



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:40 AM UTC

PDB ID : 1XFB / pdb_00001xfb
Title : Human Brain Fructose 1,6-(bis)phosphate Aldolase (C isozyme)
Authors : Arakaki, T.L.; Pezza, J.A.; Cronin, M.A.; Hopkins, C.E.; Zimmer, D.B.; Tolan, D.R.; Allen, K.N.
Deposited on : 2004-09-14
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 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

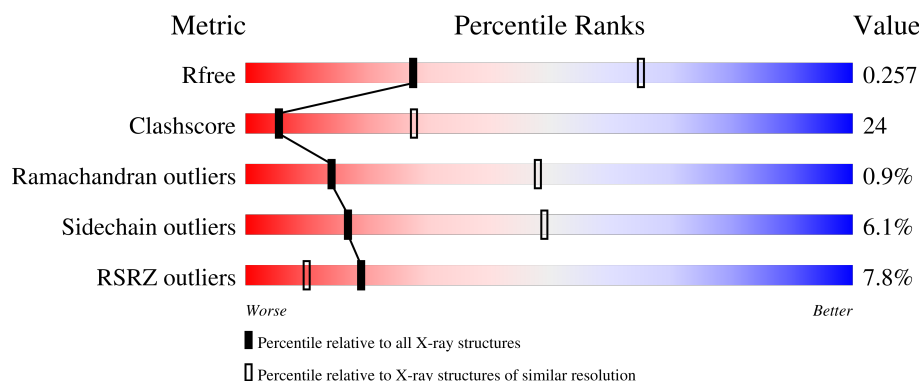
1 Overall quality at a glance

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.



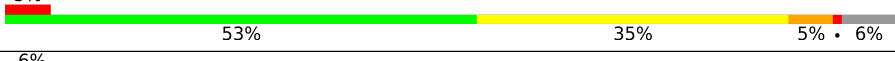
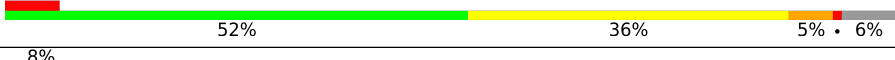
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 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 $\leq 5\%$. 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	365	
1	B	365	
1	C	365	
1	D	365	
1	E	365	

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Mol	Chain	Length	Quality of chain
1	F	365	
1	G	365	
1	H	365	
1	I	365	
1	J	365	
1	K	365	
1	L	365	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31476 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.

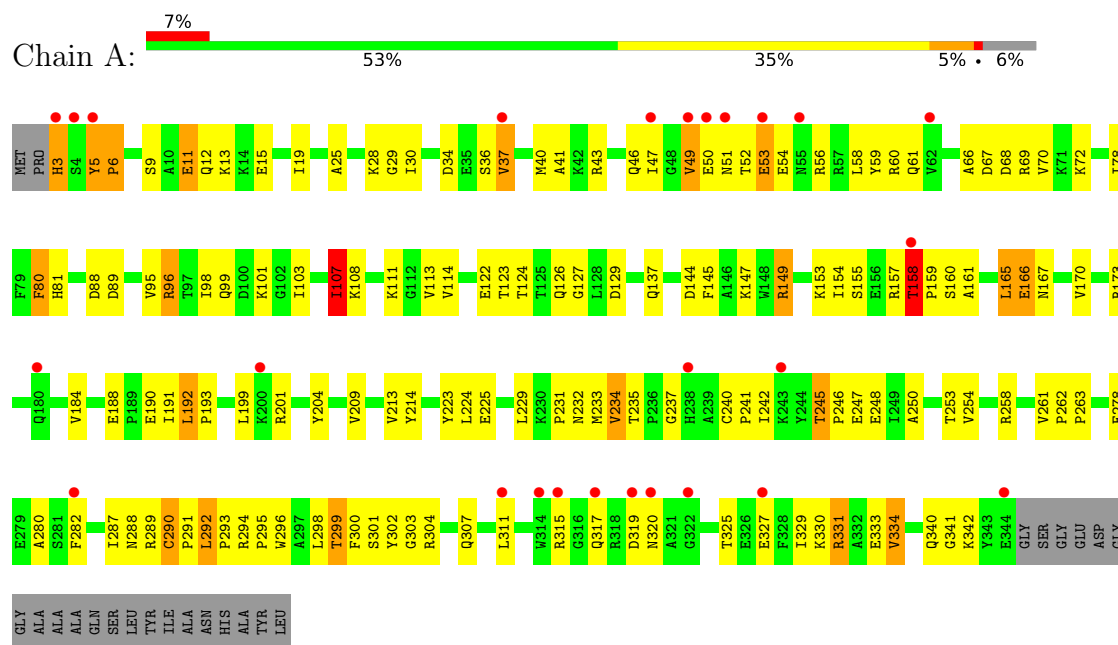
- Molecule 1 is a protein called Aldolase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	B	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	C	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	D	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	E	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	F	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	G	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	H	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	I	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	J	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	K	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			
1	L	342	Total	C	N	O	S	0	0	0
			2623	1651	465	497	10			

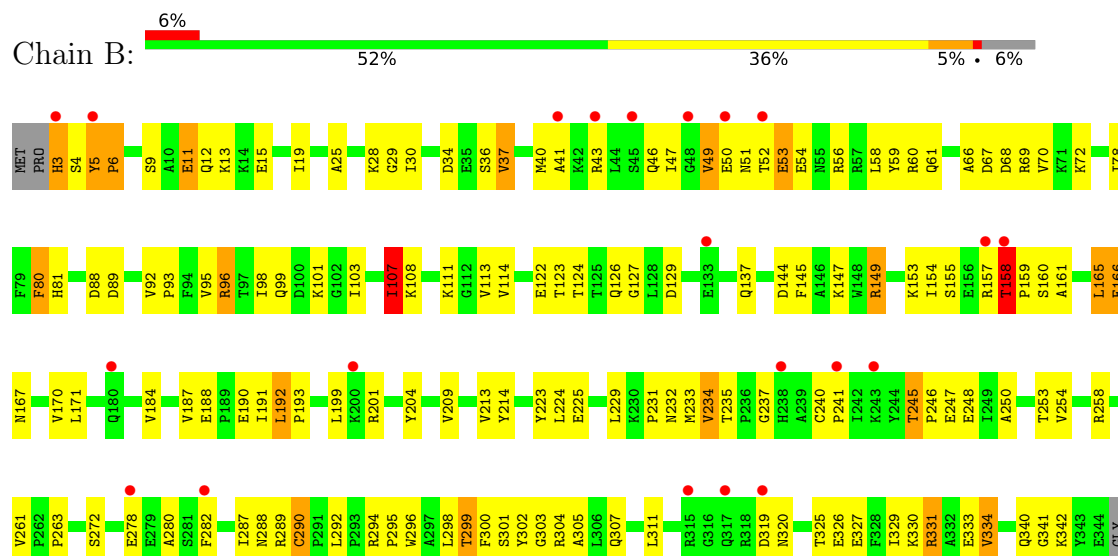
3 Residue-property plots [i](#)

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: Aldolase C



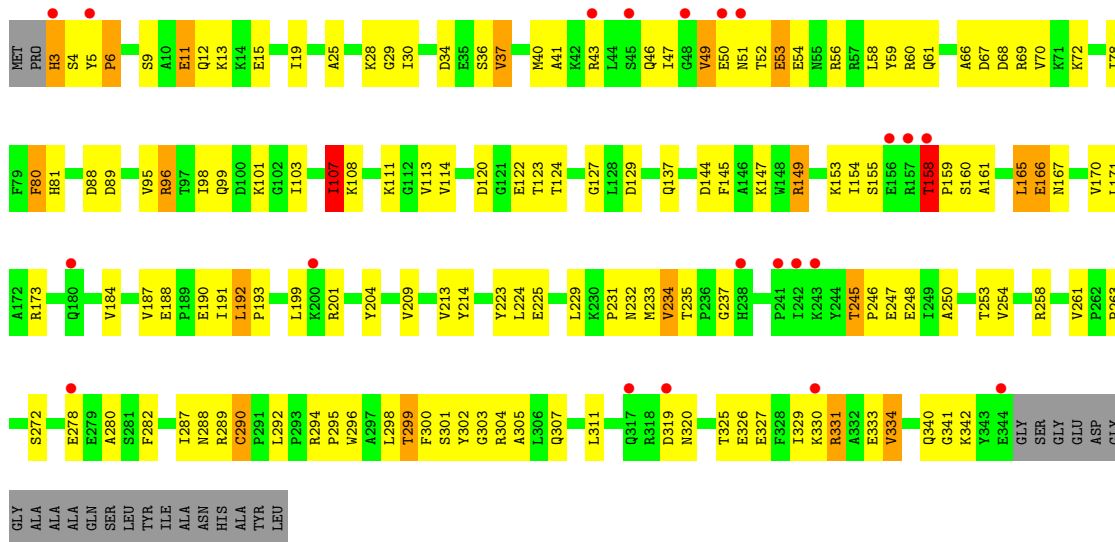
• Molecule 1: Aldolase C



SER
GLY
GLU
ASP
GLY
GLY
ALA
ALA
ALA
GLN
SER
LEU
TVR
ILE
ASN
HIS
ALA
TVR
LEU

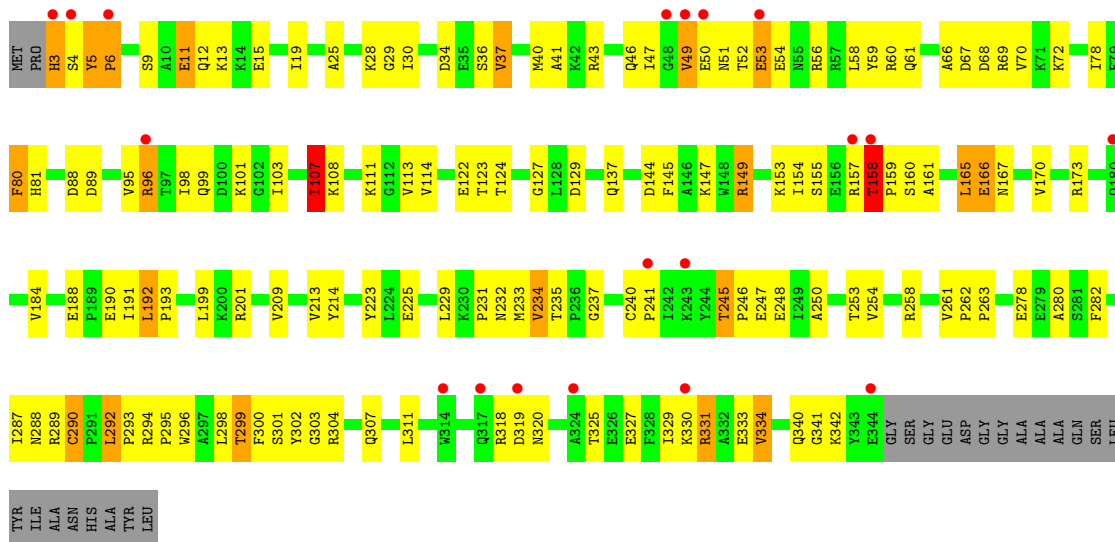
• Molecule 1: Aldolase C

Chain C: 6% 53% 35% 5% • 6%



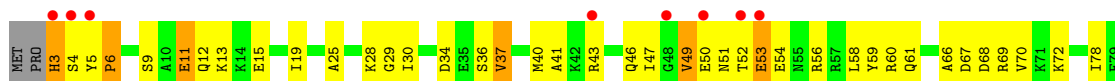
• Molecule 1: Aldolase C

Chain D: 5% 54% 34% 5% • 6%



• Molecule 1: Aldolase C

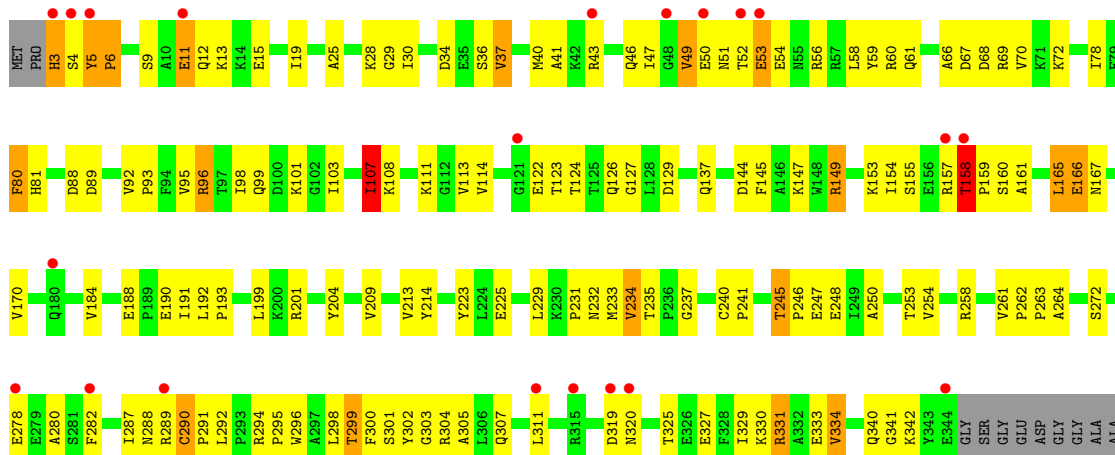
Chain E: 5% 53% 35% 5% • 6%





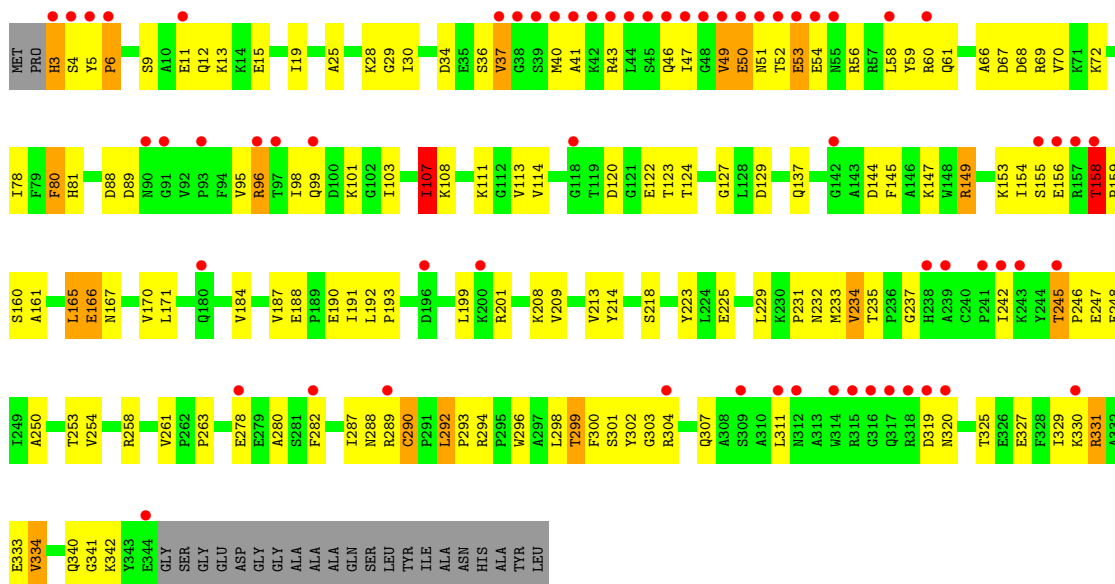
GLY
ALA
ALA
ALA
GLN
SER
SER
LEU
LEU
TYR
ILE
ALA
ASN
HIS
ALA
TYR
LEU

• Molecule 1: Aldolase C



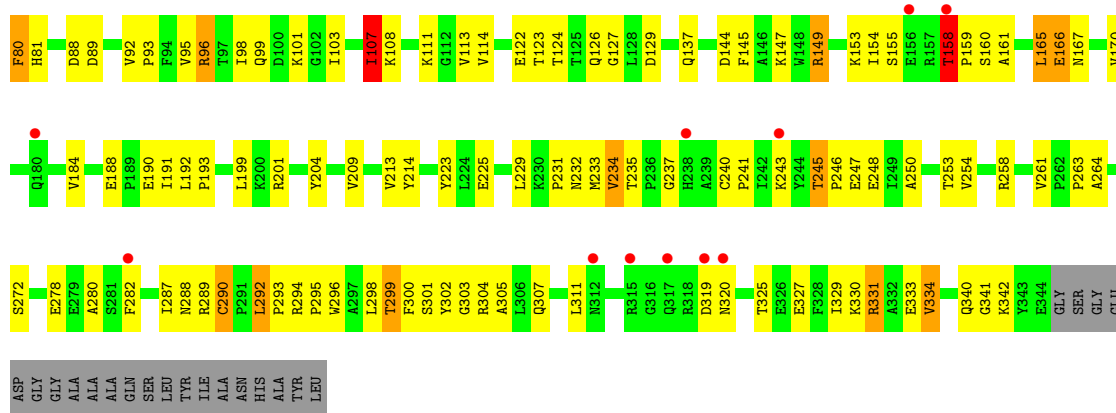
ALA
GLN
SER
SER
LEU
TYR
ILE
ALA
ASN
HIS
ALA
TYR
LEU

• Molecule 1: Aldolase C

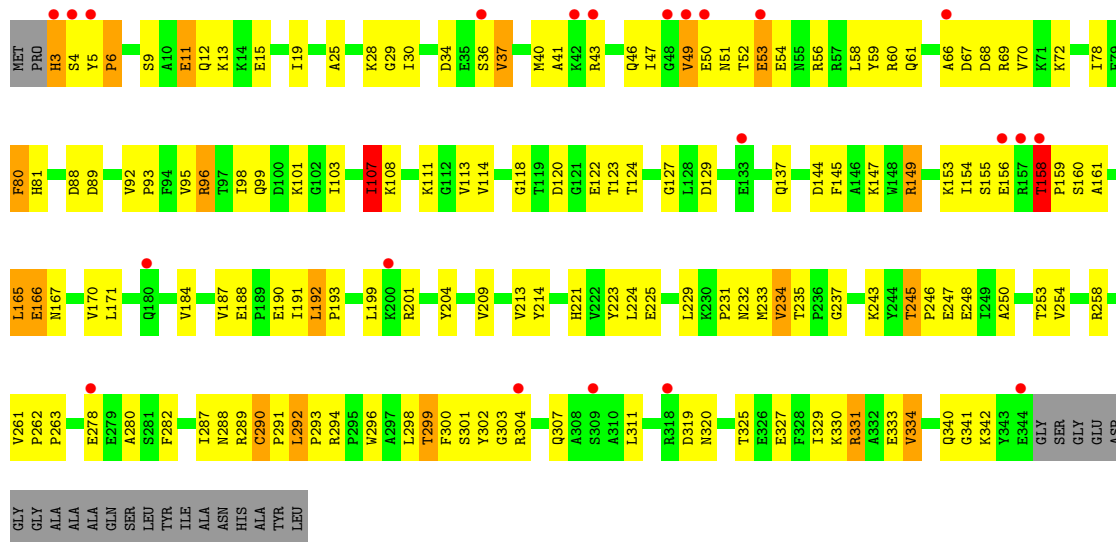


• Molecule 1: Aldolase C

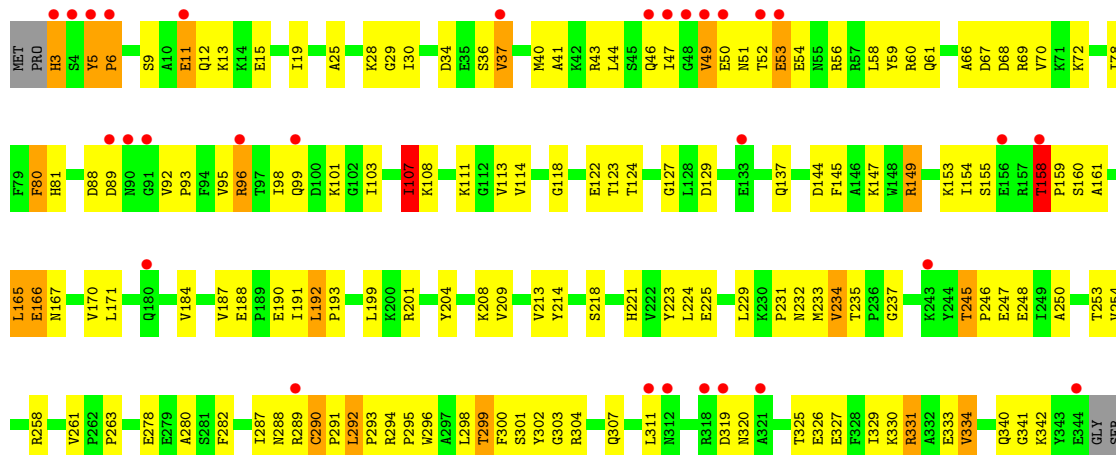




• Molecule 1: Aldolase C



• Molecule 1: Aldolase C



GLY
GLU
ASP
GLY
GLY
ALA
ALA
ALA
GLN
SER
LEU
TYR
ILE
ALA
ASN
HIS
ALA
TYR
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.87Å 121.99Å 129.52Å 107.96° 108.58° 97.39°	Depositor
Resolution (Å)	79.24 – 3.00 79.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (79.24-3.00) 97.2 (79.24-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.261 0.250 , 0.257	Depositor DCC
R_{free} test set	8700 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	31476	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.48	0/2672	1.09	23/3623 (0.6%)
1	B	0.48	0/2672	1.09	23/3623 (0.6%)
1	C	0.48	0/2672	1.09	23/3623 (0.6%)
1	D	0.48	0/2672	1.09	22/3623 (0.6%)
1	E	0.48	0/2672	1.09	23/3623 (0.6%)
1	F	0.48	0/2672	1.09	22/3623 (0.6%)
1	G	0.48	0/2672	1.09	22/3623 (0.6%)
1	H	0.48	0/2672	1.09	22/3623 (0.6%)
1	I	0.48	0/2672	1.09	22/3623 (0.6%)
1	J	0.48	0/2672	1.09	22/3623 (0.6%)
1	K	0.48	0/2672	1.09	23/3623 (0.6%)
1	L	0.48	0/2672	1.09	23/3623 (0.6%)
All	All	0.48	0/32064	1.09	270/43476 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	12

There are no bond length outliers.

