ASP:H	1.35	0.88
1:D:78:ARG:NH2	1:D:188:ASP:OD1	2.06	0.87
1:D:133:ARG:HE	1:D:133:ARG:HA	1.36	0.87
1:B:383:GLY:C	1:B:385:GLU:H	1.73	0.87
1:F:391:ALA:O	1:F:395:LEU:HD12	1.73	0.87
1:C:333:ASP:HB3	1:C:335:ALA:N	1.88	0.87
1:C:102:ARG:N	1:C:105:LEU:CD1	2.35	0.86
1:A:99:TYR:HE2	1:A:131:PRO:HB3	1.39	0.86
1:B:385:GLU:OE2	1:B:464:ILE:HD13	1.75	0.85
1:A:99:TYR:HE2	1:A:131:PRO:HB2	1.20	0.84
1:A:131:PRO:O	1:A:132:TYR:HB2	0.94	0.84
1:D:377:MET:HA	1:D:380:LEU:HD21	1.60	0.83
1:C:99:TYR:CZ	1:C:133:ARG:HB3	2.12	0.83
1:D:415:ALA:HB1	1:D:418:GLU:CA	2.08	0.83
1:F:125:ALA:O	1:F:126:ARG:C	2.13	0.83
1:F:127:GLU:OE2	1:F:143:LYS:NZ	2.12	0.83
1:C:382:LEU:HD13	1:C:385:GLU:CB	2.09	0.82
1:C:383:GLY:O	1:C:387:PRO:CD	2.27	0.81
1:D:415:ALA:HB1	1:D:418:GLU:HA	1.59	0.81
1:D:411:HIS:HA	1:D:414:ALA:CB	2.10	0.81
1:B:386:VAL:CG2	1:B:417:LEU:CD1	2.58	0.81
1:B:386:VAL:CG2	1:B:417:LEU:HD11	2.01	0.81
1:F:96:TYR:C	1:F:130:LEU:CD2	2.47	0.81
1:C:417:LEU:HD22	1:C:419:LEU:HD13	1.63	0.81
1:F:132:TYR:O	1:F:133:ARG:HB3	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:LEU:H	1:C:334:LEU:HD23	1.47	0.80
1:D:134:ASP:HB2	1:D:138:ARG:NH1	1.97	0.80
1:B:383:GLY:C	1:B:385:GLU:N	2.32	0.79
1:A:97:TYR:HB2	1:A:131:PRO:CG	2.10	0.79
1:D:99:TYR:OH	1:D:132:TYR:O	2.02	0.78
1:F:130:LEU:N	1:F:131:PRO:HD3	1.97	0.78
1:A:97:TYR:CD2	1:A:131:PRO:HG2	2.18	0.78
1:C:382:LEU:HD13	1:C:385:GLU:CD	2.04	0.78
1:D:135:ASP:HB2	1:D:136:PRO:HD3	1.64	0.78
1:A:380:LEU:CD2	1:A:381:LYS:H	1.95	0.78
1:B:385:GLU:HG2	1:B:464:ILE:HD13	1.64	0.78
1:C:99:TYR:CZ	1:C:131:PRO:HG3	2.16	0.78
1:C:102:ARG:HA	1:C:105:LEU:CD1	2.15	0.77
1:F:135:ASP:OD1	1:F:137:ASN:HB2	1.83	0.77
1:B:128:GLN:O	1:B:129:ASN:CB	2.30	0.77
1:B:386:VAL:N	1:B:387:PRO:HD2	2.00	0.77
1:C:382:LEU:HD12	1:C:382:LEU:O	1.83	0.77
1:A:373:ALA:O	1:A:376:VAL:HG22	1.84	0.76
1:D:382:LEU:O	1:D:385:GLU:N	2.18	0.76
1:B:386:VAL:CG1	1:B:387:PRO:CD	2.59	0.76
1:B:410:LEU:HD13	1:B:441:ILE:HD12	1.67	0.76
1:E:312:LYS:HA	1:E:348:ARG:HD3	1.66	0.75
1:F:108:MET:HE1	1:F:121:TYR:HA	1.68	0.75
1:F:96:TYR:HB2	1:F:130:LEU:CD2	2.16	0.75
1:C:102:ARG:H	1:C:105:LEU:HD12	1.49	0.75
1:A:9:PRO:O	1:A:11:PRO:CD	2.32	0.75
1:F:363:VAL:O	1:F:368:LEU:HD22	1.86	0.75
1:A:97:TYR:CG	1:A:131:PRO:HG2	2.21	0.74
1:A:97:TYR:CD2	1:A:131:PRO:CG	2.70	0.74
1:F:96:TYR:CE2	1:F:126:ARG:HA	2.23	0.74
1:F:369:GLU:OE2	1:F:369:GLU:HA	1.86	0.74
1:B:381:LYS:O	1:B:382:LEU:C	2.23	0.74
1:B:376:VAL:HG23	1:B:380:LEU:HD22	1.70	0.74
1:D:108:MET:HE1	1:D:121:TYR:HA	1.69	0.73
1:D:411:HIS:C	1:D:414:ALA:HB2	2.09	0.73
1:A:99:TYR:CZ	1:A:131:PRO:HB2	2.24	0.72
1:B:376:VAL:O	1:B:380:LEU:HB2	1.90	0.72
1:A:99:TYR:HE1	1:A:138:ARG:HB3	1.53	0.72
1:B:136:PRO:O	1:B:137:ASN:ND2	2.22	0.72
1:E:108:MET:HE1	1:E:121:TYR:HA	1.71	0.72
1:F:391:ALA:O	1:F:395:LEU:CD1	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:LEU:HD23	1:D:380:LEU:N	2.03	0.72
1:B:384:ALA:O	1:B:385:GLU:CB	2.37	0.72
1:C:334:LEU:N	1:C:334:LEU:HD23	2.04	0.72
1:C:102:ARG:HH11	1:C:102:ARG:HB2	1.54	0.71
1:D:377:MET:CA	1:D:380:LEU:HD21	2.20	0.71
1:C:382:LEU:O	1:C:385:GLU:CA	2.37	0.71
1:E:394:LEU:O	1:E:396:ALA:N	2.22	0.71
1:F:394:LEU:N	1:F:394:LEU:HD22	2.04	0.71
1:F:391:ALA:O	1:F:395:LEU:CG	2.39	0.71
1:A:132:TYR:O	1:A:133:ARG:HB2	1.88	0.71
1:A:97:TYR:CB	1:A:131:PRO:CG	2.67	0.71
1:D:339:ALA:HB1	1:D:342:ASP:HB2	1.72	0.70
1:D:381:LYS:O	1:D:384:ALA:N	2.16	0.70
1:A:380:LEU:HD23	1:A:381:LYS:N	2.03	0.70
1:F:368:LEU:HD23	1:F:456:ARG:NH2	2.05	0.70
1:C:130:LEU:HB2	1:C:131:PRO:HD3	1.74	0.70
1:C:99:TYR:OH	1:C:133:ARG:CB	2.37	0.70
1:D:432:ILE:HD11	1:D:444:THR:HG22	1.74	0.70
1:C:332:VAL:O	1:C:333:ASP:HB3	1.92	0.70
1:D:12:THR:HB	1:D:240:LYS:HE3	1.74	0.70
1:C:99:TYR:HH	1:C:133:ARG:HB3	1.55	0.70
1:D:244:ALA:C	1:D:246:ASP:N	2.41	0.70
1:C:133:ARG:O	1:C:133:ARG:HG2	1.92	0.69
1:C:235:GLY:O	1:C:237:LYS:N	2.25	0.69
1:F:96:TYR:CB	1:F:130:LEU:CD2	2.63	0.69
1:B:383:GLY:O	1:B:385:GLU:CA	2.40	0.69
1:D:383:GLY:O	1:D:387:PRO:CD	2.41	0.69
1:D:133:ARG:NE	1:D:133:ARG:HA	2.08	0.69
1:C:382:LEU:HD12	1:C:385:GLU:HB2	0.69	0.69
1:A:127:GLU:C	1:A:128:GLN:HG2	2.12	0.68
1:F:133:ARG:HG3	1:F:134:ASP:N	2.08	0.68
1:C:102:ARG:H	1:C:105:LEU:HD13	1.39	0.68
1:D:244:ALA:O	1:D:246:ASP:N	2.26	0.68
1:F:394:LEU:CD2	1:F:394:LEU:H	2.06	0.68
1:F:378:LYS:O	1:F:378:LYS:HG3	1.93	0.68
1:A:97:TYR:CG	1:A:131:PRO:CG	2.77	0.67
1:F:392:ARG:O	1:F:393:GLU:O	2.12	0.67
1:B:385:GLU:OE1	1:B:385:GLU:HA	1.94	0.67
1:C:102:ARG:HA	1:C:105:LEU:HB2	1.76	0.67
1:B:385:GLU:CG	1:B:464:ILE:CD1	2.70	0.67
1:D:243:GLY:C	1:D:245:ALA:H	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:LYS:NZ	1:E:378:LYS:O	2.23	0.67
1:F:10:SER:O	1:F:12:THR:HG23	1.94	0.67
1:F:372:ASP:O	1:F:376:VAL:HG23	1.94	0.67
1:D:337:GLY:N	1:D:338:PRO:HD3	2.10	0.67
1:F:125:ALA:C	1:F:126:ARG:O	2.24	0.66
1:D:135:ASP:HB2	1:D:136:PRO:CD	2.24	0.66
1:F:99:TYR:CE1	1:F:138:ARG:HB3	2.31	0.66
1:D:14:TYR:OH	1:D:244:ALA:CB	2.43	0.66
1:D:384:ALA:O	1:D:388:LEU:CD1	2.43	0.66
1:B:271:HIS:CE1	1:B:285:LEU:HD13	2.30	0.66
1:A:99:TYR:CE1	1:A:138:ARG:CB	2.79	0.66
1:F:400:GLN:N	1:F:400:GLN:OE1	2.28	0.66
1:F:11:PRO:HA	1:F:12:THR:HG1	1.60	0.66
1:A:99:TYR:CE1	1:A:138:ARG:HB3	2.31	0.66
1:C:382:LEU:CD1	1:C:385:GLU:CG	2.72	0.65
1:C:332:VAL:O	1:C:333:ASP:CB	2.45	0.65
1:C:382:LEU:O	1:C:385:GLU:HB2	1.97	0.65
1:C:102:ARG:O	1:C:103:GLU:C	2.32	0.65
1:D:246:ASP:OD1	1:D:247:VAL:N	2.30	0.65
1:E:380:LEU:O	1:E:382:LEU:N	2.30	0.65
1:F:132:TYR:O	1:F:133:ARG:CB	2.44	0.65
1:F:4:ARG:NH2	1:F:192:MET:O	2.24	0.65
1:C:102:ARG:O	1:C:103:GLU:O	2.15	0.64
1:C:102:ARG:CZ	1:C:102:ARG:HB2	2.28	0.64
1:D:384:ALA:O	1:D:388:LEU:HD12	1.97	0.64
1:D:241:ARG:O	1:D:242:THR:HG23	1.97	0.64
1:F:128:GLN:HE21	1:F:129:ASN:HB3	1.62	0.64
1:B:137:ASN:OD1	1:D:302:LYS:CE	2.42	0.64
1:B:386:VAL:N	1:B:387:PRO:CD	2.61	0.64
1:F:256:LEU:HD11	1:F:311:LEU:HD13	1.80	0.64
1:C:331:GLY:O	1:C:332:VAL:HG13	1.97	0.64
1:E:398:VAL:HG11	1:E:450:ARG:NE	2.12	0.64
1:F:320:ALA:HB1	1:F:340:ALA:HB3	1.80	0.64
1:C:89:LEU:HD21	1:C:217:LEU:CD1	2.28	0.63
1:C:333:ASP:OD2	1:C:335:ALA:HA	1.99	0.63
1:E:377:MET:HG2	1:F:380:LEU:HD13	1.80	0.63
1:F:99:TYR:HE1	1:F:138:ARG:HB3	1.63	0.63
1:A:207:THR:O	1:A:211:ILE:HG13	1.99	0.63
1:D:63:TRP:CE2	1:D:251:LYS:HG3	2.34	0.63
1:C:97:TYR:HB3	1:C:131:PRO:HG2	1.81	0.62
1:B:275:GLU:HG3	1:E:136:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ASN:CB	1:F:131:PRO:HD3	2.29	0.62
1:F:128:GLN:HG2	1:F:129:ASN:N	2.14	0.62
1:F:126:ARG:HD2	1:F:169:ASP:OD2	2.00	0.62
1:D:332:VAL:O	1:D:334:LEU:CD1	2.48	0.62
1:E:311:LEU:HD11	1:E:354:LEU:HD13	1.82	0.62
1:D:213:ILE:O	1:D:217:LEU:HD22	2.00	0.61
1:F:132:TYR:HD1	1:F:133:ARG:N	1.97	0.61
1:A:24:LEU:HD22	1:A:28:LEU:HD11	1.83	0.61
1:A:376:VAL:C	1:A:378:LYS:H	2.01	0.61
1:C:333:ASP:HB3	1:C:335:ALA:H	1.66	0.61
1:F:126:ARG:O	1:F:127:GLU:C	2.37	0.61
1:D:415:ALA:HB1	1:D:418:GLU:C	2.21	0.61
1:C:99:TYR:O	1:C:100:GLU:O	2.18	0.61
1:B:302:LYS:NZ	1:E:137:ASN:HD22	1.98	0.61
1:E:399:ASP:N	1:E:400:GLN:HA	2.15	0.61
1:F:366:GLN:O	1:F:368:LEU:HB3	2.01	0.60
1:A:130:LEU:HD23	1:A:130:LEU:N	2.14	0.60
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.65	0.60
1:C:338:PRO:HG2	1:C:447:LEU:HD22	1.83	0.60
1:B:381:LYS:O	1:B:383:GLY:N	2.34	0.60
1:C:382:LEU:O	1:C:385:GLU:CB	2.50	0.60
1:E:386:VAL:HG23	1:E:387:PRO:HD3	1.82	0.60
1:B:164:ASN:ND2	1:B:212:ASN:HD21	1.99	0.60
1:A:99:TYR:CE2	1:A:131:PRO:HB3	2.29	0.60
1:D:379:HIS:O	1:D:380:LEU:O	2.20	0.60
1:D:415:ALA:CB	1:D:418:GLU:HA	2.31	0.60
1:D:134:ASP:CB	1:D:138:ARG:NH1	2.65	0.59
1:F:129:ASN:CG	1:F:130:LEU:N	2.36	0.59
1:F:97:TYR:N	1:F:130:LEU:HD22	1.87	0.59
1:A:403:VAL:O	1:A:404:ASP:HB2	2.02	0.59
1:C:333:ASP:HB3	1:C:334:LEU:C	2.21	0.59
1:D:40:ARG:NH1	1:D:189:ASP:OD1	2.34	0.59
1:A:130:LEU:CD2	1:A:130:LEU:H	2.12	0.59
1:D:339:ALA:O	1:D:342:ASP:N	2.36	0.59
1:A:199:ARG:HD2	1:A:203:HIS:HB2	1.85	0.59
1:C:395:LEU:HD23	1:C:406:VAL:HG23	1.83	0.59
1:F:129:ASN:OD1	1:F:131:PRO:HD3	2.00	0.59
1:C:98:ALA:O	1:C:99:TYR:CD2	2.56	0.58
1:F:134:ASP:O	1:F:135:ASP:HB2	2.03	0.58
1:C:333:ASP:HB3	1:C:334:LEU:CA	2.33	0.58
1:E:394:LEU:HD13	1:E:413:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:NH2	1:C:144:ASN:O	2.36	0.58
1:C:305:TRP:CE3	1:F:136:PRO:HB3	2.38	0.58
1:F:390:LYS:NZ	1:F:393:GLU:CD	2.57	0.58
1:D:132:TYR:O	1:D:133:ARG:HB2	2.03	0.58
1:D:15:LEU:O	1:D:247:VAL:HG11	2.01	0.58
1:A:415:ALA:O	1:A:417:LEU:N	2.37	0.58
1:B:406:VAL:HG11	1:B:445:VAL:HG22	1.85	0.58
1:A:380:LEU:HD21	1:A:381:LYS:HG2	1.86	0.58
1:A:402:SER:O	1:A:406:VAL:HG13	2.04	0.58
1:F:129:ASN:O	1:F:130:LEU:CB	2.29	0.58
1:C:99:TYR:CZ	1:C:131:PRO:CG	2.77	0.57
1:F:18:GLY:HA2	1:F:230:ILE:HD13	1.85	0.57
1:F:96:TYR:CZ	1:F:126:ARG:HA	2.39	0.57
1:D:129:ASN:C	1:D:129:ASN:HD22	2.07	0.57