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	166	GLU	N-CA-C	-9.47	98.77	110.41
1	J	166	GLU	N-CA-C	-9.46	98.77	110.41
1	C	166	GLU	N-CA-C	-9.45	98.79	110.41
1	L	166	GLU	N-CA-C	-9.45	98.79	110.41
1	E	166	GLU	N-CA-C	-9.44	98.80	110.41
1	F	166	GLU	N-CA-C	-9.43	98.81	110.41
1	B	166	GLU	N-CA-C	-9.43	98.81	110.41
1	A	166	GLU	N-CA-C	-9.43	98.81	110.41
1	G	166	GLU	N-CA-C	-9.42	98.83	110.41
1	D	166	GLU	N-CA-C	-9.41	98.83	110.41
1	I	166	GLU	N-CA-C	-9.41	98.84	110.41
1	K	166	GLU	N-CA-C	-9.40	98.85	110.41
1	J	114	VAL	CA-C-N	7.65	127.41	119.76
1	J	114	VAL	C-N-CA	7.65	127.41	119.76
1	H	114	VAL	CA-C-N	7.64	127.40	119.76
1	H	114	VAL	C-N-CA	7.64	127.40	119.76
1	D	114	VAL	CA-C-N	7.62	127.38	119.76
1	D	114	VAL	C-N-CA	7.62	127.38	119.76
1	C	114	VAL	CA-C-N	7.62	127.38	119.76
1	C	114	VAL	C-N-CA	7.62	127.38	119.76
1	E	114	VAL	CA-C-N	7.62	127.38	119.76
1	E	114	VAL	C-N-CA	7.62	127.38	119.76
1	A	114	VAL	CA-C-N	7.60	127.36	119.76
1	A	114	VAL	C-N-CA	7.60	127.36	119.76
1	I	114	VAL	CA-C-N	7.60	127.36	119.76
1	I	114	VAL	C-N-CA	7.60	127.36	119.76
1	L	114	VAL	CA-C-N	7.59	127.35	119.76
1	L	114	VAL	C-N-CA	7.59	127.35	119.76
1	B	114	VAL	CA-C-N	7.59	127.35	119.76
1	B	114	VAL	C-N-CA	7.59	127.35	119.76
1	F	114	VAL	CA-C-N	7.58	127.34	119.76
1	F	114	VAL	C-N-CA	7.58	127.34	119.76
1	K	114	VAL	CA-C-N	7.58	127.34	119.76
1	K	114	VAL	C-N-CA	7.58	127.34	119.76
1	G	114	VAL	CA-C-N	7.56	127.32	119.76
1	G	114	VAL	C-N-CA	7.56	127.32	119.76
1	B	246	PRO	N-CA-C	-6.52	105.37	113.84
1	I	246	PRO	N-CA-C	-6.52	105.37	113.84
1	J	246	PRO	N-CA-C	-6.51	105.37	113.84
1	E	246	PRO	N-CA-C	-6.51	105.38	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	246	PRO	N-CA-C	-6.51	105.38	113.84
1	K	246	PRO	N-CA-C	-6.50	105.39	113.84
1	A	246	PRO	N-CA-C	-6.49	105.40	113.84
1	D	246	PRO	N-CA-C	-6.49	105.40	113.84
1	F	246	PRO	N-CA-C	-6.49	105.41	113.84
1	L	246	PRO	N-CA-C	-6.49	105.41	113.84
1	G	246	PRO	N-CA-C	-6.48	105.42	113.84
1	C	246	PRO	N-CA-C	-6.47	105.43	113.84
1	D	68	ASP	N-CA-C	6.42	120.22	112.38
1	C	53	GLU	N-CA-C	-6.42	104.36	111.36
1	C	158	THR	CA-C-N	-6.41	111.83	119.84
1	C	158	THR	C-N-CA	-6.41	111.83	119.84
1	F	53	GLU	N-CA-C	-6.41	104.38	111.36
1	D	53	GLU	N-CA-C	-6.40	104.38	111.36
1	E	53	GLU	N-CA-C	-6.40	104.38	111.36
1	G	68	ASP	N-CA-C	6.40	120.19	112.38
1	L	53	GLU	N-CA-C	-6.40	104.38	111.36
1	J	53	GLU	N-CA-C	-6.40	104.38	111.36
1	I	53	GLU	N-CA-C	-6.40	104.39	111.36
1	A	53	GLU	N-CA-C	-6.39	104.39	111.36
1	D	158	THR	CA-C-N	-6.39	111.85	119.84
1	D	158	THR	C-N-CA	-6.39	111.85	119.84
1	F	68	ASP	N-CA-C	6.39	120.17	112.38
1	H	53	GLU	N-CA-C	-6.39	104.40	111.36
1	K	53	GLU	N-CA-C	-6.39	104.40	111.36
1	G	53	GLU	N-CA-C	-6.38	104.40	111.36
1	I	68	ASP	N-CA-C	6.38	120.17	112.38
1	C	68	ASP	N-CA-C	6.38	120.17	112.38
1	B	53	GLU	N-CA-C	-6.38	104.40	111.36
1	A	68	ASP	N-CA-C	6.38	120.16	112.38
1	B	158	THR	CA-C-N	-6.38	111.87	119.84
1	B	158	THR	C-N-CA	-6.38	111.87	119.84
1	K	68	ASP	N-CA-C	6.38	120.16	112.38
1	B	68	ASP	N-CA-C	6.38	120.16	112.38
1	E	68	ASP	N-CA-C	6.37	120.16	112.38
1	K	158	THR	CA-C-N	-6.37	111.88	119.84
1	K	158	THR	C-N-CA	-6.37	111.88	119.84
1	L	68	ASP	N-CA-C	6.36	120.14	112.38
1	A	158	THR	CA-C-N	-6.36	111.89	119.84
1	A	158	THR	C-N-CA	-6.36	111.89	119.84
1	H	68	ASP	N-CA-C	6.36	120.14	112.38
1	F	158	THR	CA-C-N	-6.36	111.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	158	THR	C-N-CA	-6.36	111.89	119.84
1	J	158	THR	CA-C-N	-6.36	111.89	119.84
1	J	158	THR	C-N-CA	-6.36	111.89	119.84
1	E	158	THR	CA-C-N	-6.36	111.89	119.84
1	E	158	THR	C-N-CA	-6.36	111.89	119.84
1	H	158	THR	CA-C-N	-6.36	111.90	119.84
1	H	158	THR	C-N-CA	-6.36	111.90	119.84
1	L	158	THR	CA-C-N	-6.35	111.90	119.84
1	L	158	THR	C-N-CA	-6.35	111.90	119.84
1	J	68	ASP	N-CA-C	6.35	120.12	112.38
1	G	158	THR	CA-C-N	-6.34	111.91	119.84
1	G	158	THR	C-N-CA	-6.34	111.91	119.84
1	I	158	THR	CA-C-N	-6.33	111.93	119.84
1	I	158	THR	C-N-CA	-6.33	111.93	119.84
1	I	108	LYS	N-CA-C	-6.23	99.86	109.76
1	F	108	LYS	N-CA-C	-6.22	99.87	109.76
1	D	108	LYS	N-CA-C	-6.21	99.88	109.76
1	G	108	LYS	N-CA-C	-6.21	99.89	109.76
1	A	108	LYS	N-CA-C	-6.21	99.89	109.76
1	B	108	LYS	N-CA-C	-6.21	99.89	109.76
1	L	108	LYS	N-CA-C	-6.21	99.89	109.76
1	J	108	LYS	N-CA-C	-6.21	99.89	109.76
1	C	108	LYS	N-CA-C	-6.20	99.90	109.76
1	H	108	LYS	N-CA-C	-6.19	99.91	109.76
1	E	108	LYS	N-CA-C	-6.19	99.92	109.76
1	K	108	LYS	N-CA-C	-6.18	99.93	109.76
1	B	233	MET	N-CA-C	-6.07	101.49	110.48
1	E	233	MET	N-CA-C	-6.07	101.50	110.48
1	D	233	MET	N-CA-C	-6.07	101.50	110.48
1	J	233	MET	N-CA-C	-6.07	101.50	110.48
1	F	233	MET	N-CA-C	-6.06	101.52	110.48
1	A	233	MET	N-CA-C	-6.05	101.52	110.48
1	H	233	MET	N-CA-C	-6.05	101.52	110.48
1	I	233	MET	N-CA-C	-6.05	101.52	110.48
1	L	233	MET	N-CA-C	-6.05	101.53	110.48
1	C	233	MET	N-CA-C	-6.05	101.53	110.48
1	K	233	MET	N-CA-C	-6.04	101.54	110.48
1	G	233	MET	N-CA-C	-6.04	101.55	110.48
1	C	5	TYR	CA-C-N	5.77	127.05	119.84
1	C	5	TYR	C-N-CA	5.77	127.05	119.84
1	L	5	TYR	CA-C-N	5.75	127.03	119.84
1	L	5	TYR	C-N-CA	5.75	127.03	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	5	TYR	CA-C-N	5.75	127.03	119.84
1	K	5	TYR	C-N-CA	5.75	127.03	119.84
1	F	5	TYR	CA-C-N	5.74	127.02	119.84
1	F	5	TYR	C-N-CA	5.74	127.02	119.84
1	B	5	TYR	CA-C-N	5.74	127.01	119.84
1	B	5	TYR	C-N-CA	5.74	127.01	119.84
1	I	5	TYR	CA-C-N	5.73	127.00	119.84
1	I	5	TYR	C-N-CA	5.73	127.00	119.84
1	D	5	TYR	CA-C-N	5.73	127.00	119.84
1	D	5	TYR	C-N-CA	5.73	127.00	119.84
1	J	5	TYR	CA-C-N	5.72	127.00	119.84
1	J	5	TYR	C-N-CA	5.72	127.00	119.84
1	A	5	TYR	CA-C-N	5.72	126.99	119.84
1	A	5	TYR	C-N-CA	5.72	126.99	119.84
1	G	5	TYR	CA-C-N	5.70	126.96	119.84
1	G	5	TYR	C-N-CA	5.70	126.96	119.84
1	E	5	TYR	CA-C-N	5.69	126.96	119.84
1	E	5	TYR	C-N-CA	5.69	126.96	119.84
1	H	5	TYR	CA-C-N	5.67	126.93	119.84
1	H	5	TYR	C-N-CA	5.67	126.93	119.84
1	A	290	CYS	CA-C-N	5.66	125.33	119.05
1	A	290	CYS	C-N-CA	5.66	125.33	119.05
1	F	290	CYS	CA-C-N	5.66	125.33	119.05
1	F	290	CYS	C-N-CA	5.66	125.33	119.05
1	G	290	CYS	CA-C-N	5.65	125.32	119.05
1	G	290	CYS	C-N-CA	5.65	125.32	119.05
1	I	290	CYS	CA-C-N	5.65	125.33	119.05
1	I	290	CYS	C-N-CA	5.65	125.33	119.05
1	L	290	CYS	CA-C-N	5.65	125.32	119.05
1	L	290	CYS	C-N-CA	5.65	125.32	119.05
1	B	290	CYS	CA-C-N	5.65	125.32	119.05
1	B	290	CYS	C-N-CA	5.65	125.32	119.05
1	D	290	CYS	CA-C-N	5.65	125.32	119.05
1	D	290	CYS	C-N-CA	5.65	125.32	119.05
1	C	290	CYS	CA-C-N	5.64	125.31	119.05
1	C	290	CYS	C-N-CA	5.64	125.31	119.05
1	E	80	PHE	N-CA-C	-5.64	100.52	109.76
1	J	290	CYS	CA-C-N	5.63	125.31	119.05
1	J	290	CYS	C-N-CA	5.63	125.31	119.05
1	E	290	CYS	CA-C-N	5.63	125.30	119.05
1	E	290	CYS	C-N-CA	5.63	125.30	119.05
1	F	80	PHE	N-CA-C	-5.63	100.52	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	80	PHE	N-CA-C	-5.63	100.53	109.76
1	C	80	PHE	N-CA-C	-5.62	100.54	109.76
1	L	80	PHE	N-CA-C	-5.62	100.54	109.76
1	G	80	PHE	N-CA-C	-5.62	100.55	109.76
1	H	290	CYS	CA-C-N	5.62	125.29	119.05
1	H	290	CYS	C-N-CA	5.62	125.29	119.05
1	D	80	PHE	N-CA-C	-5.61	100.56	109.76
1	A	80	PHE	N-CA-C	-5.61	100.56	109.76
1	K	290	CYS	CA-C-N	5.61	125.28	119.05
1	K	290	CYS	C-N-CA	5.61	125.28	119.05
1	J	80	PHE	N-CA-C	-5.61	100.56	109.76
1	K	80	PHE	N-CA-C	-5.60	100.58	109.76
1	I	80	PHE	N-CA-C	-5.60	100.58	109.76
1	B	80	PHE	N-CA-C	-5.59	100.59	109.76
1	I	192	LEU	CA-C-N	5.51	126.73	119.84
1	I	192	LEU	C-N-CA	5.51	126.73	119.84
1	D	192	LEU	CA-C-N	5.49	126.71	119.84
1	D	192	LEU	C-N-CA	5.49	126.71	119.84
1	C	192	LEU	CA-C-N	5.49	126.70	119.84
1	C	192	LEU	C-N-CA	5.49	126.70	119.84
1	F	192	LEU	CA-C-N	5.48	126.69	119.84
1	F	192	LEU	C-N-CA	5.48	126.69	119.84
1	K	192	LEU	CA-C-N	5.48	126.69	119.84
1	K	192	LEU	C-N-CA	5.48	126.69	119.84
1	E	192	LEU	CA-C-N	5.47	126.68	119.84
1	E	192	LEU	C-N-CA	5.47	126.68	119.84
1	A	192	LEU	CA-C-N	5.47	126.67	119.84
1	A	192	LEU	C-N-CA	5.47	126.67	119.84
1	G	192	LEU	CA-C-N	5.46	126.67	119.84
1	G	192	LEU	C-N-CA	5.46	126.67	119.84
1	H	192	LEU	CA-C-N	5.46	126.66	119.84
1	H	192	LEU	C-N-CA	5.46	126.66	119.84
1	B	192	LEU	CA-C-N	5.44	126.64	119.84
1	B	192	LEU	C-N-CA	5.44	126.64	119.84
1	J	192	LEU	CA-C-N	5.43	126.63	119.84
1	J	192	LEU	C-N-CA	5.43	126.63	119.84
1	L	192	LEU	CA-C-N	5.43	126.63	119.84
1	L	192	LEU	C-N-CA	5.43	126.63	119.84
1	D	124	THR	N-CA-C	-5.34	101.37	108.74
1	I	124	THR	N-CA-C	-5.33	101.39	108.74
1	G	124	THR	N-CA-C	-5.33	101.39	108.74
1	H	124	THR	N-CA-C	-5.32	101.40	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	124	THR	N-CA-C	-5.32	101.40	108.74
1	A	124	THR	N-CA-C	-5.31	101.41	108.74
1	F	124	THR	N-CA-C	-5.31	101.42	108.74
1	K	124	THR	N-CA-C	-5.30	101.42	108.74
1	B	124	THR	N-CA-C	-5.30	101.42	108.74
1	L	124	THR	N-CA-C	-5.30	101.43	108.74
1	C	124	THR	N-CA-C	-5.30	101.43	108.74
1	E	124	THR	N-CA-C	-5.29	101.44	108.74
1	L	149	ARG	N-CA-C	5.25	117.08	108.52
1	J	149	ARG	N-CA-C	5.25	117.08	108.52
1	E	149	ARG	N-CA-C	5.24	117.06	108.52
1	A	149	ARG	N-CA-C	5.24	117.06	108.52
1	H	149	ARG	N-CA-C	5.24	117.06	108.52
1	F	149	ARG	N-CA-C	5.23	117.05	108.52
1	G	149	ARG	N-CA-C	5.23	117.04	108.52
1	K	149	ARG	N-CA-C	5.23	117.04	108.52
1	B	149	ARG	N-CA-C	5.22	117.03	108.52
1	C	149	ARG	N-CA-C	5.22	117.03	108.52
1	I	149	ARG	N-CA-C	5.21	117.02	108.52
1	D	149	ARG	N-CA-C	5.21	117.00	108.52
1	E	292	LEU	CA-C-N	5.21	124.97	119.76
1	E	292	LEU	C-N-CA	5.21	124.97	119.76
1	I	292	LEU	CA-C-N	5.20	124.96	119.76
1	I	292	LEU	C-N-CA	5.20	124.96	119.76
1	L	292	LEU	CA-C-N	5.19	124.95	119.76
1	L	292	LEU	C-N-CA	5.19	124.95	119.76
1	A	292	LEU	CA-C-N	5.17	124.93	119.76
1	A	292	LEU	C-N-CA	5.17	124.93	119.76
1	F	292	LEU	CA-C-N	5.17	124.93	119.76
1	F	292	LEU	C-N-CA	5.17	124.93	119.76
1	G	292	LEU	CA-C-N	5.16	124.92	119.76
1	G	292	LEU	C-N-CA	5.16	124.92	119.76
1	B	292	LEU	CA-C-N	5.16	124.92	119.76
1	B	292	LEU	C-N-CA	5.16	124.92	119.76
1	J	292	LEU	CA-C-N	5.15	124.91	119.76
1	J	292	LEU	C-N-CA	5.15	124.91	119.76
1	D	292	LEU	CA-C-N	5.15	124.91	119.76
1	D	292	LEU	C-N-CA	5.15	124.91	119.76
1	E	107	ILE	CB-CA-C	-5.13	102.59	110.50
1	H	292	LEU	CA-C-N	5.13	124.89	119.76
1	H	292	LEU	C-N-CA	5.13	124.89	119.76
1	K	292	LEU	CA-C-N	5.13	124.89	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	292	LEU	C-N-CA	5.13	124.89	119.76
1	I	107	ILE	CB-CA-C	-5.13	102.60	110.50
1	K	107	ILE	CB-CA-C	-5.12	102.61	110.50
1	B	107	ILE	CB-CA-C	-5.12	102.61	110.50
1	C	292	LEU	CA-C-N	5.12	124.88	119.76
1	C	292	LEU	C-N-CA	5.12	124.88	119.76
1	H	107	ILE	CB-CA-C	-5.12	102.62	110.50
1	J	107	ILE	CB-CA-C	-5.11	102.63	110.50
1	A	107	ILE	CB-CA-C	-5.11	102.63	110.50
1	F	107	ILE	CB-CA-C	-5.10	102.64	110.50
1	G	107	ILE	CB-CA-C	-5.10	102.64	110.50
1	C	107	ILE	CB-CA-C	-5.10	102.65	110.50
1	L	107	ILE	CB-CA-C	-5.10	102.65	110.50
1	D	107	ILE	CB-CA-C	-5.09	102.65	110.50
1	C	224	LEU	N-CA-C	5.03	117.15	111.11
1	B	224	LEU	N-CA-C	5.02	117.13	111.11
1	L	224	LEU	N-CA-C	5.01	117.12	111.11
1	E	224	LEU	N-CA-C	5.00	117.11	111.11
1	A	224	LEU	N-CA-C	5.00	117.11	111.11
1	K	224	LEU	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	TYR	Sidechain
1	B	214	TYR	Sidechain
1	C	214	TYR	Sidechain
1	D	214	TYR	Sidechain
1	E	214	TYR	Sidechain
1	F	214	TYR	Sidechain
1	G	214	TYR	Sidechain
1	H	214	TYR	Sidechain
1	I	214	TYR	Sidechain
1	J	214	TYR	Sidechain
1	K	214	TYR	Sidechain
1	L	214	TYR	Sidechain

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	2623	0	2638	147	0
1	B	2623	0	2638	133	2
1	C	2623	0	2638	130	3
1	D	2623	0	2638	126	2
1	E	2623	0	2638	132	3
1	F	2623	0	2638	146	0
1	G	2623	0	2638	131	5
1	H	2623	0	2638	147	0
1	I	2623	0	2638	145	4
1	J	2623	0	2638	147	0
1	K	2623	0	2638	144	3
1	L	2623	0	2638	138	0
All	All	31476	0	31656	1501	11

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 24.

All (1501) 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:A:315:ARG:CG	1:H:291:PRO:HG3	1.32	1.58
1:F:238:HIS:HB3	1:J:243:LYS:CE	1.48	1.44
1:F:238:HIS:CB	1:J:243:LYS:NZ	1.80	1.43
1:F:238:HIS:CB	1:J:243:LYS:HZ3	1.30	1.43
1:A:315:ARG:HG2	1:H:291:PRO:CG	1.53	1.39
1:F:238:HIS:CA	1:J:243:LYS:HZ3	1.37	1.38
1:A:317:GLN:NE2	1:H:291:PRO:O	1.63	1.31
1:A:315:ARG:CD	1:H:291:PRO:HG3	1.61	1.27
1:F:238:HIS:HB3	1:J:243:LYS:NZ	1.38	1.26
1:F:238:HIS:CB	1:J:243:LYS:CE	2.14	1.22
1:F:238:HIS:CA	1:J:243:LYS:NZ	2.00	1.19
1:F:239:ALA:HA	1:J:243:LYS:HG2	1.36	1.08
1:A:315:ARG:HD3	1:H:291:PRO:CG	1.85	1.07
1:I:3:HIS:CD2	1:L:201:ARG:HH12	1.73	1.06
1:F:238:HIS:HA	1:J:243:LYS:HZ3	1.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:CG	1:H:291:PRO:CG	2.18	0.99
1:F:238:HIS:HB3	1:J:243:LYS:HE3	1.40	0.98
1:C:153:LYS:HD2	1:C:158:THR:HG21	1.46	0.97
1:J:153:LYS:HD2	1:J:158:THR:HG21	1.46	0.97
1:B:153:LYS:HD2	1:B:158:THR:HG21	1.46	0.97
1:F:238:HIS:CG	1:J:243:LYS:HZ3	1.83	0.96
1:H:153:LYS:HD2	1:H:158:THR:HG21	1.46	0.96
1:A:315:ARG:CD	1:H:291:PRO:CG	2.34	0.96
1:I:156:GLU:OE2	1:K:156:GLU:CG	2.14	0.96
1:A:317:GLN:CD	1:H:291:PRO:O	2.08	0.95
1:D:153:LYS:HD2	1:D:158:THR:HG21	1.46	0.95
1:E:153:LYS:HD2	1:E:158:THR:HG21	1.46	0.95
1:I:153:LYS:HD2	1:I:158:THR:HG21	1.46	0.95
1:F:153:LYS:HD2	1:F:158:THR:HG21	1.46	0.95
1:G:153:LYS:HD2	1:G:158:THR:HG21	1.46	0.95
1:I:156:GLU:CG	1:K:156:GLU:OE2	2.15	0.94
1:L:153:LYS:HD2	1:L:158:THR:HG21	1.46	0.94
1:A:153:LYS:HD2	1:A:158:THR:HG21	1.46	0.94
1:J:107:ILE:HD12	1:J:107:ILE:H	1.32	0.94
1:K:153:LYS:HD2	1:K:158:THR:HG21	1.46	0.94
1:H:107:ILE:HD12	1:H:107:ILE:H	1.32	0.94
1:K:107:ILE:HD12	1:K:107:ILE:H	1.32	0.93
1:F:238:HIS:CA	1:J:243:LYS:CE	2.25	0.93
1:D:107:ILE:H	1:D:107:ILE:HD12	1.32	0.93
1:E:107:ILE:HD12	1:E:107:ILE:H	1.32	0.93
1:A:107:ILE:HD12	1:A:107:ILE:H	1.32	0.93
1:F:107:ILE:HD12	1:F:107:ILE:H	1.32	0.92
1:L:107:ILE:HD12	1:L:107:ILE:H	1.32	0.92
1:B:107:ILE:H	1:B:107:ILE:HD12	1.32	0.91
1:G:107:ILE:H	1:G:107:ILE:HD12	1.32	0.91
1:I:107:ILE:H	1:I:107:ILE:HD12	1.32	0.91
1:C:107:ILE:HD12	1:C:107:ILE:H	1.32	0.91
1:I:156:GLU:OE2	1:K:156:GLU:HG3	1.71	0.90
1:I:201:ARG:HH12	1:L:3:HIS:CD2	1.91	0.89
1:H:234:VAL:HG13	1:H:253:THR:HA	1.55	0.88
1:J:234:VAL:HG13	1:J:253:THR:HA	1.55	0.88
1:A:229:LEU:HG	1:A:231:PRO:HD3	1.56	0.88
1:J:229:LEU:HG	1:J:231:PRO:HD3	1.56	0.88
1:D:229:LEU:HG	1:D:231:PRO:HD3	1.56	0.88
1:E:234:VAL:HG13	1:E:253:THR:HA	1.55	0.88
1:H:229:LEU:HG	1:H:231:PRO:HD3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:234:VAL:HG13	1:K:253:THR:HA	1.55	0.88
1:C:234:VAL:HG13	1:C:253:THR:HA	1.55	0.88
1:A:315:ARG:HG2	1:H:291:PRO:HG3	0.88	0.88
1:B:234:VAL:HG13	1:B:253:THR:HA	1.55	0.87
1:A:315:ARG:HG2	1:H:291:PRO:CB	2.05	0.87
1:C:229:LEU:HG	1:C:231:PRO:HD3	1.56	0.87
1:E:229:LEU:HG	1:E:231:PRO:HD3	1.56	0.87
1:K:229:LEU:HG	1:K:231:PRO:HD3	1.56	0.87
1:I:156:GLU:HG3	1:K:156:GLU:OE2	1.74	0.87
1:B:229:LEU:HG	1:B:231:PRO:HD3	1.55	0.87
1:D:234:VAL:HG13	1:D:253:THR:HA	1.55	0.86
1:A:234:VAL:HG13	1:A:253:THR:HA	1.55	0.86
1:F:238:HIS:CG	1:J:243:LYS:NZ	2.41	0.86
1:G:229:LEU:HG	1:G:231:PRO:HD3	1.56	0.86
1:I:229:LEU:HG	1:I:231:PRO:HD3	1.56	0.86
1:I:234:VAL:HG13	1:I:253:THR:HA	1.55	0.86
1:G:234:VAL:HG13	1:G:253:THR:HA	1.55	0.86
1:F:234:VAL:HG13	1:F:253:THR:HA	1.55	0.86
1:F:238:HIS:HA	1:J:243:LYS:NZ	1.80	0.86
1:L:234:VAL:HG13	1:L:253:THR:HA	1.55	0.86
1:F:229:LEU:HG	1:F:231:PRO:HD3	1.56	0.86
1:L:229:LEU:HG	1:L:231:PRO:HD3	1.56	0.85
1:F:67:ASP:OD2	1:F:69:ARG:HG2	1.78	0.84
1:L:67:ASP:OD2	1:L:69:ARG:HG2	1.78	0.84
1:H:67:ASP:OD2	1:H:69:ARG:HG2	1.78	0.84
1:C:67:ASP:OD2	1:C:69:ARG:HG2	1.78	0.83
1:J:67:ASP:OD2	1:J:69:ARG:HG2	1.78	0.83
1:K:67:ASP:OD2	1:K:69:ARG:HG2	1.78	0.83
1:B:67:ASP:OD2	1:B:69:ARG:HG2	1.78	0.83
1:D:67:ASP:OD2	1:D:69:ARG:HG2	1.78	0.83
1:E:67:ASP:OD2	1:E:69:ARG:HG2	1.78	0.82
1:G:67:ASP:OD2	1:G:69:ARG:HG2	1.78	0.82
1:I:3:HIS:HD2	1:L:201:ARG:HH12	1.20	0.82
1:I:67:ASP:OD2	1:I:69:ARG:HG2	1.78	0.82
1:A:67:ASP:OD2	1:A:69:ARG:HG2	1.78	0.82
1:E:4:SER:HB3	1:H:204:TYR:CD1	2.15	0.81
1:C:166:GLU:O	1:C:167:ASN:HB2	1.82	0.80
1:B:166:GLU:O	1:B:167:ASN:HB2	1.82	0.80
1:G:107:ILE:HD12	1:G:107:ILE:N	1.97	0.80
1:H:107:ILE:HD12	1:H:107:ILE:N	1.97	0.80
1:H:166:GLU:O	1:H:167:ASN:HB2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:ILE:HD12	1:I:107:ILE:N	1.97	0.80
1:J:107:ILE:HD12	1:J:107:ILE:N	1.97	0.80
1:F:201:ARG:HH12	1:G:3:HIS:CD2	2.00	0.79
1:F:238:HIS:HB3	1:J:243:LYS:HZ1	1.43	0.79
1:J:166:GLU:O	1:J:167:ASN:HB2	1.82	0.79
1:A:107:ILE:HD12	1:A:107:ILE:N	1.97	0.78
1:D:166:GLU:O	1:D:167:ASN:HB2	1.82	0.78
1:E:107:ILE:HD12	1:E:107:ILE:N	1.97	0.78
1:E:166:GLU:O	1:E:167:ASN:HB2	1.82	0.78
1:G:166:GLU:O	1:G:167:ASN:HB2	1.82	0.78
1:H:155:SER:OG	1:H:158:THR:HG23	1.84	0.78
1:I:166:GLU:O	1:I:167:ASN:HB2	1.82	0.78
1:A:166:GLU:O	1:A:167:ASN:HB2	1.82	0.78
1:B:107:ILE:HD12	1:B:107:ILE:N	1.97	0.78
1:D:107:ILE:HD12	1:D:107:ILE:N	1.97	0.78
1:J:155:SER:OG	1:J:158:THR:HG23	1.84	0.78
1:K:107:ILE:HD12	1:K:107:ILE:N	1.97	0.78
1:A:5:TYR:OH	1:B:157:ARG:HD3	1.83	0.78
1:K:166:GLU:O	1:K:167:ASN:HB2	1.82	0.78
1:C:107:ILE:HD12	1:C:107:ILE:N	1.97	0.78
1:K:155:SER:OG	1:K:158:THR:HG23	1.84	0.77
1:C:155:SER:OG	1:C:158:THR:HG23	1.84	0.77
1:E:155:SER:OG	1:E:158:THR:HG23	1.84	0.77
1:L:166:GLU:O	1:L:167:ASN:HB2	1.82	0.77
1:I:155:SER:OG	1:I:158:THR:HG23	1.84	0.77
1:B:155:SER:OG	1:B:158:THR:HG23	1.84	0.77
1:F:107:ILE:HD12	1:F:107:ILE:N	1.97	0.77
1:F:155:SER:OG	1:F:158:THR:HG23	1.84	0.77
1:F:166:GLU:O	1:F:167:ASN:HB2	1.82	0.77
1:G:155:SER:OG	1:G:158:THR:HG23	1.84	0.77
1:D:155:SER:OG	1:D:158:THR:HG23	1.84	0.77
1:L:155:SER:OG	1:L:158:THR:HG23	1.84	0.77
1:A:155:SER:OG	1:A:158:THR:HG23	1.84	0.76
1:H:158:THR:O	1:H:160:SER:N	2.20	0.75
1:J:158:THR:O	1:J:160:SER:N	2.20	0.75
1:D:158:THR:O	1:D:160:SER:N	2.20	0.75
1:G:5:TYR:OH	1:H:157:ARG:HD3	1.85	0.75
1:A:158:THR:O	1:A:160:SER:N	2.20	0.75
1:L:107:ILE:HD12	1:L:107:ILE:N	1.97	0.75
1:G:167:ASN:H	1:G:170:VAL:HG23	1.52	0.75
1:H:167:ASN:H	1:H:170:VAL:HG23	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:ASN:H	1:I:170:VAL:HG23	1.52	0.75
1:A:167:ASN:H	1:A:170:VAL:HG23	1.52	0.74
1:J:167:ASN:H	1:J:170:VAL:HG23	1.52	0.74
1:K:158:THR:O	1:K:160:SER:N	2.20	0.74
1:I:158:THR:O	1:I:160:SER:N	2.20	0.74
1:F:158:THR:O	1:F:160:SER:N	2.20	0.74
1:F:167:ASN:H	1:F:170:VAL:HG23	1.52	0.74
1:G:158:THR:O	1:G:160:SER:N	2.20	0.74
1:L:167:ASN:H	1:L:170:VAL:HG23	1.52	0.74
1:E:158:THR:O	1:E:160:SER:N	2.20	0.74
1:L:158:THR:O	1:L:160:SER:N	2.20	0.74
1:B:61:GLN:HE21	1:B:88:ASP:HB2	1.53	0.74
1:C:61:GLN:HE21	1:C:88:ASP:HB2	1.53	0.74
1:D:167:ASN:H	1:D:170:VAL:HG23	1.53	0.74
1:B:158:THR:O	1:B:160:SER:N	2.20	0.74
1:C:158:THR:O	1:C:160:SER:N	2.20	0.74
1:F:61:GLN:HE21	1:F:88:ASP:HB2	1.53	0.74
1:H:61:GLN:HE21	1:H:88:ASP:HB2	1.53	0.73
1:I:156:GLU:CD	1:K:156:GLU:CD	2.55	0.73
1:L:61:GLN:HE21	1:L:88:ASP:HB2	1.53	0.73
1:E:61:GLN:HE21	1:E:88:ASP:HB2	1.53	0.73
1:K:167:ASN:H	1:K:170:VAL:HG23	1.52	0.73
1:E:167:ASN:H	1:E:170:VAL:HG23	1.53	0.73
1:E:61:GLN:HE22	1:E:89:ASP:H	1.37	0.73
1:K:61:GLN:HE22	1:K:89:ASP:H	1.37	0.73
1:K:61:GLN:HE21	1:K:88:ASP:HB2	1.53	0.73
1:J:61:GLN:HE21	1:J:88:ASP:HB2	1.53	0.73
1:J:61:GLN:HE22	1:J:89:ASP:H	1.37	0.73
1:A:61:GLN:HE21	1:A:88:ASP:HB2	1.53	0.73
1:C:167:ASN:H	1:C:170:VAL:HG23	1.52	0.73
1:B:167:ASN:H	1:B:170:VAL:HG23	1.52	0.73
1:J:263:PRO:HG2	1:K:296:TRP:CH2	2.24	0.73
1:H:61:GLN:HE22	1:H:89:ASP:H	1.37	0.72
1:A:61:GLN:HE22	1:A:89:ASP:H	1.37	0.72
1:D:61:GLN:HE22	1:D:89:ASP:H	1.37	0.72
1:I:61:GLN:HE21	1:I:88:ASP:HB2	1.53	0.72
1:G:61:GLN:HE21	1:G:88:ASP:HB2	1.53	0.71
1:D:61:GLN:HE21	1:D:88:ASP:HB2	1.53	0.71
1:I:61:GLN:HE22	1:I:89:ASP:H	1.37	0.71
1:A:340:GLN:HB2	1:A:342:LYS:HG2	1.73	0.71
1:G:61:GLN:HE22	1:G:89:ASP:H	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:201:ARG:HG3	1:L:201:ARG:HH11	1.56	0.71
1:D:340:GLN:HB2	1:D:342:LYS:HG2	1.73	0.71
1:G:19:ILE:HD13	1:G:144:ASP:HB3	1.73	0.71
1:F:201:ARG:HH11	1:F:201:ARG:HG3	1.56	0.71
1:H:201:ARG:HG3	1:H:201:ARG:HH11	1.56	0.71
1:I:19:ILE:HD13	1:I:144:ASP:HB3	1.73	0.71
1:B:340:GLN:HB2	1:B:342:LYS:HG2	1.73	0.71
1:F:61:GLN:HE22	1:F:89:ASP:H	1.37	0.71
1:J:201:ARG:HG3	1:J:201:ARG:HH11	1.56	0.71
1:K:201:ARG:HH11	1:K:201:ARG:HG3	1.56	0.71
1:K:340:GLN:HB2	1:K:342:LYS:HG2	1.73	0.71
1:L:61:GLN:HE22	1:L:89:ASP:H	1.37	0.71
1:E:201:ARG:HG3	1:E:201:ARG:HH11	1.56	0.71
1:E:340:GLN:HB2	1:E:342:LYS:HG2	1.73	0.71
1:F:19:ILE:HD13	1:F:144:ASP:HB3	1.73	0.71
1:L:19:ILE:HD13	1:L:144:ASP:HB3	1.73	0.71
1:E:296:TRP:CH2	1:H:263:PRO:HG2	2.26	0.71
1:J:19:ILE:HD13	1:J:144:ASP:HB3	1.73	0.71
1:C:61:GLN:HE22	1:C:89:ASP:H	1.37	0.70
1:H:19:ILE:HD13	1:H:144:ASP:HB3	1.73	0.70
1:L:340:GLN:HB2	1:L:342:LYS:HG2	1.72	0.70
1:F:201:ARG:HH12	1:G:3:HIS:HD2	1.38	0.70
1:F:340:GLN:HB2	1:F:342:LYS:HG2	1.73	0.70
1:H:340:GLN:HB2	1:H:342:LYS:HG2	1.73	0.70
1:J:340:GLN:HB2	1:J:342:LYS:HG2	1.73	0.70
1:A:3:HIS:N	1:B:157:ARG:NH2	2.39	0.70
1:B:61:GLN:HE22	1:B:89:ASP:H	1.37	0.70
1:C:340:GLN:HB2	1:C:342:LYS:HG2	1.73	0.70
1:A:19:ILE:HD13	1:A:144:ASP:HB3	1.73	0.70
1:K:19:ILE:HD13	1:K:144:ASP:HB3	1.73	0.70
1:E:19:ILE:HD13	1:E:144:ASP:HB3	1.73	0.70
1:G:340:GLN:HB2	1:G:342:LYS:HG2	1.73	0.70
1:B:201:ARG:HG3	1:B:201:ARG:HH11	1.56	0.70
1:G:201:ARG:HG3	1:G:201:ARG:HH11	1.56	0.70
1:E:234:VAL:CG1	1:E:253:THR:HA	2.22	0.70
1:B:19:ILE:HD13	1:B:144:ASP:HB3	1.73	0.69
1:C:19:ILE:HD13	1:C:144:ASP:HB3	1.73	0.69
1:I:201:ARG:HG3	1:I:201:ARG:HH11	1.56	0.69
1:I:340:GLN:HB2	1:I:342:LYS:HG2	1.73	0.69
1:K:234:VAL:CG1	1:K:253:THR:HA	2.22	0.69
1:I:3:HIS:CD2	1:L:201:ARG:NH1	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLN:NE2	1:B:89:ASP:H	1.91	0.69
1:C:201:ARG:HG3	1:C:201:ARG:HH11	1.56	0.69
1:C:61:GLN:NE2	1:C:89:ASP:H	1.91	0.69
1:A:201:ARG:HH11	1:A:201:ARG:HG3	1.56	0.69
1:D:201:ARG:HG3	1:D:201:ARG:HH11	1.56	0.69
1:D:19:ILE:HD13	1:D:144:ASP:HB3	1.73	0.69
1:B:4:SER:HB3	1:C:204:TYR:CD1	2.27	0.69
1:D:234:VAL:CG1	1:D:253:THR:HA	2.22	0.69
1:I:61:GLN:NE2	1:I:89:ASP:H	1.90	0.69
1:G:61:GLN:NE2	1:G:89:ASP:H	1.91	0.69
1:H:234:VAL:CG1	1:H:253:THR:HA	2.22	0.69
1:A:61:GLN:NE2	1:A:89:ASP:H	1.91	0.68
1:A:113:VAL:HG22	1:A:123:THR:HB	1.76	0.68
1:B:52:THR:HG22	1:B:54:GLU:H	1.59	0.68
1:I:234:VAL:CG1	1:I:253:THR:HA	2.22	0.68
1:G:234:VAL:CG1	1:G:253:THR:HA	2.22	0.68
1:H:111:LYS:HG3	1:H:127:GLY:HA2	1.75	0.68
1:J:111:LYS:HG3	1:J:127:GLY:HA2	1.75	0.68
1:J:234:VAL:CG1	1:J:253:THR:HA	2.22	0.68
1:A:234:VAL:CG1	1:A:253:THR:HA	2.22	0.68
1:C:52:THR:HG22	1:C:54:GLU:H	1.59	0.68
1:D:113:VAL:HG22	1:D:123:THR:HB	1.76	0.68
1:H:61:GLN:NE2	1:H:89:ASP:H	1.91	0.68
1:A:52:THR:HG22	1:A:54:GLU:H	1.59	0.68
1:D:52:THR:HG22	1:D:54:GLU:H	1.59	0.68
1:K:61:GLN:NE2	1:K:89:ASP:H	1.90	0.68
1:B:191:ILE:H	1:B:232:ASN:HD22	1.42	0.68