1:D:132:TYR:CD2	1:D:133:ARG:N	2.71	0.57
1:B:450:ARG:O	1:B:454:LEU:HD12	2.04	0.57
1:C:417:LEU:HD22	1:C:419:LEU:CD1	2.34	0.57
1:E:129:ASN:HB2	1:E:131:PRO:CD	2.35	0.57
1:F:128:GLN:HE21	1:F:129:ASN:H	1.51	0.57
1:F:121:TYR:OH	1:F:124:ALA:O	2.19	0.57
1:B:138:ARG:HG2	1:B:138:ARG:NH1	2.20	0.57
1:F:368:LEU:O	1:F:369:GLU:HG2	2.04	0.57
1:C:382:LEU:C	1:C:385:GLU:H	1.97	0.56
1:D:335:ALA:O	1:D:336:ALA:HB3	2.05	0.56
1:B:108:MET:HE1	1:B:122:ASP:N	2.19	0.56
1:C:97:TYR:CG	1:C:131:PRO:HB2	2.40	0.56
1:F:366:GLN:HG3	1:F:366:GLN:O	2.05	0.56
1:A:239:SER:O	1:A:244:ALA:HB2	2.05	0.56
1:F:135:ASP:C	1:F:137:ASN:H	2.09	0.56
1:A:99:TYR:OH	1:A:132:TYR:CA	2.53	0.56
1:B:55:ASP:O	1:B:59:GLU:HG3	2.06	0.56
1:A:415:ALA:O	1:A:416:ALA:C	2.43	0.56
1:C:382:LEU:CD1	1:C:385:GLU:CD	2.72	0.56
1:A:453:ALA:O	1:A:457:ILE:HG13	2.06	0.56
1:F:327:LEU:O	1:F:329:LYS:O	2.23	0.56
1:A:138:ARG:O	1:A:138:ARG:HG3	2.06	0.56
1:D:190:TRP:CD1	1:D:219:ALA:HB1	2.41	0.56
1:D:411:HIS:O	1:D:414:ALA:HB2	2.04	0.55
1:C:333:ASP:HB3	1:C:334:LEU:HA	1.89	0.55
1:E:239:SER:O	1:E:242:THR:HG22	2.06	0.55
1:A:323:LEU:HD13	1:A:357:MET:HE2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLY:O	1:B:22:THR:HG23	2.06	0.55
1:B:428:LEU:O	1:B:432:ILE:HG23	2.05	0.55
1:F:376:VAL:O	1:F:379:HIS:HB3	2.06	0.55
1:B:126:ARG:NH2	1:B:144:ASN:O	2.39	0.55
1:D:338:PRO:O	1:D:339:ALA:HB3	2.06	0.55
1:E:391:ALA:O	1:E:395:LEU:HB2	2.07	0.55
1:A:32:ARG:NH1	1:A:286:PHE:O	2.40	0.55
1:A:382:LEU:HD22	1:A:382:LEU:H	1.70	0.55
1:D:339:ALA:O	1:D:340:ALA:C	2.45	0.55
1:B:382:LEU:HD12	1:B:382:LEU:O	2.07	0.55
1:C:382:LEU:HD13	1:C:385:GLU:CG	2.37	0.55
1:B:312:LYS:HA	1:B:348:ARG:HD2	1.90	0.54
1:D:452:GLY:O	1:D:456:ARG:HG3	2.07	0.54
1:F:366:GLN:HG3	1:F:368:LEU:CB	2.23	0.54
1:E:51:GLN:NE2	1:E:54:ILE:HD11	2.22	0.54
1:F:132:TYR:CD1	1:F:133:ARG:N	2.74	0.54
1:A:332:VAL:CG2	1:A:365:TYR:HB3	2.37	0.54
1:A:380:LEU:CD2	1:A:381:LYS:HG2	2.38	0.54
1:B:386:VAL:H	1:B:387:PRO:HD2	1.71	0.54
1:D:334:LEU:N	1:D:334:LEU:CD1	2.71	0.54
1:E:390:LYS:HG3	1:E:417:LEU:HD21	1.88	0.54
1:B:378:LYS:O	1:B:381:LYS:NZ	2.36	0.54
1:F:390:LYS:O	1:F:393:GLU:HB3	2.08	0.54
1:B:351:VAL:HG21	1:B:357:MET:HG3	1.88	0.54
1:B:376:VAL:HG23	1:B:380:LEU:CD2	2.38	0.54
1:F:99:TYR:CE1	1:F:138:ARG:CB	2.91	0.53
1:F:391:ALA:O	1:F:395:LEU:HG	2.08	0.53
1:C:5:THR:HG21	1:C:26:CYS:O	2.08	0.53
1:E:100:GLU:N	1:E:100:GLU:OE2	2.41	0.53
1:E:138:ARG:O	1:E:139:VAL:HG13	2.09	0.53
1:E:386:VAL:HG23	1:E:387:PRO:CD	2.38	0.53
1:B:385:GLU:HG3	1:B:461:LEU:HD12	1.90	0.53
1:D:339:ALA:CB	1:D:342:ASP:HB2	2.37	0.53
1:E:130:LEU:N	1:E:131:PRO:CD	2.72	0.53
1:B:90:LEU:HD21	1:B:97:TYR:CZ	2.43	0.53
1:B:305:TRP:HZ2	1:E:134:ASP:HB3	1.74	0.53
1:F:96:TYR:CE2	1:F:126:ARG:CA	2.90	0.53
1:C:100:GLU:HB2	1:C:105:LEU:HD11	1.91	0.53
1:C:334:LEU:CD2	1:C:334:LEU:H	2.13	0.53
1:E:441:ILE:HA	1:E:444:THR:HG23	1.91	0.53
1:F:108:MET:CE	1:F:121:TYR:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:TYR:OH	1:A:131:PRO:HB2	2.09	0.53
1:C:333:ASP:CB	1:C:334:LEU:CA	2.87	0.53
1:A:310:TYR:HA	1:A:313:THR:HG22	1.90	0.53
1:A:380:LEU:CG	1:A:381:LYS:N	2.72	0.53
1:F:129:ASN:C	1:F:131:PRO:HD3	2.29	0.53
1:B:432:ILE:HD12	1:B:432:ILE:O	2.08	0.52
1:B:344:VAL:O	1:B:348:ARG:HG3	2.09	0.52
1:B:440:ASP:O	1:B:444:THR:HG23	2.10	0.52
1:C:207:THR:O	1:C:211:ILE:HG23	2.09	0.52
1:B:385:GLU:OE2	1:B:464:ILE:CD1	2.52	0.52
1:D:333:ASP:O	1:D:335:ALA:N	2.43	0.52
1:B:130:LEU:N	1:B:130:LEU:CD1	2.73	0.52
1:E:320:ALA:HB3	1:E:321:PRO:HD3	1.92	0.52
1:C:156:ILE:HD12	1:C:291:VAL:CG2	2.40	0.52
1:D:63:TRP:NE1	1:D:251:LYS:HG3	2.25	0.52
1:D:337:GLY:N	1:D:338:PRO:CD	2.70	0.52
1:E:398:VAL:C	1:E:400:GLN:HA	2.30	0.52
1:F:376:VAL:O	1:F:379:HIS:CB	2.58	0.52
1:A:262:ASN:HD21	1:A:276:LEU:HA	1.75	0.51
1:A:364:TRP:CH2	1:A:444:THR:HB	2.45	0.51
1:C:381:LYS:O	1:C:382:LEU:C	2.46	0.51
1:A:62:GLN:HG2	1:E:336:ALA:HB2	1.92	0.51
1:B:386:VAL:O	1:B:390:LYS:HB2	2.10	0.51
1:E:311:LEU:HD12	1:E:319:ILE:HD13	1.92	0.51
1:F:368:LEU:HD23	1:F:456:ARG:HH22	1.74	0.51
1:B:18:GLY:HA2	1:B:230:ILE:HD13	1.93	0.51
1:F:398:VAL:HG13	1:F:398:VAL:O	2.10	0.51
1:B:386:VAL:CG2	1:B:417:LEU:HD12	2.40	0.51
1:D:181:TYR:O	1:D:185:VAL:HG13	2.10	0.51
1:D:32:ARG:HG3	1:D:283:LEU:O	2.11	0.51
1:C:368:LEU:HB2	1:C:456:ARG:HE	1.75	0.51
1:F:135:ASP:O	1:F:137:ASN:N	2.43	0.51
1:D:334:LEU:N	1:D:334:LEU:HD12	2.25	0.51