1:C:113:VAL:HG22	1:C:123:THR:HB	1.75	0.68
1:C:234:VAL:CG1	1:C:253:THR:HA	2.22	0.68
1:D:111:LYS:HG3	1:D:127:GLY:HA2	1.75	0.68
1:E:191:ILE:H	1:E:232:ASN:ND2	1.92	0.68
1:F:234:VAL:CG1	1:F:253:THR:HA	2.22	0.68
1:J:61:GLN:NE2	1:J:89:ASP:H	1.91	0.68
1:L:234:VAL:CG1	1:L:253:THR:HA	2.22	0.68
1:K:191:ILE:H	1:K:232:ASN:ND2	1.92	0.68
1:E:61:GLN:NE2	1:E:89:ASP:H	1.90	0.68
1:F:52:THR:HG22	1:F:54:GLU:H	1.58	0.68
1:F:61:GLN:NE2	1:F:89:ASP:H	1.90	0.68
1:L:61:GLN:NE2	1:L:89:ASP:H	1.91	0.68
1:B:111:LYS:HG3	1:B:127:GLY:HA2	1.75	0.67
1:C:191:ILE:H	1:C:232:ASN:HD22	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:GLN:NE2	1:D:89:ASP:H	1.90	0.67
1:J:191:ILE:H	1:J:232:ASN:ND2	1.92	0.67
1:A:111:LYS:HG3	1:A:127:GLY:HA2	1.75	0.67
1:B:113:VAL:HG22	1:B:123:THR:HB	1.76	0.67
1:C:111:LYS:HG3	1:C:127:GLY:HA2	1.75	0.67
1:H:191:ILE:H	1:H:232:ASN:ND2	1.92	0.67
1:B:191:ILE:H	1:B:232:ASN:ND2	1.92	0.67
1:L:52:THR:HG22	1:L:54:GLU:H	1.59	0.67
1:A:191:ILE:H	1:A:232:ASN:ND2	1.92	0.67
1:F:3:HIS:CD2	1:G:201:ARG:HH12	2.13	0.67
1:C:191:ILE:H	1:C:232:ASN:ND2	1.92	0.67
1:H:113:VAL:HG22	1:H:123:THR:HB	1.76	0.67
1:I:113:VAL:HG22	1:I:123:THR:HB	1.76	0.67
1:I:191:ILE:H	1:I:232:ASN:HD22	1.41	0.67
1:J:113:VAL:HG22	1:J:123:THR:HB	1.76	0.67
1:F:191:ILE:H	1:F:232:ASN:ND2	1.92	0.67
1:L:111:LYS:HG3	1:L:127:GLY:HA2	1.75	0.67
1:L:191:ILE:H	1:L:232:ASN:ND2	1.92	0.67
1:D:330:LYS:O	1:D:334:VAL:HG12	1.95	0.67
1:G:191:ILE:H	1:G:232:ASN:HD22	1.41	0.67
1:I:111:LYS:HG3	1:I:127:GLY:HA2	1.75	0.67
1:K:113:VAL:HG22	1:K:123:THR:HB	1.76	0.67
1:A:330:LYS:O	1:A:334:VAL:HG12	1.95	0.67
1:B:234:VAL:CG1	1:B:253:THR:HA	2.22	0.67
1:D:191:ILE:H	1:D:232:ASN:ND2	1.92	0.67
1:G:111:LYS:HG3	1:G:127:GLY:HA2	1.75	0.67
1:F:111:LYS:HG3	1:F:127:GLY:HA2	1.75	0.67
1:F:113:VAL:HG22	1:F:123:THR:HB	1.76	0.67
1:G:52:THR:HG22	1:G:54:GLU:H	1.59	0.67
1:G:113:VAL:HG22	1:G:123:THR:HB	1.76	0.67
1:J:52:THR:HG22	1:J:54:GLU:H	1.59	0.67
1:D:191:ILE:H	1:D:232:ASN:HD22	1.41	0.67
1:E:330:LYS:O	1:E:334:VAL:HG12	1.95	0.66
1:I:52:THR:HG22	1:I:54:GLU:H	1.59	0.66
1:G:191:ILE:H	1:G:232:ASN:ND2	1.92	0.66
1:H:52:THR:HG22	1:H:54:GLU:H	1.59	0.66
1:I:156:GLU:HG2	1:K:156:GLU:OE2	1.93	0.66
1:J:204:TYR:CD1	1:K:4:SER:HB3	2.29	0.66
1:L:113:VAL:HG22	1:L:123:THR:HB	1.76	0.66
1:E:113:VAL:HG22	1:E:123:THR:HB	1.75	0.66
1:I:156:GLU:CG	1:K:156:GLU:CD	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:H	1:A:232:ASN:HD22	1.42	0.66
1:F:330:LYS:O	1:F:334:VAL:HG12	1.95	0.66
1:I:191:ILE:H	1:I:232:ASN:ND2	1.92	0.66
1:K:330:LYS:O	1:K:334:VAL:HG12	1.95	0.66
1:L:330:LYS:O	1:L:334:VAL:HG12	1.95	0.66
1:E:111:LYS:HG3	1:E:127:GLY:HA2	1.75	0.66
1:E:191:ILE:H	1:E:232:ASN:HD22	1.42	0.66
1:E:204:TYR:CG	1:H:4:SER:HB3	2.31	0.66
1:H:191:ILE:H	1:H:232:ASN:HD22	1.42	0.66
1:K:111:LYS:HG3	1:K:127:GLY:HA2	1.75	0.66
1:B:330:LYS:O	1:B:334:VAL:HG12	1.95	0.66
1:C:158:THR:OG1	1:C:159:PRO:HD3	1.96	0.66
1:K:191:ILE:H	1:K:232:ASN:HD22	1.42	0.66
1:F:191:ILE:H	1:F:232:ASN:HD22	1.42	0.66
1:G:129:ASP:OD1	1:H:126:GLN:HB2	1.96	0.66
1:G:158:THR:OG1	1:G:159:PRO:HD3	1.96	0.66
1:G:330:LYS:O	1:G:334:VAL:HG12	1.95	0.66
1:A:317:GLN:HG2	1:H:291:PRO:HA	1.78	0.66
1:B:158:THR:OG1	1:B:159:PRO:HD3	1.96	0.66
1:I:158:THR:OG1	1:I:159:PRO:HD3	1.96	0.66
1:J:191:ILE:H	1:J:232:ASN:HD22	1.42	0.66
1:I:330:LYS:O	1:I:334:VAL:HG12	1.95	0.66
1:K:52:THR:HG22	1:K:54:GLU:H	1.59	0.66
1:E:52:THR:HG22	1:E:54:GLU:H	1.59	0.65
1:L:191:ILE:H	1:L:232:ASN:HD22	1.42	0.65
1:H:158:THR:OG1	1:H:159:PRO:HD3	1.96	0.65
1:A:158:THR:OG1	1:A:159:PRO:HD3	1.96	0.65
1:I:156:GLU:CD	1:K:156:GLU:CG	2.69	0.65
1:F:158:THR:OG1	1:F:159:PRO:HD3	1.96	0.65
1:J:330:LYS:O	1:J:334:VAL:HG12	1.95	0.65
1:C:330:LYS:O	1:C:334:VAL:HG12	1.95	0.65
1:J:158:THR:OG1	1:J:159:PRO:HD3	1.96	0.65
1:E:158:THR:OG1	1:E:159:PRO:HD3	1.96	0.65
1:H:330:LYS:O	1:H:334:VAL:HG12	1.95	0.65
1:L:158:THR:OG1	1:L:159:PRO:HD3	1.96	0.65
1:K:158:THR:OG1	1:K:159:PRO:HD3	1.96	0.65
1:J:3:HIS:CD2	1:K:201:ARG:HH12	2.14	0.65
1:A:315:ARG:HD3	1:H:291:PRO:CD	2.26	0.64
1:F:98:ILE:HG23	1:F:103:ILE:HB	1.80	0.64
1:K:98:ILE:HG23	1:K:103:ILE:HB	1.79	0.64
1:L:98:ILE:HG23	1:L:103:ILE:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:THR:OG1	1:D:159:PRO:HD3	1.96	0.64
1:E:98:ILE:HG23	1:E:103:ILE:HB	1.80	0.64
1:B:98:ILE:HG23	1:B:103:ILE:HB	1.80	0.64
1:E:263:PRO:CG	1:H:295:PRO:HG2	2.28	0.64
1:G:98:ILE:HG23	1:G:103:ILE:HB	1.80	0.64
1:A:263:PRO:HG2	1:D:296:TRP:CH2	2.32	0.64
1:C:129:ASP:HB2	1:D:129:ASP:OD2	1.98	0.64
1:I:98:ILE:HG23	1:I:103:ILE:HB	1.80	0.64
1:E:29:GLY:HA3	1:E:300:PHE:CZ	2.33	0.64
1:K:29:GLY:HA3	1:K:300:PHE:CZ	2.33	0.64
1:C:98:ILE:HG23	1:C:103:ILE:HB	1.79	0.64
1:E:147:LYS:HE3	1:E:188:GLU:OE1	1.98	0.64
1:J:4:SER:HB3	1:K:204:TYR:CG	2.34	0.63
1:J:98:ILE:HG23	1:J:103:ILE:HB	1.80	0.63
1:K:147:LYS:HE3	1:K:188:GLU:OE1	1.98	0.63
1:D:98:ILE:HG23	1:D:103:ILE:HB	1.79	0.63
1:F:147:LYS:HE3	1:F:188:GLU:OE1	1.98	0.63
1:A:98:ILE:HG23	1:A:103:ILE:HB	1.80	0.63
1:L:147:LYS:HE3	1:L:188:GLU:OE1	1.98	0.63
1:A:29:GLY:HA3	1:A:300:PHE:CZ	2.33	0.63
1:F:29:GLY:HA3	1:F:300:PHE:CZ	2.33	0.63
1:H:98:ILE:HG23	1:H:103:ILE:HB	1.80	0.63
1:D:29:GLY:HA3	1:D:300:PHE:CZ	2.33	0.63
1:G:29:GLY:HA3	1:G:300:PHE:CZ	2.33	0.63
1:I:29:GLY:HA3	1:I:300:PHE:CZ	2.33	0.63
1:L:29:GLY:HA3	1:L:300:PHE:CZ	2.33	0.63
1:I:156:GLU:OE2	1:K:156:GLU:HG2	1.96	0.63
1:G:294:ARG:HG2	1:G:298:LEU:HD11	1.81	0.63
1:I:294:ARG:HG2	1:I:298:LEU:HD11	1.81	0.63
1:B:204:TYR:CD1	1:C:4:SER:HB3	2.34	0.62
1:A:147:LYS:HE3	1:A:188:GLU:OE1	1.98	0.62
1:B:29:GLY:HA3	1:B:300:PHE:CZ	2.33	0.62
1:B:147:LYS:HE3	1:B:188:GLU:OE1	1.98	0.62
1:H:29:GLY:HA3	1:H:300:PHE:CZ	2.33	0.62
1:H:147:LYS:HE3	1:H:188:GLU:OE1	1.98	0.62
1:J:201:ARG:HH12	1:K:3:HIS:CD2	2.17	0.62
1:A:263:PRO:HB2	1:D:258:ARG:HB2	1.82	0.62
1:C:29:GLY:HA3	1:C:300:PHE:CZ	2.33	0.62
1:C:147:LYS:HE3	1:C:188:GLU:OE1	1.98	0.62
1:D:147:LYS:HE3	1:D:188:GLU:OE1	1.98	0.62
1:G:147:LYS:HE3	1:G:188:GLU:OE1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ARG:HG2	1:E:298:LEU:HD11	1.81	0.62
1:I:147:LYS:HE3	1:I:188:GLU:OE1	1.98	0.62
1:K:59:TYR:OH	1:K:307:GLN:HB2	2.00	0.62
1:B:59:TYR:OH	1:B:307:GLN:HB2	2.00	0.62
1:E:59:TYR:OH	1:E:307:GLN:HB2	2.00	0.62
1:I:3:HIS:NE2	1:L:201:ARG:NH2	2.48	0.62
1:J:29:GLY:HA3	1:J:300:PHE:CZ	2.33	0.62
1:J:147:LYS:HE3	1:J:188:GLU:OE1	1.98	0.62
1:F:294:ARG:HG2	1:F:298:LEU:HD11	1.81	0.62
1:K:294:ARG:HG2	1:K:298:LEU:HD11	1.81	0.62
1:I:52:THR:HG22	1:I:53:GLU:N	2.15	0.62
1:I:129:ASP:HB2	1:J:129:ASP:OD2	2.00	0.62
1:I:201:ARG:HH12	1:L:3:HIS:HD2	1.45	0.62
1:L:294:ARG:HG2	1:L:298:LEU:HD11	1.81	0.62
1:B:52:THR:HG22	1:B:53:GLU:N	2.15	0.62
1:C:52:THR:HG22	1:C:53:GLU:N	2.15	0.62
1:C:59:TYR:OH	1:C:307:GLN:HB2	2.00	0.62
1:G:52:THR:HG22	1:G:53:GLU:N	2.15	0.62
1:A:59:TYR:OH	1:A:307:GLN:HB2	2.00	0.61
1:C:294:ARG:HG2	1:C:298:LEU:HD11	1.81	0.61
1:J:59:TYR:OH	1:J:307:GLN:HB2	2.00	0.61
1:K:52:THR:HG22	1:K:53:GLU:N	2.15	0.61
1:D:52:THR:HG22	1:D:53:GLU:N	2.15	0.61
1:G:59:TYR:OH	1:G:307:GLN:HB2	2.00	0.61
1:H:59:TYR:OH	1:H:307:GLN:HB2	2.00	0.61
1:F:52:THR:HG22	1:F:53:GLU:N	2.15	0.61
1:J:294:ARG:HG2	1:J:298:LEU:HD11	1.81	0.61
1:L:52:THR:HG22	1:L:53:GLU:N	2.15	0.61
1:D:59:TYR:OH	1:D:307:GLN:HB2	2.00	0.61
1:I:59:TYR:OH	1:I:307:GLN:HB2	2.00	0.61
1:A:52:THR:HG22	1:A:53:GLU:N	2.15	0.61
1:E:52:THR:HG22	1:E:53:GLU:N	2.15	0.61
1:B:294:ARG:HG2	1:B:298:LEU:HD11	1.81	0.61
1:A:294:ARG:HG2	1:A:298:LEU:HD11	1.81	0.61
1:F:59:TYR:OH	1:F:307:GLN:HB2	2.00	0.61
1:J:3:HIS:HD2	1:K:201:ARG:HH12	1.49	0.61
1:L:59:TYR:OH	1:L:307:GLN:HB2	2.00	0.61
1:H:294:ARG:HG2	1:H:298:LEU:HD11	1.81	0.60
1:D:294:ARG:HG2	1:D:298:LEU:HD11	1.81	0.60
1:J:52:THR:HG22	1:J:53:GLU:N	2.15	0.60
1:B:25:ALA:O	1:B:28:LYS:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ALA:O	1:C:28:LYS:HB2	2.02	0.60
1:H:25:ALA:O	1:H:28:LYS:HB2	2.02	0.60
1:H:52:THR:HG22	1:H:53:GLU:N	2.15	0.60
1:H:29:GLY:HA3	1:H:300:PHE:CE2	2.37	0.60
1:J:25:ALA:O	1:J:28:LYS:HB2	2.02	0.60
1:J:29:GLY:HA3	1:J:300:PHE:CE2	2.37	0.60
1:C:29:GLY:HA3	1:C:300:PHE:CE2	2.37	0.59
1:E:280:ALA:HB1	1:E:302:TYR:CE1	2.37	0.59
1:A:29:GLY:HA3	1:A:300:PHE:CE2	2.37	0.59
1:K:25:ALA:O	1:K:28:LYS:HB2	2.02	0.59
1:K:280:ALA:HB1	1:K:302:TYR:CE1	2.37	0.59
1:E:25:ALA:O	1:E:28:LYS:HB2	2.02	0.59
1:B:201:ARG:HG3	1:B:201:ARG:NH1	2.17	0.59
1:F:29:GLY:HA3	1:F:300:PHE:CE2	2.37	0.59
1:B:29:GLY:HA3	1:B:300:PHE:CE2	2.37	0.59
1:C:280:ALA:HB1	1:C:302:TYR:CE1	2.37	0.59
1:D:29:GLY:HA3	1:D:300:PHE:CE2	2.37	0.59
1:D:280:ALA:HB1	1:D:302:TYR:CE1	2.37	0.59
1:E:29:GLY:HA3	1:E:300:PHE:CE2	2.37	0.59
1:F:25:ALA:O	1:F:28:LYS:HB2	2.02	0.59
1:G:29:GLY:HA3	1:G:300:PHE:CE2	2.37	0.59
1:J:201:ARG:HG3	1:J:201:ARG:NH1	2.17	0.59
1:A:250:ALA:HB1	1:A:287:ILE:HA	1.85	0.59
1:F:280:ALA:HB1	1:F:302:TYR:CE1	2.37	0.59
1:G:280:ALA:HB1	1:G:302:TYR:CE1	2.37	0.59
1:I:25:ALA:O	1:I:28:LYS:HB2	2.02	0.59
1:I:29:GLY:HA3	1:I:300:PHE:CE2	2.37	0.59
1:J:280:ALA:HB1	1:J:302:TYR:CE1	2.37	0.59
1:L:29:GLY:HA3	1:L:300:PHE:CE2	2.37	0.59
1:D:25:ALA:O	1:D:28:LYS:HB2	2.02	0.59
1:G:25:ALA:O	1:G:28:LYS:HB2	2.02	0.59
1:H:201:ARG:HG3	1:H:201:ARG:NH1	2.17	0.59
1:K:29:GLY:HA3	1:K:300:PHE:CE2	2.37	0.59
1:L:280:ALA:HB1	1:L:302:TYR:CE1	2.37	0.59
1:A:280:ALA:HB1	1:A:302:TYR:CE1	2.37	0.59
1:D:201:ARG:HG3	1:D:201:ARG:NH1	2.17	0.59
1:D:250:ALA:HB1	1:D:287:ILE:HA	1.85	0.59
1:H:250:ALA:HB1	1:H:287:ILE:HA	1.85	0.59
1:J:250:ALA:HB1	1:J:287:ILE:HA	1.85	0.59
1:B:280:ALA:HB1	1:B:302:TYR:CE1	2.37	0.58
1:I:250:ALA:HB1	1:I:287:ILE:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:280:ALA:HB1	1:I:302:TYR:CE1	2.37	0.58
1:L:25:ALA:O	1:L:28:LYS:HB2	2.02	0.58
1:C:201:ARG:HG3	1:C:201:ARG:NH1	2.17	0.58
1:H:280:ALA:HB1	1:H:302:TYR:CE1	2.37	0.58
1:A:3:HIS:CD2	1:D:201:ARG:HH12	2.21	0.58
1:E:201:ARG:HG3	1:E:201:ARG:NH1	2.17	0.58
1:G:250:ALA:HB1	1:G:287:ILE:HA	1.85	0.58
1:A:25:ALA:O	1:A:28:LYS:HB2	2.02	0.58
1:F:238:HIS:CB	1:J:243:LYS:HZ1	2.02	0.58
1:A:129:ASP:OD1	1:B:126:GLN:HB2	2.03	0.58
1:F:238:HIS:CB	1:J:243:LYS:HE2	2.03	0.58
1:K:201:ARG:HG3	1:K:201:ARG:NH1	2.17	0.58
1:L:201:ARG:HG3	1:L:201:ARG:NH1	2.17	0.58
1:B:296:TRP:CH2	1:C:263:PRO:HG2	2.37	0.58
1:G:126:GLN:HB2	1:H:129:ASP:OD1	2.03	0.58
1:F:201:ARG:HG3	1:F:201:ARG:NH1	2.17	0.58
1:F:250:ALA:HB1	1:F:287:ILE:HA	1.85	0.58
1:G:303:GLY:O	1:G:307:GLN:HG2	2.03	0.58
1:H:303:GLY:O	1:H:307:GLN:HG2	2.03	0.58
1:I:303:GLY:O	1:I:307:GLN:HG2	2.03	0.58
1:B:250:ALA:HB1	1:B:287:ILE:HA	1.85	0.57
1:E:263:PRO:HG3	1:H:295:PRO:HG2	1.86	0.57
1:K:303:GLY:O	1:K:307:GLN:HG2	2.03	0.57
1:L:250:ALA:HB1	1:L:287:ILE:HA	1.85	0.57
1:C:250:ALA:HB1	1:C:287:ILE:HA	1.85	0.57
1:J:261:VAL:O	1:J:296:TRP:CZ3	2.58	0.57
1:A:261:VAL:O	1:A:296:TRP:CZ3	2.58	0.57
1:E:303:GLY:O	1:E:307:GLN:HG2	2.03	0.57
1:F:261:VAL:O	1:F:296:TRP:CZ3	2.58	0.57
1:H:261:VAL:O	1:H:296:TRP:CZ3	2.58	0.57
1:L:261:VAL:O	1:L:296:TRP:CZ3	2.58	0.57
1:C:303:GLY:O	1:C:307:GLN:HG2	2.03	0.57
1:J:296:TRP:CH2	1:K:263:PRO:HG2	2.39	0.57
1:J:303:GLY:O	1:J:307:GLN:HG2	2.03	0.57
1:E:261:VAL:O	1:E:296:TRP:CZ3	2.58	0.57
1:F:46:GLN:HE22	1:F:304:ARG:NH2	2.03	0.57
1:F:204:TYR:CG	1:G:4:SER:HB3	2.39	0.57
1:F:303:GLY:O	1:F:307:GLN:HG2	2.03	0.57
1:K:250:ALA:HB1	1:K:287:ILE:HA	1.85	0.57
1:L:46:GLN:HE22	1:L:304:ARG:NH2	2.03	0.57
1:L:303:GLY:O	1:L:307:GLN:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:O	1:A:307:GLN:HG2	2.03	0.57
1:B:261:VAL:O	1:B:296:TRP:CZ3	2.58	0.57
1:D:303:GLY:O	1:D:307:GLN:HG2	2.03	0.57
1:E:250:ALA:HB1	1:E:287:ILE:HA	1.85	0.57
1:G:149:ARG:NH1	1:G:190:GLU:OE1	2.38	0.57
1:B:303:GLY:O	1:B:307:GLN:HG2	2.03	0.57
1:C:261:VAL:O	1:C:296:TRP:CZ3	2.58	0.57
1:D:261:VAL:O	1:D:296:TRP:CZ3	2.58	0.57
1:F:155:SER:N	1:F:158:THR:OG1	2.38	0.57
1:I:149:ARG:NH1	1:I:190:GLU:OE1	2.38	0.57
1:I:261:VAL:O	1:I:296:TRP:CZ3	2.58	0.57
1:A:46:GLN:HE22	1:A:304:ARG:NH2	2.03	0.57
1:G:261:VAL:O	1:G:296:TRP:CZ3	2.58	0.57
1:K:261:VAL:O	1:K:296:TRP:CZ3	2.58	0.57
1:L:155:SER:N	1:L:158:THR:OG1	2.38	0.57
1:A:149:ARG:NH1	1:A:190:GLU:OE1	2.38	0.56
1:C:149:ARG:NH1	1:C:190:GLU:OE1	2.38	0.56
1:D:149:ARG:NH1	1:D:190:GLU:OE1	2.38	0.56
1:E:56:ARG:O	1:E:60:ARG:HG2	2.05	0.56
1:K:56:ARG:O	1:K:60:ARG:HG2	2.05	0.56
1:K:155:SER:N	1:K:158:THR:OG1	2.38	0.56
1:C:46:GLN:HE22	1:C:304:ARG:NH2	2.03	0.56
1:E:155:SER:N	1:E:158:THR:OG1	2.38	0.56
1:K:46:GLN:HE22	1:K:304:ARG:NH2	2.03	0.56
1:B:46:GLN:HE22	1:B:304:ARG:NH2	2.03	0.56
1:D:46:GLN:HE22	1:D:304:ARG:NH2	2.03	0.56
1:E:46:GLN:HE22	1:E:304:ARG:NH2	2.03	0.56
1:G:201:ARG:HG3	1:G:201:ARG:NH1	2.17	0.56
1:H:46:GLN:HE22	1:H:304:ARG:NH2	2.03	0.56
1:H:155:SER:N	1:H:158:THR:OG1	2.38	0.56
1:J:155:SER:N	1:J:158:THR:OG1	2.38	0.56
1:B:149:ARG:NH1	1:B:190:GLU:OE1	2.38	0.56
1:E:156:GLU:CG	1:G:156:GLU:OE2	2.53	0.56
1:A:56:ARG:O	1:A:60:ARG:HG2	2.05	0.56
1:A:155:SER:N	1:A:158:THR:OG1	2.38	0.56
1:B:56:ARG:O	1:B:60:ARG:HG2	2.05	0.56
1:C:56:ARG:O	1:C:60:ARG:HG2	2.05	0.56
1:D:155:SER:N	1:D:158:THR:OG1	2.38	0.56
1:L:149:ARG:NH1	1:L:190:GLU:OE1	2.38	0.56
1:A:201:ARG:HG3	1:A:201:ARG:NH1	2.17	0.56
1:G:56:ARG:O	1:G:60:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:ARG:HG3	1:I:201:ARG:NH1	2.17	0.56
1:D:69:ARG:HB2	1:D:72:LYS:NZ	2.21	0.56
1:F:69:ARG:HB2	1:F:72:LYS:NZ	2.21	0.56
1:F:149:ARG:NH1	1:F:190:GLU:OE1	2.38	0.56
1:G:155:SER:N	1:G:158:THR:OG1	2.38	0.56
1:I:56:ARG:O	1:I:60:ARG:HG2	2.05	0.56
1:I:155:SER:N	1:I:158:THR:OG1	2.38	0.56
1:C:155:SER:N	1:C:158:THR:OG1	2.38	0.56
1:J:46:GLN:HE22	1:J:304:ARG:NH2	2.03	0.56
1:L:69:ARG:HB2	1:L:72:LYS:NZ	2.21	0.56
1:B:25:ALA:HB3	1:B:28:LYS:HD2	1.88	0.56
1:D:234:VAL:HG13	1:D:253:THR:CA	2.33	0.56
1:G:46:GLN:HE22	1:G:304:ARG:NH2	2.03	0.56
1:K:69:ARG:HB2	1:K:72:LYS:NZ	2.21	0.56
1:A:69:ARG:HB2	1:A:72:LYS:NZ	2.21	0.56
1:B:155:SER:N	1:B:158:THR:OG1	2.38	0.56
1:E:69:ARG:HB2	1:E:72:LYS:NZ	2.21	0.56
1:G:69:ARG:HB2	1:G:72:LYS:NZ	2.21	0.56
1:I:46:GLN:HE22	1:I:304:ARG:NH2	2.03	0.56
1:J:69:ARG:HB2	1:J:72:LYS:NZ	2.21	0.56
1:J:149:ARG:NH1	1:J:190:GLU:OE1	2.38	0.56
1:A:248:GLU:OE1	1:I:96:ARG:NH2	2.38	0.55
1:C:25:ALA:HB3	1:C:28:LYS:HD2	1.88	0.55
1:H:56:ARG:O	1:H:60:ARG:HG2	2.05	0.55
1:I:69:ARG:HB2	1:I:72:LYS:NZ	2.21	0.55
1:J:25:ALA:HB3	1:J:28:LYS:HD2	1.88	0.55
1:K:149:ARG:NH1	1:K:190:GLU:OE1	2.38	0.55
1:L:25:ALA:HB3	1:L:28:LYS:HD2	1.88	0.55
1:C:234:VAL:HG13	1:C:253:THR:CA	2.33	0.55
1:E:149:ARG:NH1	1:E:190:GLU:OE1	2.38	0.55
1:E:156:GLU:OE2	1:G:156:GLU:CG	2.53	0.55
1:L:56:ARG:O	1:L:60:ARG:HG2	2.05	0.55
1:L:289:ARG:HD2	1:L:341:GLY:O	2.07	0.55
1:B:72:LYS:HE2	1:B:333:GLU:HG2	1.89	0.55
1:B:234:VAL:HG13	1:B:253:THR:CA	2.33	0.55
1:F:25:ALA:HB3	1:F:28:LYS:HD2	1.88	0.55
1:F:289:ARG:HD2	1:F:341:GLY:O	2.07	0.55
1:H:25:ALA:HB3	1:H:28:LYS:HD2	1.88	0.55
1:C:72:LYS:HE2	1:C:333:GLU:HG2	1.89	0.55
1:D:289:ARG:HD2	1:D:341:GLY:O	2.07	0.55
1:E:3:HIS:CD2	1:H:201:ARG:HH12	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:LYS:HE2	1:F:333:GLU:HG2	1.88	0.55
1:J:56:ARG:O	1:J:60:ARG:HG2	2.05	0.55
1:B:69:ARG:HB2	1:B:72:LYS:NZ	2.21	0.55
1:B:263:PRO:HG2	1:C:296:TRP:CH2	2.41	0.55
1:E:4:SER:HB3	1:H:204:TYR:CE1	2.42	0.55
1:F:56:ARG:O	1:F:60:ARG:HG2	2.05	0.55
1:G:289:ARG:HD2	1:G:341:GLY:O	2.07	0.55
1:H:69:ARG:HB2	1:H:72:LYS:NZ	2.21	0.55
1:J:72:LYS:HE2	1:J:333:GLU:HG2	1.89	0.55
1:H:72:LYS:HE2	1:H:333:GLU:HG2	1.89	0.55
1:H:149:ARG:NH1	1:H:190:GLU:OE1	2.38	0.55
1:I:289:ARG:HD2	1:I:341:GLY:O	2.07	0.55
1:D:56:ARG:O	1:D:60:ARG:HG2	2.05	0.55
1:J:234:VAL:HG13	1:J:253:THR:CA	2.33	0.55
1:L:72:LYS:HE2	1:L:333:GLU:HG2	1.89	0.55
1:A:289:ARG:HD2	1:A:341:GLY:O	2.07	0.55
1:D:25:ALA:HB3	1:D:28:LYS:HD2	1.88	0.55
1:E:299:THR:OG1	1:E:300:PHE:N	2.39	0.55
1:F:15:GLU:O	1:F:19:ILE:HG13	2.07	0.55
1:I:296:TRP:CH2	1:L:263:PRO:HG2	2.42	0.55
1:C:69:ARG:HB2	1:C:72:LYS:NZ	2.21	0.55
1:D:72:LYS:HE2	1:D:333:GLU:HG2	1.89	0.55
1:F:34:ASP:HB3	1:F:78:ILE:HG22	1.89	0.55
1:H:289:ARG:HD2	1:H:341:GLY:O	2.07	0.55
1:I:15:GLU:O	1:I:19:ILE:HG13	2.07	0.55
1:I:201:ARG:NH2	1:L:3:HIS:NE2	2.54	0.55
1:L:15:GLU:O	1:L:19:ILE:HG13	2.07	0.55
1:L:34:ASP:HB3	1:L:78:ILE:HG22	1.89	0.55
1:B:289:ARG:HD2	1:B:341:GLY:O	2.07	0.54
1:C:34:ASP:HB3	1:C:78:ILE:HG22	1.89	0.54
1:G:15:GLU:O	1:G:19:ILE:HG13	2.07	0.54
1:G:25:ALA:HB3	1:G:28:LYS:HD2	1.88	0.54
1:H:234:VAL:HG13	1:H:253:THR:CA	2.33	0.54
1:B:34:ASP:HB3	1:B:78:ILE:HG22	1.89	0.54
1:C:289:ARG:HD2	1:C:341:GLY:O	2.07	0.54
1:A:72:LYS:HE2	1:A:333:GLU:HG2	1.89	0.54
1:F:238:HIS:ND1	1:J:243:LYS:NZ	2.54	0.54
1:K:299:THR:OG1	1:K:300:PHE:N	2.39	0.54
1:A:25:ALA:HB3	1:A:28:LYS:HD2	1.88	0.54
1:E:15:GLU:O	1:E:19:ILE:HG13	2.07	0.54
1:H:15:GLU:O	1:H:19:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:ALA:HB3	1:I:28:LYS:HD2	1.88	0.54
1:I:218:SER:O	1:L:208:LYS:NZ	2.40	0.54
1:J:289:ARG:HD2	1:J:341:GLY:O	2.07	0.54
1:C:40:MET:HE3	1:C:40:MET:HA	1.89	0.54
1:G:72:LYS:HE2	1:G:333:GLU:HG2	1.89	0.54
1:I:72:LYS:HE2	1:I:333:GLU:HG2	1.88	0.54
1:L:40:MET:HE3	1:L:40:MET:HA	1.89	0.54
1:D:15:GLU:O	1:D:19:ILE:HG13	2.07	0.54
1:E:72:LYS:HE2	1:E:333:GLU:HG2	1.89	0.54
1:F:296:TRP:CH2	1:G:263:PRO:HG2	2.42	0.54
1:F:299:THR:OG1	1:F:300:PHE:N	2.39	0.54
1:J:15:GLU:O	1:J:19:ILE:HG13	2.07	0.54
1:K:9:SER:OG	1:K:12:GLN:HG3	2.08	0.54
1:K:72:LYS:HE2	1:K:333:GLU:HG2	1.88	0.54
1:A:9:SER:OG	1:A:12:GLN:HG3	2.08	0.54
1:A:234:VAL:HG13	1:A:253:THR:CA	2.33	0.54
1:D:9:SER:OG	1:D:12:GLN:HG3	2.08	0.54
1:E:34:ASP:HB3	1:E:78:ILE:HG22	1.89	0.54
1:H:34:ASP:HB3	1:H:78:ILE:HG22	1.89	0.54
1:J:40:MET:HA	1:J:40:MET:HE3	1.89	0.54
1:L:299:THR:OG1	1:L:300:PHE:N	2.39	0.54
1:C:299:THR:OG1	1:C:300:PHE:N	2.39	0.54
1:D:40:MET:HE3	1:D:40:MET:HA	1.89	0.54
1:E:9:SER:OG	1:E:12:GLN:HG3	2.08	0.54
1:J:34:ASP:HB3	1:J:78:ILE:HG22	1.90	0.54
1:K:15:GLU:O	1:K:19:ILE:HG13	2.07	0.54
1:B:40:MET:HE3	1:B:40:MET:HA	1.89	0.54
1:C:15:GLU:O	1:C:19:ILE:HG13	2.07	0.54
1:F:40:MET:HE3	1:F:40:MET:HA	1.89	0.54
1:H:40:MET:HE3	1:H:40:MET:HA	1.89	0.54
1:K:25:ALA:HB3	1:K:28:LYS:HD2	1.88	0.54
1:K:34:ASP:HB3	1:K:78:ILE:HG22	1.90	0.54
1:A:299:THR:OG1	1:A:300:PHE:N	2.39	0.54
1:F:9:SER:OG	1:F:12:GLN:HG3	2.08	0.54
1:E:40:MET:HA	1:E:40:MET:HE3	1.89	0.53
1:G:40:MET:HE3	1:G:40:MET:HA	1.89	0.53
1:J:9:SER:OG	1:J:12:GLN:HG3	2.08	0.53
1:A:15:GLU:O	1:A:19:ILE:HG13	2.07	0.53
1:A:40:MET:HE3	1:A:40:MET:HA	1.89	0.53
1:B:15:GLU:O	1:B:19:ILE:HG13	2.07	0.53
1:E:25:ALA:HB3	1:E:28:LYS:HD2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:TYR:CD2	1:H:4:SER:HB3	2.43	0.53
1:I:40:MET:HE3	1:I:40:MET:HA	1.89	0.53
1:K:40:MET:HE3	1:K:40:MET:HA	1.89	0.53
1:B:61:GLN:HE21	1:B:88:ASP:CB	2.22	0.53
1:H:9:SER:OG	1:H:12:GLN:HG3	2.08	0.53
1:I:34:ASP:HB3	1:I:78:ILE:HG22	1.89	0.53
1:L:9:SER:OG	1:L:12:GLN:HG3	2.08	0.53
1:E:289:ARG:HD2	1:E:341:GLY:O	2.07	0.53
1:B:9:SER:OG	1:B:12:GLN:HG3	2.08	0.53
1:C:61:GLN:HE21	1:C:88:ASP:CB	2.22	0.53
1:G:9:SER:OG	1:G:12:GLN:HG3	2.08	0.53
1:G:34:ASP:HB3	1:G:78:ILE:HG22	1.90	0.53
1:J:295:PRO:HG2	1:K:263:PRO:CG	2.39	0.53
1:K:289:ARG:HD2	1:K:341:GLY:O	2.07	0.53
1:A:296:TRP:CH2	1:D:263:PRO:HG2	2.44	0.53
1:A:315:ARG:HG2	1:H:291:PRO:HB3	1.90	0.53
1:B:299:THR:OG1	1:B:300:PHE:N	2.39	0.53
1:C:9:SER:OG	1:C:12:GLN:HG3	2.08	0.53
1:D:34:ASP:HB3	1:D:78:ILE:HG22	1.89	0.53
1:H:3:HIS:N	1:H:3:HIS:CD2	2.77	0.53
1:I:9:SER:OG	1:I:12:GLN:HG3	2.08	0.53
1:A:34:ASP:HB3	1:A:78:ILE:HG22	1.89	0.53
1:G:3:HIS:CD2	1:G:3:HIS:N	2.77	0.53
1:I:3:HIS:CD2	1:I:3:HIS:N	2.77	0.53
1:J:3:HIS:CD2	1:J:3:HIS:N	2.77	0.53
1:B:3:HIS:N	1:B:3:HIS:CD2	2.77	0.53
1:J:331:ARG:HA	1:J:334:VAL:CG1	2.39	0.53
1:C:3:HIS:N	1:C:3:HIS:CD2	2.77	0.53
1:D:299:THR:OG1	1:D:300:PHE:N	2.39	0.53
1:G:331:ARG:HA	1:G:334:VAL:CG1	2.39	0.53
1:H:331:ARG:HA	1:H:334:VAL:CG1	2.39	0.53
1:B:331:ARG:HA	1:B:334:VAL:CG1	2.39	0.52
1:E:331:ARG:HA	1:E:334:VAL:CG1	2.39	0.52
1:I:167:ASN:N	1:I:170:VAL:HG23	2.23	0.52
1:I:331:ARG:HA	1:I:334:VAL:CG1	2.39	0.52
1:K:331:ARG:HA	1:K:334:VAL:CG1	2.39	0.52
1:A:126:GLN:HB2	1:B:129:ASP:OD1	2.08	0.52
1:G:167:ASN:N	1:G:170:VAL:HG23	2.23	0.52
1:F:263:PRO:HG2	1:G:296:TRP:CH2	2.44	0.52
1:J:165:LEU:C	1:J:165:LEU:HD23	2.35	0.52
1:B:165:LEU:C	1:B:165:LEU:HD23	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:HIS:CD2	1:E:3:HIS:N	2.77	0.52
1:H:165:LEU:C	1:H:165:LEU:HD23	2.35	0.52
1:I:263:PRO:HB2	1:L:258:ARG:HB2	1.92	0.52
1:A:261:VAL:HB	1:A:296:TRP:CH2	2.45	0.52
1:C:331:ARG:HA	1:C:334:VAL:CG1	2.39	0.52
1:D:3:HIS:N	1:D:3:HIS:CD2	2.77	0.52
1:D:261:VAL:HB	1:D:296:TRP:CH2	2.45	0.52
1:F:165:LEU:C	1:F:165:LEU:HD23	2.35	0.52
1:I:258:ARG:HB2	1:L:263:PRO:HB2	1.92	0.52
1:K:165:LEU:HD23	1:K:165:LEU:C	2.35	0.52
1:L:165:LEU:C	1:L:165:LEU:HD23	2.35	0.52
1:D:167:ASN:N	1:D:170:VAL:HG23	2.23	0.52
1:E:165:LEU:C	1:E:165:LEU:HD23	2.35	0.52
1:G:299:THR:OG1	1:G:300:PHE:N	2.39	0.52
1:I:156:GLU:CD	1:K:156:GLU:HG3	2.34	0.52
1:K:3:HIS:CD2	1:K:3:HIS:N	2.77	0.52
1:L:245:THR:HG22	1:L:247:GLU:OE1	2.10	0.52
1:L:261:VAL:HB	1:L:296:TRP:CH2	2.45	0.52
1:L:331:ARG:HA	1:L:334:VAL:CG1	2.39	0.52
1:A:315:ARG:HD3	1:H:291:PRO:HG2	1.86	0.52
1:C:165:LEU:C	1:C:165:LEU:HD23	2.35	0.52
1:E:261:VAL:HB	1:E:296:TRP:CH2	2.45	0.52
1:F:3:HIS:CD2	1:F:3:HIS:N	2.77	0.52
1:F:245:THR:HG22	1:F:247:GLU:OE1	2.10	0.52
1:I:299:THR:OG1	1:I:300:PHE:N	2.39	0.52
1:A:3:HIS:N	1:A:3:HIS:CD2	2.77	0.52
1:C:129:ASP:OD2	1:D:129:ASP:HB2	2.10	0.52
1:D:165:LEU:HD23	1:D:165:LEU:C	2.35	0.52
1:F:261:VAL:HB	1:F:296:TRP:CH2	2.45	0.52
1:F:331:ARG:HA	1:F:334:VAL:CG1	2.39	0.52
1:K:261:VAL:HB	1:K:296:TRP:CH2	2.45	0.52
1:L:3:HIS:CD2	1:L:3:HIS:N	2.77	0.52
1:A:331:ARG:HA	1:A:334:VAL:CG1	2.39	0.52
1:C:245:THR:HG22	1:C:247:GLU:OE1	2.10	0.52
1:D:245:THR:HG22	1:D:247:GLU:OE1	2.10	0.52
1:H:245:THR:HG22	1:H:247:GLU:OE1	2.10	0.52
1:H:261:VAL:HB	1:H:296:TRP:CH2	2.45	0.52