1:D:28:LEU:O	1:D:32:ARG:HB2	2.11	0.51
1:D:332:VAL:O	1:D:334:LEU:HD12	2.11	0.51
1:F:133:ARG:CG	1:F:134:ASP:N	2.74	0.51
1:B:17:ILE:HG12	1:B:264:LEU:HD21	1.93	0.50
1:D:384:ALA:O	1:D:388:LEU:HD13	2.10	0.50
1:D:264:LEU:HD23	1:D:267:LEU:HD12	1.92	0.50
1:B:22:THR:HG22	1:B:227:MET:CE	2.41	0.50
1:D:381:LYS:HD2	1:D:423:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:SER:OG	1:E:444:THR:HG21	2.11	0.50
1:A:257:PRO:HD3	1:A:322:GLN:HE22	1.76	0.50
1:C:130:LEU:CB	1:C:131:PRO:HD3	2.40	0.50
1:C:347:LEU:O	1:C:351:VAL:HG22	2.11	0.50
1:D:17:ILE:CD1	1:D:264:LEU:HD21	2.41	0.50
1:D:320:ALA:HB1	1:D:340:ALA:HB3	1.94	0.50
1:F:128:GLN:CG	1:F:129:ASN:N	2.73	0.50
1:D:432:ILE:HD13	1:D:445:VAL:HA	1.93	0.50
1:F:11:PRO:HA	1:F:12:THR:CB	2.41	0.50
1:F:11:PRO:C	1:F:12:THR:HG23	2.32	0.50
1:C:332:VAL:C	1:C:334:LEU:HA	2.32	0.49
1:D:4:ARG:HD2	1:D:36:GLN:HE21	1.78	0.49
1:F:99:TYR:HH	1:F:133:ARG:HB3	1.77	0.49
1:C:100:GLU:CB	1:C:105:LEU:HD11	2.42	0.49
1:D:240:LYS:O	1:D:242:THR:N	2.35	0.49
1:E:411:HIS:HA	1:E:421:MET:HE1	1.93	0.49
1:B:302:LYS:O	1:B:306:VAL:HG12	2.12	0.49
1:C:198:ILE:HD12	1:C:198:ILE:N	2.27	0.49
1:F:309:HIS:CE1	1:F:313:THR:HG21	2.48	0.49
1:A:127:GLU:O	1:A:128:GLN:HG2	2.12	0.49
1:A:149:THR:HG22	1:A:163:ALA:HA	1.95	0.49
1:E:129:ASN:HB2	1:E:131:PRO:HD2	1.95	0.49
1:A:130:LEU:CD2	1:A:130:LEU:N	2.73	0.49
1:B:381:LYS:C	1:B:383:GLY:N	2.63	0.49
1:E:271:HIS:CE1	1:E:285:LEU:CD1	2.96	0.49
1:F:373:ALA:O	1:F:377:MET:HG2	2.12	0.49
1:B:120:ARG:HG2	1:B:168:ASP:HB3	1.94	0.49
1:B:15:LEU:HD13	1:B:57:ILE:HG23	1.95	0.49
1:F:391:ALA:O	1:F:395:LEU:HB2	2.12	0.49
1:B:140:ILE:HD12	1:B:173:PHE:HB3	1.96	0.48
1:B:416:ALA:O	1:B:417:LEU:HB3	2.13	0.48
1:A:43:ASP:OD1	1:A:76:THR:HG23	2.13	0.48
1:A:90:LEU:HD21	1:A:97:TYR:CE2	2.47	0.48
1:C:156:ILE:HD12	1:C:291:VAL:HG22	1.95	0.48
1:D:14:TYR:OH	1:D:244:ALA:HB1	2.13	0.48
1:D:29:GLU:OE1	1:D:33:ARG:NH2	2.46	0.48
1:C:378:LYS:HG3	1:C:379:HIS:N	2.27	0.48
1:D:377:MET:C	1:D:380:LEU:HD21	2.34	0.48
1:F:335:ALA:HB3	1:F:367:PRO:HD3	1.94	0.48
1:A:432:ILE:O	1:A:456:ARG:NH1	2.45	0.48
1:D:323:LEU:CD2	1:D:343:VAL:HG13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:ASP:HB3	1:E:302:LYS:HB2	1.95	0.48
1:D:14:TYR:OH	1:D:244:ALA:HB2	2.12	0.48
1:F:127:GLU:O	1:F:128:GLN:HB2	2.13	0.48
1:F:128:GLN:NE2	1:F:129:ASN:HB3	2.28	0.48
1:D:170:MET:HE2	1:D:209:ARG:HB3	1.94	0.47
1:F:32:ARG:HG3	1:F:283:LEU:O	2.14	0.47
1:B:136:PRO:C	1:B:138:ARG:H	2.17	0.47
1:D:404:ASP:O	1:D:407:SER:HB3	2.14	0.47
1:A:380:LEU:CD2	1:A:381:LYS:N	2.70	0.47
1:A:60:ALA:HB1	1:A:247:VAL:HG21	1.96	0.47
1:F:99:TYR:OH	1:F:133:ARG:HB3	2.14	0.47
1:A:9:PRO:HD2	1:A:40:ARG:O	2.14	0.47
1:B:385:GLU:HG2	1:B:464:ILE:HG21	1.96	0.47
1:F:129:ASN:HB2	1:F:131:PRO:HD3	1.94	0.47
1:F:134:ASP:O	1:F:135:ASP:CB	2.62	0.47
1:F:368:LEU:CD2	1:F:456:ARG:NH2	2.76	0.47
1:D:134:ASP:HA	1:D:138:ARG:HH11	1.80	0.47
1:F:90:LEU:CD2	1:F:97:TYR:CE2	2.97	0.47
1:C:457:ILE:O	1:C:461:LEU:N	2.44	0.47
1:E:231:LEU:HD22	1:E:235:GLY:O	2.15	0.47
1:B:22:THR:HG22	1:B:227:MET:HE1	1.95	0.47
1:B:373:ALA:O	1:B:376:VAL:HG12	2.14	0.47
1:C:162:ILE:HD12	1:C:208:PRO:HG3	1.97	0.47
1:D:333:ASP:C	1:D:335:ALA:H	2.18	0.47
1:F:128:GLN:CG	1:F:129:ASN:H	2.27	0.47
1:F:203:HIS:HA	1:F:206:ASN:HD22	1.79	0.47
1:C:31:ARG:NH1	1:C:69:ASP:OD1	2.48	0.46
1:A:98:ALA:HB1	1:A:100:GLU:OE2	2.16	0.46
1:A:134:ASP:O	1:A:135:ASP:C	2.54	0.46
1:F:135:ASP:C	1:F:137:ASN:N	2.69	0.46
1:A:386:VAL:HB	1:A:387:PRO:HD3	1.97	0.46
1:A:402:SER:HA	1:A:446:TYR:CE1	2.51	0.46
1:D:278:THR:OG1	1:D:281:GLU:HG3	2.15	0.46
1:F:402:SER:O	1:F:406:VAL:HG23	2.15	0.46
1:B:385:GLU:HG2	1:B:464:ILE:CD1	2.41	0.46
1:D:404:ASP:N	1:D:404:ASP:OD1	2.48	0.46
1:D:63:TRP:CB	1:D:248:MET:HE1	2.46	0.46
1:E:32:ARG:HG3	1:E:283:LEU:O	2.14	0.46
1:C:186:VAL:CG2	1:C:210:GLN:HG2	2.46	0.46
1:F:126:ARG:O	1:F:127:GLU:O	2.34	0.46
1:F:4:ARG:HD2	1:F:36:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:SER:O	1:B:406:VAL:HG23	2.16	0.46
1:C:97:TYR:HB2	1:C:131:PRO:HD2	1.98	0.46
1:C:21:ARG:CZ	1:C:230:ILE:HD11	2.46	0.46
1:D:133:ARG:NE	1:D:133:ARG:CA	2.78	0.46
1:E:108:MET:CE	1:E:121:TYR:HA	2.44	0.46
1:B:262:ASN:C	1:B:262:ASN:HD22	2.18	0.46
1:B:417:LEU:CD2	1:B:419:LEU:HB2	2.45	0.46
1:C:102:ARG:CZ	1:C:102:ARG:CB	2.93	0.46
1:C:338:PRO:HG3	1:C:447:LEU:HA	1.97	0.46
1:C:98:ALA:O	1:C:99:TYR:CG	2.69	0.46
1:D:257:PRO:O	1:D:261:ILE:HG23	2.16	0.46