1:A:61:GLN:HE21	1:A:88:ASP:CB	2.22	0.52
1:A:165:LEU:C	1:A:165:LEU:HD23	2.35	0.52
1:A:245:THR:HG22	1:A:247:GLU:OE1	2.10	0.52
1:B:245:THR:HG22	1:B:247:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:VAL:HB	1:B:296:TRP:CH2	2.45	0.52
1:G:61:GLN:HE21	1:G:88:ASP:CB	2.22	0.52
1:H:167:ASN:N	1:H:170:VAL:HG23	2.23	0.52
1:I:61:GLN:HE21	1:I:88:ASP:CB	2.22	0.52
1:I:156:GLU:HG3	1:K:156:GLU:CD	2.34	0.52
1:J:245:THR:HG22	1:J:247:GLU:OE1	2.10	0.52
1:A:167:ASN:N	1:A:170:VAL:HG23	2.23	0.51
1:B:167:ASN:N	1:B:170:VAL:HG23	2.23	0.51
1:C:261:VAL:HB	1:C:296:TRP:CH2	2.45	0.51
1:J:261:VAL:HB	1:J:296:TRP:CH2	2.45	0.51
1:B:325:THR:O	1:B:329:ILE:HG13	2.11	0.51
1:C:41:ALA:HB2	1:C:51:ASN:ND2	2.26	0.51
1:A:41:ALA:HB2	1:A:51:ASN:ND2	2.26	0.51
1:B:41:ALA:HB2	1:B:51:ASN:ND2	2.26	0.51
1:C:325:THR:O	1:C:329:ILE:HG13	2.11	0.51
1:G:234:VAL:HG13	1:G:253:THR:CA	2.33	0.51
1:G:261:VAL:HB	1:G:296:TRP:CH2	2.45	0.51
1:I:261:VAL:HB	1:I:296:TRP:CH2	2.45	0.51
1:A:242:ILE:HG12	1:I:99:GLN:OE1	2.09	0.51
1:A:258:ARG:HB2	1:D:263:PRO:HB2	1.91	0.51
1:A:325:THR:O	1:A:329:ILE:HG13	2.11	0.51
1:D:331:ARG:HA	1:D:334:VAL:CG1	2.39	0.51
1:E:156:GLU:HG3	1:G:156:GLU:OE2	2.11	0.51
1:G:165:LEU:C	1:G:165:LEU:HD23	2.35	0.51
1:D:41:ALA:HB2	1:D:51:ASN:ND2	2.26	0.51
1:D:325:THR:O	1:D:329:ILE:HG13	2.11	0.51
1:E:245:THR:HG22	1:E:247:GLU:OE1	2.10	0.51
1:F:325:THR:O	1:F:329:ILE:HG13	2.11	0.51
1:G:245:THR:HG22	1:G:247:GLU:OE1	2.10	0.51
1:H:41:ALA:HB2	1:H:51:ASN:ND2	2.25	0.51
1:I:245:THR:HG22	1:I:247:GLU:OE1	2.10	0.51
1:J:167:ASN:N	1:J:170:VAL:HG23	2.23	0.51
1:L:234:VAL:HG13	1:L:253:THR:CA	2.33	0.51
1:B:113:VAL:HG22	1:B:123:THR:CB	2.41	0.51
1:E:61:GLN:HE21	1:E:88:ASP:CB	2.22	0.51
1:I:234:VAL:HG13	1:I:253:THR:CA	2.33	0.51
1:K:245:THR:HG22	1:K:247:GLU:OE1	2.10	0.51
1:L:325:THR:O	1:L:329:ILE:HG13	2.11	0.51
1:I:165:LEU:HD23	1:I:165:LEU:C	2.35	0.51
1:C:120:ASP:HB2	1:D:5:TYR:CZ	2.45	0.51
1:K:41:ALA:HB2	1:K:51:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:N	1:B:157:ARG:CZ	2.74	0.51
1:D:59:TYR:CE1	1:D:311:LEU:HD13	2.46	0.51
1:E:325:THR:O	1:E:329:ILE:HG13	2.11	0.51
1:F:122:GLU:OE1	1:F:158:THR:O	2.29	0.51
1:G:113:VAL:HG22	1:G:123:THR:CB	2.41	0.51
1:G:157:ARG:HD3	1:H:5:TYR:OH	2.11	0.51
1:H:325:THR:O	1:H:329:ILE:HG13	2.11	0.51
1:I:113:VAL:HG22	1:I:123:THR:CB	2.41	0.51
1:J:41:ALA:HB2	1:J:51:ASN:ND2	2.26	0.51
1:K:325:THR:O	1:K:329:ILE:HG13	2.11	0.51
1:L:122:GLU:OE1	1:L:158:THR:O	2.29	0.51
1:D:61:GLN:HE21	1:D:88:ASP:CB	2.22	0.51
1:J:40:MET:HE3	1:J:43:ARG:HB2	1.93	0.51
1:K:113:VAL:HG22	1:K:123:THR:CB	2.41	0.51
1:E:41:ALA:HB2	1:E:51:ASN:ND2	2.26	0.50
1:E:167:ASN:N	1:E:170:VAL:HG23	2.23	0.50
1:G:40:MET:HE3	1:G:43:ARG:HB2	1.93	0.50
1:K:167:ASN:N	1:K:170:VAL:HG23	2.23	0.50
1:A:59:TYR:CE1	1:A:311:LEU:HD13	2.46	0.50
1:A:95:VAL:O	1:A:99:GLN:HG3	2.11	0.50
1:D:113:VAL:HG22	1:D:123:THR:CB	2.41	0.50
1:F:234:VAL:HG13	1:F:253:THR:CA	2.33	0.50
1:G:41:ALA:HB2	1:G:51:ASN:ND2	2.26	0.50
1:H:40:MET:HE3	1:H:43:ARG:HB2	1.93	0.50
1:I:40:MET:HE3	1:I:43:ARG:HB2	1.93	0.50
1:K:61:GLN:HE21	1:K:88:ASP:CB	2.22	0.50
1:A:40:MET:HE3	1:A:43:ARG:HB2	1.93	0.50
1:C:59:TYR:CE1	1:C:311:LEU:HD13	2.46	0.50
1:C:113:VAL:HG22	1:C:123:THR:CB	2.41	0.50
1:G:122:GLU:OE1	1:G:158:THR:O	2.29	0.50
1:I:41:ALA:HB2	1:I:51:ASN:ND2	2.26	0.50
1:I:59:TYR:CE1	1:I:311:LEU:HD13	2.46	0.50
1:J:325:THR:O	1:J:329:ILE:HG13	2.11	0.50
1:K:118:GLY:HA3	1:L:221:HIS:CD2	2.45	0.50
1:K:234:VAL:HG13	1:K:253:THR:CA	2.33	0.50
1:B:59:TYR:CE1	1:B:311:LEU:HD13	2.46	0.50
1:C:167:ASN:N	1:C:170:VAL:HG23	2.23	0.50
1:D:95:VAL:O	1:D:99:GLN:HG3	2.11	0.50
1:G:59:TYR:CE1	1:G:311:LEU:HD13	2.46	0.50
1:G:95:VAL:O	1:G:99:GLN:HG3	2.11	0.50
1:H:95:VAL:O	1:H:99:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:THR:OG1	1:H:300:PHE:N	2.39	0.50
1:I:95:VAL:O	1:I:99:GLN:HG3	2.11	0.50
1:J:299:THR:OG1	1:J:300:PHE:N	2.39	0.50
1:C:40:MET:HE3	1:C:43:ARG:HB2	1.93	0.50
1:E:59:TYR:CE1	1:E:311:LEU:HD13	2.46	0.50
1:E:122:GLU:OE1	1:E:158:THR:O	2.29	0.50
1:F:41:ALA:HB2	1:F:51:ASN:ND2	2.26	0.50
1:G:325:THR:O	1:G:329:ILE:HG13	2.10	0.50
1:L:59:TYR:CE1	1:L:311:LEU:HD13	2.46	0.50
1:D:40:MET:HE3	1:D:43:ARG:HB2	1.93	0.50
1:E:234:VAL:HG13	1:E:253:THR:CA	2.33	0.50
1:E:258:ARG:O	1:H:264:ALA:HB2	2.12	0.50
1:F:59:TYR:CE1	1:F:311:LEU:HD13	2.46	0.50
1:I:122:GLU:OE1	1:I:158:THR:O	2.29	0.50
1:I:263:PRO:HG2	1:L:296:TRP:CH2	2.47	0.50
1:K:59:TYR:CE1	1:K:311:LEU:HD13	2.46	0.50
1:K:122:GLU:OE1	1:K:158:THR:O	2.29	0.50
1:L:41:ALA:HB2	1:L:51:ASN:ND2	2.26	0.50
1:C:122:GLU:OE1	1:C:158:THR:O	2.29	0.50
1:D:122:GLU:OE1	1:D:158:THR:O	2.29	0.50
1:I:325:THR:O	1:I:329:ILE:HG13	2.11	0.50
1:J:4:SER:HB3	1:K:204:TYR:CD1	2.47	0.50
1:J:122:GLU:OE1	1:J:158:THR:O	2.29	0.50
1:J:295:PRO:HG2	1:K:263:PRO:HG3	1.94	0.50
1:B:40:MET:HE3	1:B:43:ARG:HB2	1.93	0.50
1:C:95:VAL:O	1:C:99:GLN:HG3	2.11	0.50
1:D:300:PHE:HB2	1:D:302:TYR:CD2	2.47	0.50
1:J:95:VAL:O	1:J:99:GLN:HG3	2.12	0.50
1:K:95:VAL:O	1:K:99:GLN:HG3	2.11	0.50
1:L:113:VAL:HG22	1:L:123:THR:CB	2.41	0.50
1:A:300:PHE:HB2	1:A:302:TYR:CD2	2.47	0.49
1:B:95:VAL:O	1:B:99:GLN:HG3	2.11	0.49
1:B:122:GLU:OE1	1:B:158:THR:O	2.29	0.49
1:F:113:VAL:HG22	1:F:123:THR:CB	2.41	0.49
1:H:59:TYR:CE1	1:H:311:LEU:HD13	2.46	0.49
1:A:122:GLU:OE1	1:A:158:THR:O	2.29	0.49
1:C:173:ARG:HD2	1:D:166:GLU:OE2	2.11	0.49
1:G:158:THR:HG1	1:G:159:PRO:HD3	1.76	0.49
1:H:300:PHE:HB2	1:H:302:TYR:CD2	2.47	0.49
1:J:300:PHE:HB2	1:J:302:TYR:CD2	2.47	0.49
1:A:107:ILE:N	1:A:107:ILE:CD1	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:HD3	1:H:291:PRO:HD3	1.93	0.49
1:E:4:SER:HB3	1:H:204:TYR:CG	2.47	0.49
1:F:167:ASN:N	1:F:170:VAL:HG23	2.23	0.49
1:L:167:ASN:N	1:L:170:VAL:HG23	2.23	0.49
1:L:300:PHE:HB2	1:L:302:TYR:CD2	2.47	0.49
1:B:46:GLN:HE22	1:B:304:ARG:HH21	1.61	0.49
1:F:300:PHE:HB2	1:F:302:TYR:CD2	2.47	0.49
1:H:122:GLU:OE1	1:H:158:THR:O	2.29	0.49
1:J:61:GLN:HE21	1:J:88:ASP:CB	2.22	0.49
1:K:40:MET:HE3	1:K:43:ARG:HB2	1.93	0.49
1:C:46:GLN:HE22	1:C:304:ARG:HH21	1.61	0.49
1:C:300:PHE:HB2	1:C:302:TYR:CD2	2.47	0.49
1:F:40:MET:HE3	1:F:43:ARG:HB2	1.93	0.49
1:F:96:ARG:NH1	1:F:96:ARG:HG2	2.28	0.49
1:H:61:GLN:HE21	1:H:88:ASP:CB	2.22	0.49
1:L:40:MET:HE3	1:L:43:ARG:HB2	1.93	0.49
1:E:40:MET:HE3	1:E:43:ARG:HB2	1.93	0.49
1:E:113:VAL:HG22	1:E:123:THR:CB	2.41	0.49
1:E:158:THR:HG1	1:E:159:PRO:HD3	1.78	0.49
1:F:61:GLN:HE21	1:F:88:ASP:CB	2.22	0.49
1:F:238:HIS:CG	1:J:243:LYS:HZ1	2.26	0.49
1:G:96:ARG:NH1	1:G:96:ARG:HG2	2.28	0.49
1:I:96:ARG:HG2	1:I:96:ARG:NH1	2.28	0.49
1:J:59:TYR:CE1	1:J:311:LEU:HD13	2.46	0.49
1:K:300:PHE:HB2	1:K:302:TYR:CD2	2.47	0.49
1:L:96:ARG:NH1	1:L:96:ARG:HG2	2.28	0.49
1:E:95:VAL:O	1:E:99:GLN:HG3	2.12	0.49
1:E:96:ARG:NH1	1:E:96:ARG:HG2	2.28	0.49
1:E:300:PHE:HB2	1:E:302:TYR:CD2	2.47	0.49
1:A:46:GLN:HE22	1:A:304:ARG:HH21	1.61	0.49
1:A:113:VAL:HG22	1:A:123:THR:CB	2.41	0.49
1:E:46:GLN:HE22	1:E:304:ARG:HH21	1.61	0.49
1:B:300:PHE:HB2	1:B:302:TYR:CD2	2.47	0.49
1:K:46:GLN:HE22	1:K:304:ARG:HH21	1.61	0.49
1:K:96:ARG:NH1	1:K:96:ARG:HG2	2.28	0.49
1:L:61:GLN:HE21	1:L:88:ASP:CB	2.22	0.49
1:B:96:ARG:NH1	1:B:96:ARG:HG2	2.28	0.48
1:D:43:ARG:HG2	1:D:304:ARG:HH22	1.78	0.48
1:G:46:GLN:HE22	1:G:304:ARG:HH21	1.61	0.48
1:A:43:ARG:HG2	1:A:304:ARG:HH22	1.79	0.48
1:B:263:PRO:CG	1:C:295:PRO:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ARG:HG2	1:F:304:ARG:HH22	1.78	0.48
1:F:95:VAL:O	1:F:99:GLN:HG3	2.11	0.48
1:G:300:PHE:HB2	1:G:302:TYR:CD2	2.47	0.48
1:I:46:GLN:HE22	1:I:304:ARG:HH21	1.61	0.48
1:I:300:PHE:HB2	1:I:302:TYR:CD2	2.47	0.48
1:D:46:GLN:HE22	1:D:304:ARG:HH21	1.61	0.48
1:L:95:VAL:O	1:L:99:GLN:HG3	2.11	0.48
1:C:96:ARG:NH1	1:C:96:ARG:HG2	2.28	0.48
1:D:199:LEU:CD1	1:D:235:THR:HA	2.44	0.48
1:L:43:ARG:HG2	1:L:304:ARG:HH22	1.79	0.48
1:A:199:LEU:CD1	1:A:235:THR:HA	2.44	0.48
1:B:43:ARG:HG2	1:B:304:ARG:HH22	1.79	0.48
1:B:107:ILE:N	1:B:107:ILE:CD1	2.67	0.48
1:E:261:VAL:O	1:E:296:TRP:HZ3	1.96	0.48
1:H:96:ARG:NH1	1:H:96:ARG:HG2	2.28	0.48
1:H:113:VAL:HG22	1:H:123:THR:CB	2.41	0.48
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.28	0.48
1:D:261:VAL:O	1:D:296:TRP:HZ3	1.96	0.48
1:F:160:SER:O	1:F:161:ALA:C	2.57	0.48
1:F:288:ASN:HA	1:F:294:ARG:NH2	2.29	0.48
1:J:46:GLN:HE22	1:J:304:ARG:HH21	1.61	0.48
1:L:160:SER:O	1:L:161:ALA:C	2.57	0.48
1:A:157:ARG:HD3	1:B:5:TYR:OH	2.13	0.48
1:A:242:ILE:HD11	1:I:99:GLN:HB3	1.96	0.48
1:D:96:ARG:NH1	1:D:96:ARG:HG2	2.28	0.48
1:G:61:GLN:HE22	1:G:89:ASP:N	2.10	0.48
1:H:46:GLN:HE22	1:H:304:ARG:HH21	1.61	0.48
1:I:43:ARG:HG2	1:I:304:ARG:HH22	1.79	0.48
1:I:158:THR:HG1	1:I:159:PRO:HD3	1.78	0.48
1:C:199:LEU:CD1	1:C:235:THR:HA	2.44	0.48
1:D:288:ASN:HA	1:D:294:ARG:NH2	2.29	0.48
1:G:43:ARG:HG2	1:G:304:ARG:HH22	1.79	0.48
1:I:61:GLN:HE22	1:I:89:ASP:N	2.10	0.48
1:J:113:VAL:HG22	1:J:123:THR:CB	2.41	0.48
1:K:261:VAL:O	1:K:296:TRP:HZ3	1.96	0.48
1:L:288:ASN:HA	1:L:294:ARG:NH2	2.29	0.48
1:C:43:ARG:HG2	1:C:304:ARG:HH22	1.79	0.48
1:C:158:THR:HG1	1:C:159:PRO:HD3	1.76	0.48
1:D:160:SER:O	1:D:161:ALA:C	2.57	0.48
1:G:160:SER:O	1:G:161:ALA:C	2.57	0.48
1:G:288:ASN:HA	1:G:294:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:288:ASN:HA	1:I:294:ARG:NH2	2.29	0.48
1:A:288:ASN:HA	1:A:294:ARG:NH2	2.29	0.48
1:E:199:LEU:CD1	1:E:235:THR:HA	2.44	0.48
1:F:199:LEU:CD1	1:F:235:THR:HA	2.44	0.48
1:H:13:LYS:HB3	1:H:223:TYR:CZ	2.49	0.48
1:I:160:SER:O	1:I:161:ALA:C	2.57	0.48
1:J:96:ARG:NH1	1:J:96:ARG:HG2	2.28	0.48
1:K:160:SER:O	1:K:161:ALA:C	2.57	0.48
1:K:199:LEU:CD1	1:K:235:THR:HA	2.44	0.48
1:A:261:VAL:O	1:A:296:TRP:HZ3	1.96	0.47
1:B:261:VAL:O	1:B:296:TRP:HZ3	1.96	0.47
1:C:37:VAL:HG23	1:C:56:ARG:NH1	2.29	0.47
1:E:288:ASN:HA	1:E:294:ARG:NH2	2.29	0.47
1:F:4:SER:HB3	1:G:204:TYR:CD1	2.48	0.47
1:F:37:VAL:HG23	1:F:56:ARG:NH1	2.29	0.47
1:G:37:VAL:HG23	1:G:56:ARG:NH1	2.29	0.47
1:H:37:VAL:HG23	1:H:56:ARG:NH1	2.29	0.47
1:H:288:ASN:HA	1:H:294:ARG:NH2	2.29	0.47
1:J:37:VAL:HG23	1:J:56:ARG:NH1	2.29	0.47
1:J:288:ASN:HA	1:J:294:ARG:NH2	2.29	0.47
1:L:37:VAL:HG23	1:L:56:ARG:NH1	2.29	0.47
1:L:199:LEU:CD1	1:L:235:THR:HA	2.44	0.47
1:B:37:VAL:HG23	1:B:56:ARG:NH1	2.29	0.47
1:C:166:GLU:OE2	1:D:173:ARG:HD2	2.14	0.47
1:E:13:LYS:HB3	1:E:223:TYR:CZ	2.49	0.47
1:J:13:LYS:HB3	1:J:223:TYR:CZ	2.49	0.47
1:J:43:ARG:HG2	1:J:304:ARG:HH22	1.78	0.47
1:J:199:LEU:CD1	1:J:235:THR:HA	2.44	0.47
1:K:13:LYS:HB3	1:K:223:TYR:CZ	2.49	0.47
1:K:288:ASN:HA	1:K:294:ARG:NH2	2.29	0.47
1:B:199:LEU:CD1	1:B:235:THR:HA	2.44	0.47
1:E:160:SER:O	1:E:161:ALA:C	2.57	0.47
1:F:13:LYS:HB3	1:F:223:TYR:CZ	2.49	0.47
1:H:199:LEU:CD1	1:H:235:THR:HA	2.44	0.47
1:H:278:GLU:OE2	1:H:331:ARG:NH2	2.48	0.47
1:I:37:VAL:HG23	1:I:56:ARG:NH1	2.29	0.47
1:L:13:LYS:HB3	1:L:223:TYR:CZ	2.49	0.47
1:L:46:GLN:HE22	1:L:304:ARG:HH21	1.61	0.47
1:A:154:ILE:HA	1:A:158:THR:HG1	1.80	0.47
1:B:278:GLU:OE2	1:B:331:ARG:NH2	2.48	0.47