1:E:432:ILE:HD13	1:E:448:ALA:HB2	1.97	0.46
1:F:391:ALA:O	1:F:395:LEU:CB	2.64	0.46
1:A:97:TYR:CD2	1:A:131:PRO:CD	2.98	0.46
1:B:385:GLU:CD	1:B:464:ILE:CD1	2.71	0.46
1:C:102:ARG:CA	1:C:105:LEU:CD1	2.76	0.46
1:D:170:MET:HE3	1:D:213:ILE:HD11	1.98	0.46
1:E:377:MET:HA	1:F:380:LEU:HD22	1.97	0.46
1:A:60:ALA:HB1	1:A:247:VAL:CG2	2.46	0.46
1:A:460:ALA:O	1:A:464:ILE:HG13	2.16	0.46
1:D:415:ALA:CA	1:D:419:LEU:H	2.26	0.46
1:A:24:LEU:HD22	1:A:28:LEU:CD1	2.46	0.45
1:C:32:ARG:HG3	1:C:283:LEU:O	2.15	0.45
1:D:21:ARG:NH1	1:D:230:ILE:HD11	2.31	0.45
1:F:366:GLN:C	1:F:368:LEU:N	2.69	0.45
1:C:150:VAL:HG23	1:C:211:ILE:HD11	1.98	0.45
1:D:17:ILE:HD12	1:D:264:LEU:HD21	1.97	0.45
1:A:327:LEU:HB3	1:A:332:VAL:HG11	1.99	0.45
1:E:386:VAL:O	1:E:390:LYS:HB2	2.16	0.45
1:F:97:TYR:HB2	1:F:130:LEU:HA	1.99	0.45
1:A:388:LEU:HD22	1:A:457:ILE:HG23	1.99	0.45
1:D:90:LEU:HD21	1:D:97:TYR:CE2	2.52	0.45
1:E:453:ALA:O	1:E:457:ILE:HG13	2.16	0.45
1:B:21:ARG:NE	1:B:230:ILE:HD11	2.31	0.45
1:B:441:ILE:O	1:B:445:VAL:HG13	2.16	0.45
1:D:344:VAL:O	1:D:348:ARG:HB2	2.17	0.45
1:D:88:GLN:HG2	1:D:92:GLN:HE21	1.81	0.45
1:A:128:GLN:HB2	1:A:129:ASN:H	1.50	0.45
1:A:379:HIS:O	1:A:380:LEU:C	2.55	0.45
1:D:207:THR:N	1:D:208:PRO:HD2	2.31	0.45
1:B:138:ARG:C	1:B:139:VAL:HG13	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:VAL:HG23	1:D:387:PRO:HD3	1.99	0.45
1:D:399:ASP:C	1:D:401:TRP:HA	2.37	0.45
1:F:144:ASN:ND2	1:F:212:ASN:HD22	2.13	0.45
1:D:411:HIS:O	1:D:414:ALA:CB	2.65	0.45
1:F:242:THR:OG1	1:F:243:GLY:N	2.50	0.45
1:A:429:ARG:O	1:A:433:THR:HB	2.18	0.44
1:D:411:HIS:O	1:D:411:HIS:ND1	2.50	0.44
1:C:133:ARG:CG	1:C:133:ARG:O	2.64	0.44
1:D:262:ASN:HD22	1:D:262:ASN:C	2.20	0.44
1:D:377:MET:CA	1:D:380:LEU:CD2	2.76	0.44
1:D:391:ALA:O	1:D:395:LEU:HD22	2.16	0.44
1:E:64:LEU:HD21	1:E:260:LEU:HD23	1.98	0.44
1:A:90:LEU:HD11	1:A:140:ILE:HG23	1.99	0.44
1:B:4:ARG:HD3	1:B:36:GLN:HE21	1.83	0.44
1:D:245:ALA:O	1:D:246:ASP:HB3	2.17	0.44
1:E:149:THR:HG22	1:E:163:ALA:HA	1.98	0.44
1:F:122:ASP:O	1:F:124:ALA:N	2.50	0.44
1:A:364:TRP:HH2	1:A:444:THR:HB	1.82	0.44
1:F:347:LEU:HD21	1:F:439:PRO:HG3	2.00	0.44
1:A:31:ARG:NH2	1:A:69:ASP:OD1	2.50	0.44
1:C:377:MET:SD	1:C:378:LYS:N	2.90	0.44
1:F:124:ALA:O	1:F:125:ALA:HB3	2.17	0.44
1:C:302:LYS:HG2	1:F:136:PRO:O	2.18	0.44
1:C:155:LEU:HD21	1:C:223:LYS:HG3	2.00	0.44
1:C:308:GLN:O	1:C:312:LYS:HG3	2.18	0.44
1:D:21:ARG:CZ	1:D:230:ILE:HD11	2.48	0.44
1:D:243:GLY:O	1:D:244:ALA:HB3	2.18	0.44
1:F:135:ASP:OD1	1:F:137:ASN:N	2.47	0.44
1:F:120:ARG:HG2	1:F:168:ASP:HB3	2.00	0.44
1:A:108:MET:HE2	1:A:121:TYR:HA	2.00	0.44
1:A:171:VAL:O	1:A:180:THR:HG21	2.18	0.44
1:E:410:LEU:HD21	1:E:428:LEU:HD23	1.98	0.44
1:F:128:GLN:NE2	1:F:129:ASN:HD22	2.16	0.44
1:A:47:GLN:O	1:A:49:SER:N	2.51	0.44
1:C:179:PRO:CG	1:C:184:ALA:HB2	2.48	0.44
1:C:384:ALA:O	1:C:387:PRO:HD2	2.18	0.44
1:E:28:LEU:HD11	1:E:282:LEU:HD13	2.00	0.44
1:A:376:VAL:HG21	1:B:376:VAL:CG1	2.48	0.43
1:A:380:LEU:HG	1:A:381:LYS:N	2.32	0.43
1:D:380:LEU:H	1:D:380:LEU:CD2	2.05	0.43
1:E:394:LEU:HD22	1:E:412:ASP:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LEU:CD2	1:C:406:VAL:HG23	2.47	0.43
1:D:162:ILE:HD12	1:D:208:PRO:HG3	1.98	0.43
1:A:183:PHE:O	1:A:187:VAL:HG23	2.18	0.43
1:B:382:LEU:C	1:B:384:ALA:N	2.72	0.43
1:E:182:ASN:OD1	1:E:206:ASN:HB3	2.18	0.43
1:F:394:LEU:CD2	1:F:394:LEU:N	2.72	0.43
1:B:136:PRO:C	1:B:138:ARG:N	2.72	0.43
1:C:333:ASP:CB	1:C:334:LEU:C	2.85	0.43
1:F:29:GLU:OE2	1:F:32:ARG:NH2	2.50	0.43
1:A:131:PRO:HB2	1:A:132:TYR:H	1.53	0.43
1:A:207:THR:N	1:A:208:PRO:HD2	2.32	0.43
1:F:328:ALA:C	1:F:329:LYS:O	2.57	0.43
1:C:382:LEU:HD13	1:C:385:GLU:HB2	1.70	0.43
1:D:132:TYR:CG	1:D:133:ARG:N	2.85	0.43
1:D:388:LEU:HD11	1:D:427:PRO:HB2	2.01	0.43
1:E:311:LEU:HD11	1:E:354:LEU:CD1	2.47	0.43
1:E:438:SER:HG	1:E:444:THR:HG21	1.83	0.43
1:D:327:LEU:HB3	1:D:358:ALA:HB1	2.00	0.43
1:D:399:ASP:O	1:D:401:TRP:HA	2.18	0.43
1:F:230:ILE:HG22	1:F:298:LEU:HD12	2.01	0.43
1:D:243:GLY:C	1:D:245:ALA:N	2.68	0.43
1:E:21:ARG:CZ	1:E:230:ILE:HD11	2.49	0.43
1:E:99:TYR:CE2	1:E:138:ARG:HG3	2.54	0.43
1:F:309:HIS:O	1:F:313:THR:HG23	2.19	0.43
1:B:418:GLU:O	1:B:418:GLU:HG3	2.18	0.43
1:C:333:ASP:N	1:C:334:LEU:HA	2.34	0.43
1:E:18:GLY:HA2	1:E:230:ILE:HD13	2.00	0.43
1:F:162:ILE:HD12	1:F:208:PRO:HG3	2.01	0.43
1:B:164:ASN:HD21	1:B:212:ASN:HD21	1.67	0.43
1:B:144:ASN:ND2	1:B:212:ASN:HD22	2.16	0.43
1:F:125:ALA:O	1:F:128:GLN:HB3	2.19	0.43
1:A:440:ASP:O	1:A:444:THR:HG23	2.18	0.42
1:C:372:ASP:HB3	1:C:375:ALA:HB3	2.01	0.42
1:E:108:MET:SD	1:E:122:ASP:OD1	2.77	0.42
1:E:133:ARG:C	1:E:134:ASP:O	2.57	0.42
1:D:337:GLY:O	1:D:365:TYR:CZ	2.72	0.42
1:E:463:LYS:HB3	1:F:377:MET:HE2	2.00	0.42
1:E:130:LEU:N	1:E:131:PRO:HD3	2.34	0.42
1:B:179:PRO:HG2	1:B:184:ALA:HB2	2.00	0.42
1:C:156:ILE:HD11	1:C:288:VAL:HG22	2.02	0.42
1:C:333:ASP:CB	1:C:335:ALA:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:GLY:O	1:C:387:PRO:HD2	2.17	0.42
1:F:132:TYR:HD1	1:F:133:ARG:C	2.16	0.42
1:D:126:ARG:NH2	1:D:144:ASN:O	2.52	0.42
1:D:337:GLY:H	1:D:338:PRO:HD3	1.81	0.42
1:E:29:GLU:OE2	1:E:288:VAL:HG12	2.20	0.42
1:D:21:ARG:CZ	1:D:230:ILE:CD1	2.98	0.42
1:E:380:LEU:HD22	1:E:381:LYS:N	2.34	0.42
1:F:278:THR:HG23	1:F:281:GLU:OE2	2.19	0.42
1:A:151:VAL:CG2	1:A:161:GLU:HG3	2.50	0.42
1:B:136:PRO:C	1:B:137:ASN:ND2	2.73	0.42
1:D:2:ALA:O	1:D:195:THR:HG21	2.20	0.42
1:A:126:ARG:NH2	1:A:144:ASN:O	2.53	0.42
1:B:207:THR:N	1:B:208:PRO:HD2	2.34	0.42
1:D:31:ARG:NH2	1:D:69:ASP:OD1	2.50	0.42
1:E:139:VAL:HG23	1:E:139:VAL:O	2.19	0.42
1:C:406:VAL:HG11	1:C:445:VAL:HG13	2.01	0.42
1:B:96:TYR:CE2	1:B:126:ARG:HA	2.55	0.41
1:C:38:VAL:HG21	1:C:192:MET:CE	2.50	0.41
1:D:15:LEU:C	1:D:247:VAL:HG11	2.40	0.41
1:D:382:LEU:C	1:D:384:ALA:N	2.72	0.41
1:E:417:LEU:HD12	1:E:419:LEU:HD11	2.02	0.41
1:D:244:ALA:O	1:D:245:ALA:HB3	2.19	0.41
1:D:63:TRP:HB3	1:D:248:MET:HE1	2.02	0.41
1:F:156:ILE:HG12	1:F:291:VAL:HG22	2.02	0.41
1:B:302:LYS:HG2	1:E:136:PRO:HB2	2.02	0.41
1:F:144:ASN:HD21	1:F:212:ASN:HD22	1.68	0.41
1:B:256:LEU:HD11	1:B:311:LEU:CD1	2.50	0.41
1:D:205:ASN:N	1:D:205:ASN:HD22	2.18	0.41
1:A:134:ASP:HB3	1:A:135:ASP:H	1.37	0.41
1:B:162:ILE:HD12	1:B:208:PRO:HG3	2.02	0.41
1:C:379:HIS:CG	1:C:379:HIS:O	2.74	0.41
1:D:240:LYS:C	1:D:242:THR:N	2.74	0.41
1:F:458:ASP:O	1:F:462:THR:HG23	2.20	0.41
1:A:83:GLN:HG2	1:A:173:PHE:CZ	2.56	0.41
1:A:376:VAL:C	1:A:378:LYS:N	2.71	0.41
1:B:336:ALA:HB3	1:B:365:TYR:O	2.20	0.41
1:C:263:TYR:OH	1:C:298:LEU:HD23	2.20	0.41
1:B:438:SER:OG	1:B:444:THR:HG21	2.20	0.41
1:C:103:GLU:O	1:C:106:ASP:N	2.53	0.41
1:E:395:LEU:C	1:E:397:ALA:H	2.23	0.41
1:A:33:ARG:NH1	2:A:501:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:GLY:O	1:B:385:GLU:HA	2.15	0.41
1:D:14:TYR:CE1	1:D:244:ALA:HB1	2.56	0.41
1:D:243:GLY:O	1:D:245:ALA:N	2.54	0.41
1:F:159:ARG:C	1:F:160:ILE:HD12	2.41	0.41
1:F:392:ARG:C	1:F:393:GLU:O	2.59	0.41
1:D:386:VAL:HG23	1:D:387:PRO:CD	2.51	0.41
1:E:90:LEU:HD21	1:E:97:TYR:CE2	2.56	0.41
1:F:124:ALA:O	1:F:125:ALA:CB	2.69	0.41
1:B:99:TYR:CE2	1:B:138:ARG:HB2	2.56	0.41
1:C:256:LEU:HD23	1:C:354:LEU:HD11	2.02	0.41
1:D:402:SER:O	1:D:406:VAL:HG13	2.20	0.41
1:F:15:LEU:O	1:F:247:VAL:HG13	2.21	0.41
1:A:232:ASP:N	1:A:236:THR:O	2.47	0.41
1:D:60:ALA:HA	1:D:248:MET:CE	2.51	0.41
1:B:130:LEU:HA	1:B:131:PRO:HD3	1.85	0.40
1:C:256:LEU:CD2	1:C:354:LEU:HD11	2.51	0.40
1:D:135:ASP:CB	1:D:136:PRO:CD	2.97	0.40
1:E:75:GLN:HG3	1:E:82:TYR:OH	2.21	0.40
1:A:127:GLU:O	1:A:128:GLN:CB	2.69	0.40
1:A:382:LEU:O	1:A:385:GLU:HG2	2.22	0.40
1:C:100:GLU:HB3	1:C:105:LEU:CD1	2.52	0.40
1:C:153:ASP:N	1:C:153:ASP:OD1	2.54	0.40
1:E:302:LYS:O	1:E:306:VAL:HG12	2.20	0.40
1:F:128:GLN:HE21	1:F:129:ASN:CB	2.30	0.40
1:C:18:GLY:HA2	1:C:230:ILE:HD13	2.03	0.40
1:F:79:VAL:HG23	1:F:178:LEU:HD12	2.03	0.40
1:F:17:ILE:CD1	1:F:264:LEU:HD21	2.52	0.40
1:F:357:MET:O	1:F:361:ALA:N	2.53	0.40
1:A:380:LEU:C	1:A:381:LYS:O	2.56	0.40
1:B:124:ALA:O	1:B:128:GLN:NE2	2.55	0.40
1:B:60:ALA:HB1	1:B:247:VAL:HG21	2.02	0.40
1:D:129:ASN:ND2	1:D:129:ASN:C	2.73	0.40
1:D:132:TYR:HD2	1:D:133:ARG:H	1.66	0.40
1:F:308:GLN:HE21	1:F:312:LYS:HE2	1.86	0.40
1:A:26:CYS:SG	1:A:198:ILE:HB	2.61	0.40
1:C:131:PRO:HB3	1:C:132:TYR:HA	2.03	0.40
1:C:88:GLN:HE21	1:C:92:GLN:NE2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/488 (95%)	418 (90%)	35 (8%)	10 (2%)	6	31
1	B	456/488 (93%)	418 (92%)	31 (7%)	7 (2%)	10	42
1	C	445/488 (91%)	395 (89%)	36 (8%)	14 (3%)	4	23
1	D	463/488 (95%)	417 (90%)	28 (6%)	18 (4%)	3	17
1	E	463/488 (95%)	426 (92%)	26 (6%)	11 (2%)	6	29
1	F	463/488 (95%)	412 (89%)	31 (7%)	20 (4%)	2	15
All	All	2753/2928 (94%)	2486 (90%)	187 (7%)	80 (3%)	4	24

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	132	TYR
1	A	133	ARG