1:B:288:ASN:HA	1:B:294:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:OE2	1:C:331:ARG:NH2	2.48	0.47
1:J:278:GLU:OE2	1:J:331:ARG:NH2	2.48	0.47
1:K:43:ARG:HG2	1:K:304:ARG:HH22	1.79	0.47
1:L:278:GLU:OE2	1:L:331:ARG:NH2	2.48	0.47
1:A:160:SER:O	1:A:161:ALA:C	2.57	0.47
1:C:288:ASN:HA	1:C:294:ARG:NH2	2.29	0.47
1:D:37:VAL:HG23	1:D:56:ARG:NH1	2.29	0.47
1:E:278:GLU:OE2	1:E:331:ARG:NH2	2.48	0.47
1:F:278:GLU:OE2	1:F:331:ARG:NH2	2.48	0.47
1:H:261:VAL:O	1:H:296:TRP:HZ3	1.96	0.47
1:J:261:VAL:O	1:J:296:TRP:HZ3	1.96	0.47
1:D:13:LYS:HB3	1:D:223:TYR:CZ	2.49	0.47
1:E:37:VAL:HG23	1:E:56:ARG:NH1	2.30	0.47
1:E:46:GLN:NE2	1:E:304:ARG:NH2	2.63	0.47
1:H:43:ARG:HG2	1:H:304:ARG:HH22	1.79	0.47
1:I:199:LEU:CD1	1:I:235:THR:HA	2.44	0.47
1:K:37:VAL:HG23	1:K:56:ARG:NH1	2.29	0.47
1:L:245:THR:HB	1:L:248:GLU:H	1.80	0.47
1:A:13:LYS:HB3	1:A:223:TYR:CZ	2.49	0.47
1:B:4:SER:HB3	1:C:204:TYR:CG	2.49	0.47
1:B:59:TYR:CZ	1:B:311:LEU:HD13	2.50	0.47
1:C:59:TYR:CZ	1:C:311:LEU:HD13	2.50	0.47
1:C:154:ILE:HA	1:C:158:THR:HG1	1.80	0.47
1:C:261:VAL:O	1:C:296:TRP:HZ3	1.96	0.47
1:E:43:ARG:HG2	1:E:304:ARG:HH22	1.79	0.47
1:E:204:TYR:CD1	1:H:4:SER:HB3	2.50	0.47
1:F:46:GLN:HE22	1:F:304:ARG:HH21	1.61	0.47
1:F:204:TYR:CD1	1:G:4:SER:HB3	2.49	0.47
1:F:245:THR:HB	1:F:248:GLU:H	1.80	0.47
1:G:191:ILE:HB	1:G:232:ASN:ND2	2.30	0.47
1:G:278:GLU:OE2	1:G:331:ARG:NH2	2.48	0.47
1:I:191:ILE:HB	1:I:232:ASN:ND2	2.30	0.47
1:K:46:GLN:NE2	1:K:304:ARG:NH2	2.63	0.47
1:K:129:ASP:OD2	1:L:129:ASP:N	2.45	0.47
1:K:221:HIS:CD2	1:L:118:GLY:HA3	2.50	0.47
1:K:278:GLU:OE2	1:K:331:ARG:NH2	2.48	0.47
1:B:13:LYS:HB3	1:B:223:TYR:CZ	2.49	0.47
1:E:59:TYR:CZ	1:E:311:LEU:HD13	2.50	0.47
1:E:191:ILE:HB	1:E:232:ASN:ND2	2.30	0.47
1:G:261:VAL:O	1:G:296:TRP:HZ3	1.96	0.47
1:I:59:TYR:CZ	1:I:311:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:278:GLU:OE2	1:I:331:ARG:NH2	2.48	0.47
1:J:46:GLN:NE2	1:J:304:ARG:NH2	2.63	0.47
1:K:191:ILE:HB	1:K:232:ASN:ND2	2.30	0.47
1:A:37:VAL:HG23	1:A:56:ARG:NH1	2.29	0.47
1:C:13:LYS:HB3	1:C:223:TYR:CZ	2.49	0.47
1:C:129:ASP:OD2	1:D:129:ASP:N	2.44	0.47
1:G:46:GLN:NE2	1:G:304:ARG:NH2	2.63	0.47
1:G:59:TYR:CZ	1:G:311:LEU:HD13	2.50	0.47
1:G:199:LEU:CD1	1:G:235:THR:HA	2.44	0.47
1:I:13:LYS:HB3	1:I:223:TYR:CZ	2.49	0.47
1:I:261:VAL:O	1:I:296:TRP:HZ3	1.96	0.47
1:K:154:ILE:HA	1:K:158:THR:HG1	1.80	0.47
1:A:191:ILE:HB	1:A:232:ASN:ND2	2.30	0.47
1:G:245:THR:HB	1:G:248:GLU:H	1.80	0.47
1:I:46:GLN:NE2	1:I:304:ARG:NH2	2.63	0.47
1:J:264:ALA:HB2	1:K:258:ARG:O	2.15	0.47
1:C:245:THR:HB	1:C:248:GLU:H	1.80	0.46
1:E:11:GLU:H	1:E:11:GLU:HG2	1.51	0.46
1:F:61:GLN:HE22	1:F:89:ASP:N	2.10	0.46
1:G:13:LYS:HB3	1:G:223:TYR:CZ	2.49	0.46
1:H:11:GLU:H	1:H:11:GLU:HG2	1.50	0.46
1:H:46:GLN:NE2	1:H:304:ARG:NH2	2.63	0.46
1:H:191:ILE:HB	1:H:232:ASN:ND2	2.30	0.46
1:I:245:THR:HB	1:I:248:GLU:H	1.80	0.46
1:K:59:TYR:CZ	1:K:311:LEU:HD13	2.50	0.46
1:E:201:ARG:HH12	1:H:3:HIS:HD2	1.63	0.46
1:F:59:TYR:CZ	1:F:311:LEU:HD13	2.50	0.46
1:H:245:THR:HB	1:H:248:GLU:H	1.80	0.46
1:L:61:GLN:HE22	1:L:89:ASP:N	2.10	0.46
1:B:154:ILE:HA	1:B:158:THR:HG1	1.80	0.46
1:D:154:ILE:HA	1:D:158:THR:HG1	1.80	0.46
1:J:160:SER:O	1:J:161:ALA:C	2.57	0.46
1:L:59:TYR:CZ	1:L:311:LEU:HD13	2.50	0.46
1:A:46:GLN:NE2	1:A:304:ARG:NH2	2.63	0.46
1:D:278:GLU:OE2	1:D:331:ARG:NH2	2.48	0.46
1:I:154:ILE:HA	1:I:158:THR:HG1	1.80	0.46
1:J:191:ILE:HB	1:J:232:ASN:ND2	2.30	0.46
1:B:61:GLN:HE22	1:B:89:ASP:N	2.10	0.46
1:D:245:THR:HB	1:D:248:GLU:H	1.80	0.46
1:J:245:THR:HB	1:J:248:GLU:H	1.80	0.46
1:A:278:GLU:OE2	1:A:331:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:O	1:B:81:HIS:C	2.59	0.46
1:B:204:TYR:CE1	1:C:4:SER:HB3	2.50	0.46
1:C:191:ILE:HB	1:C:232:ASN:ND2	2.30	0.46
1:F:46:GLN:NE2	1:F:304:ARG:NH2	2.63	0.46
1:F:258:ARG:HB2	1:G:263:PRO:HB2	1.98	0.46
1:H:59:TYR:CZ	1:H:311:LEU:HD13	2.50	0.46
1:J:154:ILE:HA	1:J:158:THR:HG1	1.81	0.46
1:K:245:THR:HB	1:K:248:GLU:H	1.80	0.46
1:B:245:THR:HB	1:B:248:GLU:H	1.80	0.46
1:C:46:GLN:NE2	1:C:304:ARG:NH2	2.63	0.46
1:F:154:ILE:HA	1:F:158:THR:HG1	1.80	0.46
1:G:154:ILE:HA	1:G:158:THR:HG1	1.80	0.46
1:H:160:SER:O	1:H:161:ALA:C	2.57	0.46
1:I:4:SER:HB3	1:L:204:TYR:CG	2.51	0.46
1:K:11:GLU:H	1:K:11:GLU:HG2	1.51	0.46
1:L:46:GLN:NE2	1:L:304:ARG:NH2	2.63	0.46
1:A:157:ARG:NH2	1:B:3:HIS:N	2.64	0.46
1:B:46:GLN:NE2	1:B:304:ARG:NH2	2.63	0.46
1:D:46:GLN:NE2	1:D:304:ARG:NH2	2.63	0.46
1:H:154:ILE:HA	1:H:158:THR:HG1	1.81	0.46
1:C:160:SER:O	1:C:161:ALA:C	2.57	0.46
1:D:59:TYR:CZ	1:D:311:LEU:HD13	2.50	0.46
1:F:261:VAL:O	1:F:296:TRP:HZ3	1.96	0.46
1:L:154:ILE:HA	1:L:158:THR:HG1	1.80	0.46
1:E:154:ILE:HA	1:E:158:THR:HG1	1.80	0.46
1:E:245:THR:HB	1:E:248:GLU:H	1.80	0.46
1:J:294:ARG:HA	1:J:295:PRO:HD3	1.79	0.46
1:L:191:ILE:HB	1:L:232:ASN:ND2	2.30	0.46
1:J:59:TYR:CZ	1:J:311:LEU:HD13	2.50	0.45
1:A:245:THR:HB	1:A:248:GLU:H	1.80	0.45
1:B:160:SER:O	1:B:161:ALA:C	2.57	0.45
1:B:191:ILE:HB	1:B:232:ASN:ND2	2.30	0.45
1:F:191:ILE:HB	1:F:232:ASN:ND2	2.30	0.45
1:H:30:ILE:HB	1:H:301:SER:HA	1.99	0.45
1:K:80:PHE:O	1:K:81:HIS:C	2.59	0.45
1:L:261:VAL:O	1:L:296:TRP:HZ3	1.96	0.45
1:B:30:ILE:HB	1:B:301:SER:HA	1.99	0.45
1:C:30:ILE:HB	1:C:301:SER:HA	1.99	0.45
1:D:61:GLN:HE22	1:D:89:ASP:N	2.10	0.45
1:D:191:ILE:HB	1:D:232:ASN:ND2	2.30	0.45
1:E:263:PRO:HG3	1:H:263:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:30:ILE:HB	1:J:301:SER:HA	1.99	0.45
1:K:129:ASP:N	1:L:129:ASP:OD2	2.45	0.45
1:A:59:TYR:CZ	1:A:311:LEU:HD13	2.50	0.45
1:B:11:GLU:H	1:B:11:GLU:HG2	1.50	0.45
1:G:30:ILE:HB	1:G:301:SER:HA	1.99	0.45
1:A:52:THR:HG22	1:A:53:GLU:H	1.82	0.45
1:D:80:PHE:O	1:D:81:HIS:C	2.59	0.45
1:E:80:PHE:O	1:E:81:HIS:C	2.59	0.45
1:H:294:ARG:HA	1:H:295:PRO:HD3	1.79	0.45
1:I:30:ILE:HB	1:I:301:SER:HA	1.99	0.45
1:A:80:PHE:O	1:A:81:HIS:C	2.59	0.45
1:F:80:PHE:O	1:F:81:HIS:C	2.59	0.45
1:J:11:GLU:H	1:J:11:GLU:HG2	1.50	0.45
1:L:30:ILE:HB	1:L:301:SER:HA	1.98	0.45
1:L:80:PHE:O	1:L:81:HIS:C	2.59	0.45
1:A:317:GLN:CG	1:H:291:PRO:HA	2.44	0.45
1:F:30:ILE:HB	1:F:301:SER:HA	1.99	0.45
1:A:292:LEU:HA	1:A:293:PRO:HD3	1.78	0.45
1:D:52:THR:HG22	1:D:53:GLU:H	1.82	0.45
1:D:158:THR:HG1	1:D:159:PRO:HD3	1.80	0.45
1:I:52:THR:HG22	1:I:53:GLU:H	1.82	0.45
1:B:47:ILE:HG13	1:B:49:VAL:HG23	1.99	0.45
1:C:47:ILE:HG13	1:C:49:VAL:HG23	1.99	0.45
1:G:47:ILE:HG13	1:G:49:VAL:HG23	1.99	0.45
1:I:201:ARG:NH1	1:L:3:HIS:CD2	2.74	0.45
1:K:30:ILE:HB	1:K:301:SER:HA	1.99	0.45
1:A:61:GLN:HE22	1:A:89:ASP:N	2.10	0.45
1:B:3:HIS:CD2	1:C:201:ARG:HH12	2.35	0.45
1:C:61:GLN:HE22	1:C:89:ASP:N	2.10	0.45
1:E:30:ILE:HB	1:E:301:SER:HA	1.99	0.45
1:G:52:THR:HG22	1:G:53:GLU:H	1.82	0.45
1:H:80:PHE:O	1:H:81:HIS:C	2.59	0.45
1:I:47:ILE:HG13	1:I:49:VAL:HG23	1.98	0.45
1:I:80:PHE:O	1:I:81:HIS:C	2.59	0.45
1:J:52:THR:HG22	1:J:53:GLU:H	1.82	0.45
1:L:320:ASN:N	1:L:320:ASN:HD22	2.15	0.45
1:C:11:GLU:H	1:C:11:GLU:HG2	1.50	0.44
1:D:47:ILE:HG13	1:D:49:VAL:HG23	1.99	0.44
1:D:292:LEU:HA	1:D:293:PRO:HD3	1.78	0.44
1:E:201:ARG:HH12	1:H:3:HIS:CD2	2.34	0.44
1:F:201:ARG:NH2	1:G:3:HIS:NE2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:ASN:N	1:F:320:ASN:HD22	2.16	0.44
1:F:52:THR:HG22	1:F:53:GLU:H	1.82	0.44
1:G:80:PHE:O	1:G:81:HIS:C	2.59	0.44
1:H:47:ILE:HG13	1:H:49:VAL:HG23	1.99	0.44
1:K:192:LEU:HA	1:K:193:PRO:HD3	1.77	0.44
1:C:80:PHE:O	1:C:81:HIS:C	2.59	0.44
1:E:320:ASN:N	1:E:320:ASN:HD22	2.15	0.44
1:H:52:THR:HG22	1:H:53:GLU:H	1.82	0.44
1:J:80:PHE:O	1:J:81:HIS:C	2.59	0.44
1:A:240:CYS:HA	1:A:241:PRO:HD3	1.83	0.44
1:A:278:GLU:OE1	1:A:282:PHE:HE1	2.01	0.44
1:B:4:SER:HB3	1:C:204:TYR:CE1	2.52	0.44
1:C:52:THR:HG22	1:C:53:GLU:H	1.82	0.44
1:C:278:GLU:OE1	1:C:282:PHE:HE1	2.01	0.44
1:C:294:ARG:HA	1:C:295:PRO:HD3	1.79	0.44
1:J:47:ILE:HG13	1:J:49:VAL:HG23	1.99	0.44
1:K:129:ASP:HB2	1:L:129:ASP:OD2	2.16	0.44
1:K:165:LEU:HD23	1:K:166:GLU:N	2.33	0.44
1:K:320:ASN:HD22	1:K:320:ASN:N	2.16	0.44
1:A:11:GLU:H	1:A:11:GLU:HG2	1.51	0.44
1:E:165:LEU:HD23	1:E:166:GLU:N	2.33	0.44
1:A:47:ILE:HG13	1:A:49:VAL:HG23	1.99	0.44
1:B:278:GLU:OE1	1:B:282:PHE:HE1	2.01	0.44
1:C:320:ASN:N	1:C:320:ASN:HD22	2.15	0.44
1:D:30:ILE:HB	1:D:301:SER:HA	1.98	0.44
1:D:278:GLU:OE1	1:D:282:PHE:HE1	2.01	0.44
1:E:263:PRO:HG2	1:H:296:TRP:CH2	2.52	0.44
1:I:209:VAL:O	1:I:213:VAL:HG23	2.18	0.44
1:L:52:THR:HG22	1:L:53:GLU:H	1.82	0.44
1:L:278:GLU:OE1	1:L:282:PHE:HE1	2.01	0.44
1:A:30:ILE:HB	1:A:301:SER:HA	1.99	0.44
1:D:294:ARG:HA	1:D:295:PRO:HD3	1.79	0.44
1:E:47:ILE:HG13	1:E:49:VAL:HG23	1.99	0.44
1:E:209:VAL:O	1:E:213:VAL:HG23	2.18	0.44
1:F:3:HIS:HD2	1:G:201:ARG:HH12	1.64	0.44
1:F:278:GLU:OE1	1:F:282:PHE:HE1	2.01	0.44
1:G:3:HIS:N	1:H:157:ARG:NH2	2.65	0.44
1:K:209:VAL:O	1:K:213:VAL:HG23	2.18	0.44
1:A:245:THR:C	1:A:247:GLU:N	2.73	0.44
1:B:209:VAL:O	1:B:213:VAL:HG23	2.18	0.44
1:B:245:THR:C	1:B:247:GLU:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:VAL:O	1:G:213:VAL:HG23	2.18	0.44
1:I:165:LEU:HD23	1:I:166:GLU:N	2.33	0.44
1:B:192:LEU:HA	1:B:193:PRO:HD3	1.77	0.44
1:D:245:THR:C	1:D:247:GLU:N	2.73	0.44
1:E:61:GLN:HE22	1:E:89:ASP:N	2.10	0.44
1:E:156:GLU:OE2	1:G:156:GLU:HG3	2.18	0.44
1:G:165:LEU:HD23	1:G:166:GLU:N	2.33	0.44
1:J:204:TYR:CG	1:K:4:SER:HB3	2.53	0.44
1:K:47:ILE:HG13	1:K:49:VAL:HG23	1.99	0.44
1:K:278:GLU:OE1	1:K:282:PHE:HE1	2.01	0.44
1:B:294:ARG:HA	1:B:295:PRO:HD3	1.79	0.43
1:B:320:ASN:N	1:B:320:ASN:HD22	2.16	0.43
1:D:240:CYS:HA	1:D:241:PRO:HD3	1.83	0.43
1:J:209:VAL:O	1:J:213:VAL:HG23	2.18	0.43
1:K:52:THR:HG22	1:K:53:GLU:H	1.82	0.43
1:K:61:GLN:HE22	1:K:89:ASP:N	2.10	0.43
1:G:278:GLU:OE1	1:G:282:PHE:HE1	2.01	0.43
1:I:278:GLU:OE1	1:I:282:PHE:HE1	2.01	0.43
1:K:262:PRO:HA	1:K:263:PRO:HD3	1.93	0.43
1:B:52:THR:HG22	1:B:53:GLU:H	1.82	0.43
1:C:245:THR:C	1:C:247:GLU:N	2.73	0.43
1:E:52:THR:HG22	1:E:53:GLU:H	1.82	0.43
1:F:47:ILE:HG13	1:F:49:VAL:HG23	1.99	0.43
1:I:3:HIS:CD2	1:L:201:ARG:HH22	2.35	0.43
1:B:165:LEU:HD23	1:B:166:GLU:N	2.33	0.43
1:C:209:VAL:O	1:C:213:VAL:HG23	2.18	0.43
1:F:11:GLU:H	1:F:11:GLU:HG2	1.51	0.43
1:F:44:LEU:HD23	1:F:44:LEU:HA	1.87	0.43
1:G:245:THR:C	1:G:247:GLU:N	2.73	0.43
1:I:320:ASN:N	1:I:320:ASN:HD22	2.16	0.43
1:L:11:GLU:H	1:L:11:GLU:HG2	1.50	0.43
1:L:47:ILE:HG13	1:L:49:VAL:HG23	1.99	0.43
1:A:290:CYS:HA	1:A:291:PRO:HD3	1.87	0.43
1:D:165:LEU:HD23	1:D:166:GLU:N	2.33	0.43
1:E:278:GLU:OE1	1:E:282:PHE:HE1	2.01	0.43
1:G:320:ASN:N	1:G:320:ASN:HD22	2.16	0.43
1:H:209:VAL:O	1:H:213:VAL:HG23	2.18	0.43
1:A:193:PRO:O	1:A:237:GLY:HA2	2.19	0.43
1:I:245:THR:C	1:I:247:GLU:N	2.73	0.43
1:C:165:LEU:HD23	1:C:166:GLU:N	2.33	0.43
1:J:245:THR:C	1:J:247:GLU:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:254:VAL:HG12	1:J:258:ARG:HD2	2.01	0.43
1:L:165:LEU:HD23	1:L:166:GLU:N	2.33	0.43
1:D:193:PRO:O	1:D:237:GLY:HA2	2.19	0.43
1:D:262:PRO:HA	1:D:263:PRO:HD3	1.93	0.43
1:H:245:THR:C	1:H:247:GLU:N	2.73	0.43