1	A	134	ASP
1	A	383	GLY
1	A	404	ASP
1	B	384	ALA
1	B	385	GLU
1	C	100	GLU
1	C	332	VAL
1	C	333	ASP
1	C	335	ALA
1	C	421	MET
1	D	132	TYR
1	D	380	LEU
1	D	382	LEU
1	E	381	LYS
1	E	396	ALA
1	F	126	ARG
1	F	128	GLN

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Mol	Chain	Res	Type
1	F	129	ASN
1	F	130	LEU
1	F	132	TYR
1	F	135	ASP
1	F	369	GLU
1	F	380	LEU
1	F	393	GLU
1	B	123	GLY
1	B	400	GLN
1	B	439	PRO
1	C	99	TYR
1	C	340	ALA
1	C	420	GLY
1	D	247	VAL
1	D	334	LEU
1	D	381	LYS
1	D	414	ALA
1	E	11	PRO
1	E	134	ASP
1	E	379	HIS
1	E	398	VAL
1	F	125	ALA
1	F	127	GLU
1	F	378	LYS
1	B	336	ALA
1	C	130	LEU
1	C	337	GLY
1	D	129	ASN
1	D	245	ALA
1	D	338	PRO
1	D	339	ALA
1	D	416	ALA
1	E	128	GLN
1	E	401	TRP
1	E	465	GLY
1	F	123	GLY
1	F	136	PRO
1	F	329	LYS
1	A	131	PRO
1	A	450	ARG
1	C	103	GLU
1	C	339	ALA

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Mol	Chain	Res	Type
1	D	465	GLY
1	E	135	ASP
1	F	440	ASP
1	C	418	GLU
1	D	336	ALA
1	D	409	ALA
1	D	133	ARG
1	F	116	GLN
1	F	394	LEU
1	A	243	GLY
1	D	439	PRO
1	F	13	GLY
1	F	367	PRO
1	C	135	ASP
1	D	11	PRO
1	E	130	LEU
1	B	465	GLY
1	A	136	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/386 (95%)	321 (88%)	46 (12%)	4	20
1	B	363/386 (94%)	314 (86%)	49 (14%)	4	17
1	C	359/386 (93%)	301 (84%)	58 (16%)	2	12
1	D	367/386 (95%)	313 (85%)	54 (15%)	3	15
1	E	367/386 (95%)	300 (82%)	67 (18%)	1	9
1	F	366/386 (95%)	303 (83%)	63 (17%)	2	10
All	All	2189/2316 (94%)	1852 (85%)	337 (15%)	2	13

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	17	ILE
1	A	24	LEU
1	A	33	ARG
1	A	38	VAL
1	A	44	THR
1	A	47	GLN
1	A	48	ARG
1	A	54	ILE
1	A	83	GLN
1	A	105	LEU
1	A	113	MET
1	A	116	GLN
1	A	118	LYS
1	A	130	LEU
1	A	132	TYR
1	A	133	ARG
1	A	138	ARG
1	A	146	ILE
1	A	160	ILE
1	A	166	GLU
1	A	167	LEU
1	A	178	LEU
1	A	202	ASP
1	A	217	LEU
1	A	227	MET
1	A	240	LYS
1	A	241	ARG
1	A	270	SER
1	A	291	VAL
1	A	306	VAL
1	A	308	GLN
1	A	311	LEU
1	A	313	THR
1	A	362	VAL
1	A	368	LEU
1	A	378	LYS
1	A	381	LYS
1	A	386	VAL
1	A	395	LEU
1	A	406	VAL
1	A	421	MET
1	A	432	ILE

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Mol	Chain	Res	Type
1	A	444	THR
1	A	445	VAL
1	A	461	LEU
1	B	6	ARG
1	B	17	ILE
1	B	24	LEU
1	B	44	THR
1	B	47	GLN
1	B	55	ASP
1	B	73	ILE
1	B	113	MET
1	B	118	LYS
1	B	126	ARG
1	B	127	GLU
1	B	130	LEU
1	B	137	ASN
1	B	146	ILE
1	B	150	VAL
1	B	167	LEU
1	B	170	MET
1	B	178	LEU
1	B	199	ARG
1	B	201	ASP
1	B	202	ASP
1	B	217	LEU
1	B	262	ASN
1	B	266	ARG
1	B	293	SER
1	B	294	LYS
1	B	311	LEU
1	B	327	LEU
1	B	330	LEU
1	B	332	VAL
1	B	334	LEU
1	B	345	VAL
1	B	349	GLU
1	B	350	ARG
1	B	357	MET
1	B	363	VAL
1	B	377	MET
1	B	381	LYS
1	B	382	LEU

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Mol	Chain	Res	Type
1	B	385	GLU
1	B	392	ARG
1	B	395	LEU
1	B	400	GLN
1	B	417	LEU
1	B	423	LYS
1	B	432	ILE
1	B	445	VAL
1	B	451	GLU
1	B	461	LEU
1	C	5	THR
1	C	6	ARG
1	C	24	LEU
1	C	38	VAL
1	C	44	THR
1	C	102	ARG
1	C	104	GLU
1	C	116	GLN
1	C	130	LEU
1	C	135	ASP
1	C	137	ASN
1	C	146	ILE
1	C	150	VAL
1	C	153	ASP
1	C	155	LEU
1	C	160	ILE
1	C	165	SER
1	C	167	LEU
1	C	169	ASP
1	C	170	MET
1	C	178	LEU
1	C	182	ASN
1	C	199	ARG
1	C	211	ILE
1	C	217	LEU
1	C	223	LYS
1	C	227	MET
1	C	232	ASP
1	C	233	GLU
1	C	247	VAL
1	C	264	LEU
1	C	266	ARG

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Mol	Chain	Res	Type
1	C	273	ASP
1	C	323	LEU
1	C	330	LEU
1	C	332	VAL
1	C	334	LEU
1	C	344	VAL
1	C	347	LEU
1	C	349	GLU
1	C	370	THR
1	C	377	MET
1	C	378	LYS
1	C	379	HIS
1	C	388	LEU
1	C	392	ARG
1	C	405	SER
1	C	410	LEU
1	C	417	LEU
1	C	421	MET
1	C	426	GLN
1	C	436	GLN
1	C	438	SER
1	C	441	ILE
1	C	442	SER
1	C	451	GLU
1	C	455	LYS
1	C	464	ILE
1	D	6	ARG
1	D	10	SER
1	D	17	ILE
1	D	24	LEU
1	D	31	ARG
1	D	44	THR
1	D	46	ARG
1	D	47	GLN
1	D	49	SER
1	D	50	THR
1	D	62	GLN
1	D	101	THR
1	D	109	ARG
1	D	115	LYS
1	D	118	LYS
1	D	129	ASN

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Mol	Chain	Res	Type
1	D	133	ARG
1	D	134	ASP
1	D	146	ILE
1	D	159	ARG
1	D	162	ILE
1	D	167	LEU
1	D	174	ARG
1	D	199	ARG
1	D	204	ILE
1	D	205	ASN
1	D	217	LEU
1	D	247	VAL
1	D	261	ILE
1	D	262	ASN
1	D	291	VAL
1	D	297	ARG
1	D	311	LEU
1	D	327	LEU
1	D	332	VAL
1	D	334	LEU
1	D	344	VAL
1	D	376	VAL
1	D	377	MET
1	D	378	LYS
1	D	380	LEU
1	D	381	LYS
1	D	382	LEU
1	D	386	VAL
1	D	393	GLU
1	D	401	TRP
1	D	411	HIS
1	D	418	GLU
1	D	432	ILE
1	D	445	VAL
1	D	450	ARG
1	D	451	GLU
1	D	461	LEU
1	D	463	LYS
1	E	6	ARG
1	E	17	ILE
1	E	24	LEU
1	E	38	VAL

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Mol	Chain	Res	Type
1	E	48	ARG
1	E	83	GLN
1	E	88	GLN
1	E	102	ARG
1	E	110	GLU
1	E	113	MET
1	E	116	GLN
1	E	120	ARG
1	E	126	ARG
1	E	129	ASN
1	E	137	ASN
1	E	146	ILE
1	E	150	VAL
1	E	153	ASP
1	E	167	LEU
1	E	199	ARG
1	E	204	ILE
1	E	217	LEU
1	E	227	MET
1	E	232	ASP
1	E	233	GLU
1	E	238	LEU
1	E	240	LYS
1	E	241	ARG
1	E	262	ASN
1	E	266	ARG
1	E	270	SER
1	E	273	ASP
1	E	285	LEU
1	E	289	LYS
1	E	291	VAL
1	E	294	LYS
1	E	300	MET
1	E	302	LYS
1	E	311	LEU
1	E	327	LEU
1	E	334	LEU
1	E	342	ASP
1	E	347	LEU
1	E	348	ARG
1	E	349	GLU
1	E	354	LEU

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Mol	Chain	Res	Type
1	E	368	LEU
1	E	370	THR
1	E	377	MET
1	E	378	LYS
1	E	379	HIS
1	E	380	LEU
1	E	382	LEU
1	E	390	LYS
1	E	392	ARG
1	E	395	LEU
1	E	400	GLN
1	E	405	SER
1	E	419	LEU
1	E	432	ILE
1	E	443	GLN
1	E	444	THR
1	E	445	VAL
1	E	454	LEU
1	E	461	LEU
1	E	462	THR
1	E	463	LYS
1	F	6	ARG
1	F	10	SER
1	F	14	TYR
1	F	17	ILE
1	F	24	LEU
1	F	31	ARG
1	F	38	VAL
1	F	46	ARG
1	F	50	THR
1	F	54	ILE
1	F	55	ASP
1	F	62	GLN
1	F	68	TYR
1	F	102	ARG
1	F	103	GLU
1	F	109	ARG
1	F	117	GLU
1	F	118	LYS
1	F	129	ASN
1	F	130	LEU
1	F	133	ARG

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Mol	Chain	Res	Type
1	F	146	ILE
1	F	150	VAL
1	F	165	SER
1	F	170	MET
1	F	178	LEU
1	F	199	ARG
1	F	217	LEU
1	F	221	VAL
1	F	240	LYS
1	F	242	THR
1	F	247	VAL
1	F	262	ASN
1	F	275	GLU
1	F	285	LEU
1	F	293	SER
1	F	294	LYS
1	F	298	LEU
1	F	311	LEU
1	F	332	VAL
1	F	333	ASP
1	F	334	LEU
1	F	348	ARG
1	F	362	VAL
1	F	368	LEU
1	F	369	GLU
1	F	370	THR
1	F	377	MET
1	F	378	LYS
1	F	382	LEU
1	F	385	GLU
1	F	390	LYS
1	F	392	ARG
1	F	394	LEU
1	F	400	GLN
1	F	410	LEU
1	F	419	LEU
1	F	429	ARG
1	F	432	ILE
1	F	433	THR
1	F	442	SER
1	F	454	LEU
1	F	461	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	88	GLN
1	A	92	GLN
1	A	116	GLN
1	A	206	ASN
1	A	262	ASN
1	A	322	GLN
1	A	443	GLN
1	B	16	HIS
1	B	36	GLN
1	B	47	GLN
1	B	75	GLN
1	B	129	ASN
1	B	164	ASN
1	B	206	ASN
1	B	212	ASN
1	B	271	HIS
1	B	280	GLN
1	C	88	GLN
1	C	92	GLN
1	C	116	GLN
1	C	258	HIS
1	C	426	GLN
1	C	443	GLN
1	D	36	GLN
1	D	62	GLN
1	D	88	GLN
1	D	92	GLN
1	D	116	GLN
1	D	129	ASN
1	D	137	ASN
1	D	203	HIS
1	D	205	ASN
1	D	258	HIS
1	D	292	ASN
1	D	322	GLN
1	D	366	GLN
1	E	51	GLN
1	E	137	ASN
1	E	206	ASN
1	E	443	GLN

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Mol	Chain	Res	Type
1	F	51	GLN
1	F	128	GLN
1	F	144	ASN
1	F	308	GLN
1	F	309	HIS
1	F	366	GLN

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 carbohydrates 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, 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	465/488 (95%)	-0.19	11 (2%) 59 30	43, 66, 110, 133	0
1	B	460/488 (94%)	-0.28	7 (1%) 73 46	36, 61, 96, 124	0
1	C	455/488 (93%)	0.01	18 (3%) 38 15	56, 82, 120, 150	0
1	D	465/488 (95%)	-0.18	13 (2%) 53 25	40, 64, 111, 143	0
1	E	465/488 (95%)	-0.21	11 (2%) 59 30	42, 62, 96, 150	0
1	F	465/488 (95%)	-0.20	3 (0%) 89 72	42, 66, 114, 139	0
All	All	2775/2928 (94%)	-0.17	63 (2%) 60 31	36, 67, 111, 150	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	242	THR	3.5
1	C	466	ALA	3.5
1	C	135	ASP	3.4
1	D	114	ALA	3.4
1	C	129	ASN	3.4
1	E	114	ALA	3.3
1	D	51	GLN	3.1
1	E	237	LYS	3.1
1	A	399	ASP	3.1
1	C	117	GLU	3.1
1	B	244	ALA	3.0
1	D	241	ARG	3.0
1	D	400	GLN	3.0
1	E	130	LEU	2.9
1	F	241	ARG	2.9
1	E	400	GLN	2.9
1	F	242	THR	2.9
1	C	133	ARG	2.9
1	A	398	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	49	SER	2.9
1	C	398	VAL	2.8
1	E	243	GLY	2.7
1	B	399	ASP	2.7
1	D	245	ALA	2.7
1	A	116	GLN	2.7
1	C	239	SER	2.7
1	C	415	ALA	2.6
1	D	411	HIS	2.6
1	E	113	MET	2.6
1	D	239	SER	2.5
1	E	399	ASP	2.4
1	A	239	SER	2.4
1	E	239	SER	2.4
1	A	118	LYS	2.4
1	A	241	ARG	2.4
1	B	421	MET	2.4
1	B	386	VAL	2.4
1	A	113	MET	2.4
1	C	240	LYS	2.4
1	A	115	LYS	2.3
1	D	2	ALA	2.3
1	A	242	THR	2.3
1	C	118	LYS	2.3
1	C	113	MET	2.3
1	C	421	MET	2.3
1	C	12	THR	2.3
1	A	135	ASP	2.2
1	B	284	ASP	2.2
1	A	114	ALA	2.2
1	D	117	GLU	2.2
1	D	116	GLN	2.2
1	E	241	ARG	2.2
1	C	234	GLN	2.2
1	D	315	ASP	2.2
1	C	330	LEU	2.2
1	D	418	GLU	2.2
1	F	51	GLN	2.2
1	D	417	LEU	2.2
1	B	419	LEU	2.1
1	B	115	LYS	2.1
1	C	146	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	134	ASP	2.0
1	E	240	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.