1:H:254:VAL:HG12	1:H:258:ARG:HD2	2.01	0.43
1:H:262:PRO:HA	1:H:263:PRO:HD3	1.93	0.43
1:J:320:ASN:N	1:J:320:ASN:HD22	2.16	0.43
1:L:44:LEU:HD23	1:L:44:LEU:HA	1.87	0.43
1:A:320:ASN:N	1:A:320:ASN:HD22	2.16	0.43
1:D:209:VAL:O	1:D:213:VAL:HG23	2.18	0.43
1:E:192:LEU:HA	1:E:193:PRO:HD3	1.77	0.43
1:F:165:LEU:HD23	1:F:166:GLU:N	2.33	0.43
1:H:320:ASN:N	1:H:320:ASN:HD22	2.16	0.43
1:A:165:LEU:HD23	1:A:166:GLU:N	2.33	0.43
1:B:28:LYS:O	1:B:299:THR:HG21	2.19	0.43
1:C:331:ARG:HA	1:C:334:VAL:HG13	2.01	0.43
1:F:193:PRO:O	1:F:237:GLY:HA2	2.19	0.43
1:H:28:LYS:O	1:H:299:THR:HG21	2.19	0.43
1:J:28:LYS:O	1:J:299:THR:HG21	2.19	0.43
1:J:165:LEU:HD23	1:J:166:GLU:N	2.33	0.43
1:L:209:VAL:O	1:L:213:VAL:HG23	2.18	0.43
1:B:193:PRO:O	1:B:237:GLY:HA2	2.19	0.42
1:E:28:LYS:O	1:E:299:THR:HG21	2.19	0.42
1:F:209:VAL:O	1:F:213:VAL:HG23	2.18	0.42
1:H:165:LEU:HD23	1:H:166:GLU:N	2.33	0.42
1:J:278:GLU:OE1	1:J:282:PHE:HE1	2.01	0.42
1:L:292:LEU:HA	1:L:293:PRO:HD3	1.78	0.42
1:A:209:VAL:O	1:A:213:VAL:HG23	2.18	0.42
1:A:254:VAL:HG12	1:A:258:ARG:HD2	2.01	0.42
1:B:331:ARG:HA	1:B:334:VAL:HG13	2.01	0.42
1:C:28:LYS:O	1:C:299:THR:HG21	2.19	0.42
1:D:331:ARG:HA	1:D:334:VAL:HG13	2.01	0.42
1:F:263:PRO:HB2	1:G:258:ARG:HB2	2.01	0.42
1:H:278:GLU:OE1	1:H:282:PHE:HE1	2.01	0.42
1:I:223:TYR:CZ	1:I:225:GLU:HG2	2.54	0.42
1:I:254:VAL:HG12	1:I:258:ARG:HD2	2.01	0.42
1:L:28:LYS:O	1:L:299:THR:HG21	2.19	0.42
1:A:28:LYS:O	1:A:299:THR:HG21	2.19	0.42
1:B:263:PRO:HG3	1:C:263:PRO:HG3	2.00	0.42
1:C:223:TYR:CZ	1:C:225:GLU:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ASN:N	1:D:320:ASN:HD22	2.16	0.42
1:E:292:LEU:HA	1:E:293:PRO:HD3	1.78	0.42
1:F:331:ARG:HA	1:F:334:VAL:HG13	2.01	0.42
1:G:223:TYR:CZ	1:G:225:GLU:HG2	2.54	0.42
1:I:28:LYS:O	1:I:299:THR:HG21	2.19	0.42
1:J:223:TYR:CZ	1:J:225:GLU:HG2	2.55	0.42
1:K:28:LYS:O	1:K:299:THR:HG21	2.19	0.42
1:K:129:ASP:OD2	1:L:129:ASP:HB2	2.20	0.42
1:L:193:PRO:O	1:L:237:GLY:HA2	2.19	0.42
1:L:245:THR:C	1:L:247:GLU:N	2.73	0.42
1:L:331:ARG:HA	1:L:334:VAL:HG13	2.01	0.42
1:E:258:ARG:O	1:H:264:ALA:N	2.51	0.42
1:F:28:LYS:O	1:F:299:THR:HG21	2.19	0.42
1:I:261:VAL:O	1:I:296:TRP:CH2	2.73	0.42
1:A:3:HIS:HD2	1:D:201:ARG:HH12	1.65	0.42
1:G:28:LYS:O	1:G:299:THR:HG21	2.19	0.42
1:G:254:VAL:HG12	1:G:258:ARG:HD2	2.01	0.42
1:G:261:VAL:O	1:G:296:TRP:CH2	2.73	0.42
1:H:223:TYR:CZ	1:H:225:GLU:HG2	2.55	0.42
1:I:292:LEU:HA	1:I:293:PRO:HD3	1.78	0.42
1:K:261:VAL:O	1:K:296:TRP:CH2	2.73	0.42
1:L:261:VAL:O	1:L:296:TRP:CH2	2.73	0.42
1:A:158:THR:HG1	1:A:159:PRO:HD3	1.84	0.42
1:C:193:PRO:O	1:C:237:GLY:HA2	2.19	0.42
1:C:254:VAL:HG12	1:C:258:ARG:HD2	2.01	0.42
1:D:254:VAL:HG12	1:D:258:ARG:HD2	2.01	0.42
1:F:245:THR:C	1:F:247:GLU:N	2.73	0.42
1:F:261:VAL:O	1:F:296:TRP:CH2	2.73	0.42
1:B:223:TYR:CZ	1:B:225:GLU:HG2	2.55	0.42
1:E:261:VAL:O	1:E:296:TRP:CH2	2.73	0.42
1:E:331:ARG:HA	1:E:334:VAL:HG13	2.01	0.42
1:G:331:ARG:HA	1:G:334:VAL:HG13	2.01	0.42
1:K:331:ARG:HA	1:K:334:VAL:HG13	2.01	0.42
1:L:290:CYS:HA	1:L:291:PRO:HD3	1.87	0.42
1:A:331:ARG:HA	1:A:334:VAL:HG13	2.01	0.42
1:B:290:CYS:O	1:B:294:ARG:NH1	2.53	0.42
1:C:261:VAL:O	1:C:296:TRP:CH2	2.73	0.42
1:C:290:CYS:O	1:C:294:ARG:NH1	2.53	0.42
1:D:28:LYS:O	1:D:299:THR:HG21	2.19	0.42
1:D:36:SER:HA	1:D:80:PHE:CE1	2.55	0.42
1:E:290:CYS:O	1:E:294:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:LEU:HA	1:F:293:PRO:HD3	1.78	0.42
1:G:292:LEU:HA	1:G:293:PRO:HD3	1.78	0.42
1:H:261:VAL:O	1:H:296:TRP:CH2	2.73	0.42
1:I:263:PRO:HG3	1:L:295:PRO:HG2	2.01	0.42
1:K:107:ILE:N	1:K:107:ILE:CD1	2.67	0.42
1:L:36:SER:HA	1:L:80:PHE:CE1	2.55	0.42
1:A:36:SER:HA	1:A:80:PHE:CE1	2.55	0.42
1:B:254:VAL:HG12	1:B:258:ARG:HD2	2.01	0.42
1:B:263:PRO:HG3	1:C:295:PRO:HG2	2.01	0.42
1:E:36:SER:HA	1:E:80:PHE:CE1	2.55	0.42
1:E:223:TYR:CZ	1:E:225:GLU:HG2	2.54	0.42
1:F:36:SER:HA	1:F:80:PHE:CE1	2.55	0.42
1:F:290:CYS:O	1:F:294:ARG:NH1	2.53	0.42
1:F:290:CYS:HA	1:F:291:PRO:HD3	1.87	0.42
1:H:92:VAL:HA	1:H:93:PRO:HD3	1.88	0.42
1:I:193:PRO:O	1:I:237:GLY:HA2	2.19	0.42
1:I:331:ARG:HA	1:I:334:VAL:HG13	2.01	0.42
1:J:261:VAL:O	1:J:296:TRP:CH2	2.73	0.42
1:K:223:TYR:CZ	1:K:225:GLU:HG2	2.55	0.42
1:K:254:VAL:HG12	1:K:258:ARG:HD2	2.01	0.42
1:L:290:CYS:O	1:L:294:ARG:NH1	2.53	0.42
1:B:261:VAL:O	1:B:296:TRP:CH2	2.73	0.42
1:D:52:THR:CG2	1:D:53:GLU:N	2.83	0.42
1:D:320:ASN:N	1:D:320:ASN:ND2	2.68	0.42
1:E:245:THR:C	1:E:247:GLU:N	2.73	0.42
1:E:254:VAL:HG12	1:E:258:ARG:HD2	2.01	0.42
1:F:66:ALA:O	1:F:101:LYS:HE3	2.20	0.42
1:F:201:ARG:HH22	1:G:3:HIS:CD2	2.37	0.42
1:G:290:CYS:O	1:G:294:ARG:NH1	2.53	0.42
1:I:290:CYS:O	1:I:294:ARG:NH1	2.53	0.42
1:J:193:PRO:O	1:J:237:GLY:HA2	2.19	0.42
1:K:290:CYS:O	1:K:294:ARG:NH1	2.53	0.42
1:L:66:ALA:O	1:L:101:LYS:HE3	2.20	0.42
1:E:193:PRO:O	1:E:237:GLY:HA2	2.19	0.41
1:G:193:PRO:O	1:G:237:GLY:HA2	2.19	0.41
1:H:193:PRO:O	1:H:237:GLY:HA2	2.19	0.41
1:J:264:ALA:N	1:K:258:ARG:O	2.52	0.41
1:K:36:SER:HA	1:K:80:PHE:CE1	2.55	0.41
1:K:290:CYS:HA	1:K:291:PRO:HD3	1.87	0.41
1:B:66:ALA:O	1:B:101:LYS:HE3	2.20	0.41
1:C:66:ALA:O	1:C:101:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:VAL:O	1:D:296:TRP:CH2	2.73	0.41
1:F:92:VAL:HA	1:F:93:PRO:HD3	1.88	0.41
1:F:158:THR:HG1	1:F:159:PRO:HD3	1.84	0.41
1:J:61:GLN:HE22	1:J:89:ASP:N	2.10	0.41
1:L:223:TYR:CZ	1:L:225:GLU:HG2	2.54	0.41
1:A:294:ARG:HA	1:A:295:PRO:HD3	1.79	0.41
1:F:223:TYR:CZ	1:F:225:GLU:HG2	2.55	0.41
1:H:66:ALA:O	1:H:101:LYS:HE3	2.20	0.41
1:H:331:ARG:HA	1:H:334:VAL:HG13	2.01	0.41
1:J:92:VAL:HA	1:J:93:PRO:HD3	1.88	0.41
1:K:120:ASP:HB2	1:L:5:TYR:CZ	2.56	0.41
1:K:245:THR:C	1:K:247:GLU:N	2.73	0.41
1:L:254:VAL:HG12	1:L:258:ARG:HD2	2.01	0.41
1:A:192:LEU:HA	1:A:193:PRO:HD3	1.77	0.41
1:E:92:VAL:HA	1:E:93:PRO:HD3	1.88	0.41
1:J:58:LEU:O	1:J:61:GLN:HB3	2.21	0.41
1:J:66:ALA:O	1:J:101:LYS:HE3	2.20	0.41
1:K:193:PRO:O	1:K:237:GLY:HA2	2.19	0.41
1:K:292:LEU:HA	1:K:293:PRO:HD3	1.78	0.41
1:A:173:ARG:HD2	1:B:166:GLU:OE2	2.21	0.41
1:A:223:TYR:CZ	1:A:225:GLU:HG2	2.54	0.41
1:B:36:SER:HA	1:B:80:PHE:CE1	2.55	0.41
1:D:223:TYR:CZ	1:D:225:GLU:HG2	2.54	0.41
1:E:129:ASP:OD1	1:F:127:GLY:N	2.52	0.41
1:I:120:ASP:HB2	1:J:5:TYR:CZ	2.56	0.41
1:I:129:ASP:OD1	1:J:126:GLN:HB2	2.21	0.41
1:J:290:CYS:O	1:J:294:ARG:NH1	2.53	0.41
1:D:58:LEU:O	1:D:61:GLN:HB3	2.21	0.41
1:E:145:PHE:HA	1:E:184:VAL:O	2.21	0.41
1:F:254:VAL:HG12	1:F:258:ARG:HD2	2.01	0.41
1:G:320:ASN:N	1:G:320:ASN:ND2	2.68	0.41
1:H:58:LEU:O	1:H:61:GLN:HB3	2.21	0.41
1:J:331:ARG:HA	1:J:334:VAL:HG13	2.01	0.41
1:K:145:PHE:HA	1:K:184:VAL:O	2.21	0.41
1:L:158:THR:HG1	1:L:159:PRO:HD3	1.84	0.41
1:A:290:CYS:O	1:A:294:ARG:NH1	2.53	0.41
1:B:320:ASN:N	1:B:320:ASN:ND2	2.68	0.41
1:C:58:LEU:O	1:C:61:GLN:HB3	2.21	0.41
1:D:145:PHE:HA	1:D:184:VAL:O	2.21	0.41
1:D:290:CYS:O	1:D:294:ARG:NH1	2.53	0.41
1:G:145:PHE:HA	1:G:184:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:CYS:HA	1:H:241:PRO:HD3	1.83	0.41
1:I:320:ASN:N	1:I:320:ASN:ND2	2.68	0.41
1:A:46:GLN:NE2	1:A:304:ARG:HH21	2.19	0.41
1:A:52:THR:CG2	1:A:53:GLU:N	2.83	0.41
1:A:145:PHE:HA	1:A:184:VAL:O	2.21	0.41
1:A:262:PRO:HA	1:A:263:PRO:HD3	1.93	0.41
1:H:61:GLN:HE22	1:H:89:ASP:N	2.10	0.41
1:H:290:CYS:O	1:H:294:ARG:NH1	2.53	0.41
1:I:145:PHE:HA	1:I:184:VAL:O	2.21	0.41
1:J:240:CYS:HA	1:J:241:PRO:HD3	1.83	0.41
1:L:92:VAL:HA	1:L:93:PRO:HD3	1.88	0.41
1:A:58:LEU:O	1:A:61:GLN:HB3	2.21	0.41
1:B:58:LEU:O	1:B:61:GLN:HB3	2.21	0.41
1:B:240:CYS:HA	1:B:241:PRO:HD3	1.83	0.41
1:C:3:HIS:N	1:D:157:ARG:CZ	2.84	0.41
1:C:171:LEU:HD13	1:C:187:VAL:CG1	2.51	0.41
1:D:46:GLN:NE2	1:D:304:ARG:HH21	2.19	0.41
1:E:58:LEU:O	1:E:61:GLN:HB3	2.21	0.41
1:E:66:ALA:O	1:E:101:LYS:HE3	2.20	0.41
1:G:36:SER:HA	1:G:80:PHE:CE1	2.55	0.41
1:H:36:SER:HA	1:H:80:PHE:CE1	2.55	0.41
1:H:166:GLU:O	1:H:167:ASN:CB	2.58	0.41
1:I:36:SER:HA	1:I:80:PHE:CE1	2.55	0.41
1:I:66:ALA:O	1:I:101:LYS:HE3	2.20	0.41
1:I:208:LYS:NZ	1:L:218:SER:O	2.53	0.41
1:J:36:SER:HA	1:J:80:PHE:CE1	2.55	0.41
1:J:52:THR:CG2	1:J:53:GLU:N	2.83	0.41
1:J:166:GLU:O	1:J:167:ASN:CB	2.58	0.41
1:K:58:LEU:O	1:K:61:GLN:HB3	2.21	0.41
1:L:192:LEU:HA	1:L:193:PRO:HD3	1.77	0.41
1:A:261:VAL:O	1:A:296:TRP:CH2	2.73	0.41
1:C:36:SER:HA	1:C:80:PHE:CE1	2.55	0.41
1:C:145:PHE:HA	1:C:184:VAL:O	2.21	0.41
1:F:171:LEU:HD13	1:F:187:VAL:CG1	2.51	0.41
1:G:58:LEU:O	1:G:61:GLN:HB3	2.21	0.41
1:G:66:ALA:O	1:G:101:LYS:HE3	2.20	0.41
1:I:58:LEU:O	1:I:61:GLN:HB3	2.21	0.41
1:J:292:LEU:HA	1:J:293:PRO:HD3	1.78	0.41
1:J:320:ASN:N	1:J:320:ASN:ND2	2.68	0.41
1:K:171:LEU:HD13	1:K:187:VAL:CG1	2.51	0.41
1:A:66:ALA:O	1:A:101:LYS:HE3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:NH2	1:B:326:GLU:OE2	2.54	0.40
1:B:166:GLU:O	1:B:167:ASN:CB	2.58	0.40
1:C:166:GLU:HG3	1:C:167:ASN:N	2.37	0.40
1:D:66:ALA:O	1:D:101:LYS:HE3	2.20	0.40
1:E:171:LEU:HD13	1:E:187:VAL:CG1	2.51	0.40
1:L:171:LEU:HD13	1:L:187:VAL:CG1	2.51	0.40
1:A:204:TYR:CD1	1:D:4:SER:HB3	2.56	0.40
1:D:11:GLU:H	1:D:11:GLU:HG2	1.51	0.40
1:F:192:LEU:HA	1:F:193:PRO:HD3	1.77	0.40
1:H:145:PHE:HA	1:H:184:VAL:O	2.21	0.40
1:H:272:SER:HB2	1:H:305:ALA:HB2	2.04	0.40
1:H:320:ASN:N	1:H:320:ASN:ND2	2.68	0.40
1:I:52:THR:CG2	1:I:53:GLU:N	2.83	0.40
1:B:145:PHE:HA	1:B:184:VAL:O	2.21	0.40
1:B:171:LEU:HD13	1:B:187:VAL:CG1	2.51	0.40
1:B:272:SER:HB2	1:B:305:ALA:HB2	2.04	0.40
1:C:46:GLN:NE2	1:C:304:ARG:HH21	2.19	0.40
1:C:192:LEU:HA	1:C:193:PRO:HD3	1.77	0.40
1:C:272:SER:HB2	1:C:305:ALA:HB2	2.04	0.40
1:E:166:GLU:HG3	1:E:167:ASN:N	2.37	0.40
1:G:171:LEU:HD13	1:G:187:VAL:CG1	2.51	0.40
1:I:4:SER:HB3	1:L:204:TYR:CD1	2.57	0.40
1:I:61:GLN:NE2	1:I:89:ASP:N	2.65	0.40
1:I:166:GLU:HG3	1:I:167:ASN:N	2.37	0.40
1:K:66:ALA:O	1:K:101:LYS:HE3	2.20	0.40
1:K:120:ASP:HB2	1:L:5:TYR:CE1	2.56	0.40
1:K:166:GLU:HG3	1:K:167:ASN:N	2.37	0.40
1:L:145:PHE:HA	1:L:184:VAL:O	2.21	0.40
1:B:166:GLU:HG3	1:B:167:ASN:N	2.37	0.40
1:C:320:ASN:N	1:C:320:ASN:ND2	2.68	0.40
1:E:126:GLN:HB2	1:F:129:ASP:OD1	2.22	0.40
1:E:290:CYS:HA	1:E:291:PRO:HD3	1.87	0.40
1:F:46:GLN:NE2	1:F:304:ARG:HH21	2.19	0.40
1:F:58:LEU:O	1:F:61:GLN:HB3	2.21	0.40
1:F:145:PHE:HA	1:F:184:VAL:O	2.21	0.40
1:G:153:LYS:O	1:G:159:PRO:HG3	2.22	0.40
1:G:166:GLU:HG3	1:G:167:ASN:N	2.37	0.40
1:I:153:LYS:O	1:I:159:PRO:HG3	2.22	0.40
1:I:171:LEU:HD13	1:I:187:VAL:CG1	2.51	0.40
1:J:272:SER:HB2	1:J:305:ALA:HB2	2.04	0.40
1:L:320:ASN:N	1:L:320:ASN:ND2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:HA	1:B:93:PRO:HD3	1.88	0.40
1:C:69:ARG:NH2	1:C:326:GLU:OE2	2.54	0.40
1:D:192:LEU:HA	1:D:193:PRO:HD3	1.77	0.40
1:F:320:ASN:N	1:F:320:ASN:ND2	2.68	0.40
1:G:52:THR:CG2	1:G:53:GLU:N	2.83	0.40
1:J:145:PHE:HA	1:J:184:VAL:O	2.21	0.40
1:J:204:TYR:CE1	1:K:4:SER:HB3	2.57	0.40
1:K:92:VAL:HA	1:K:93:PRO:HD3	1.88	0.40
1:L:58:LEU:O	1:L:61:GLN:HB3	2.21	0.40
1:L:69:ARG:NH2	1:L:326:GLU:OE2	2.54	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:OD1	1:K:243:LYS:NZ[1_454]	1.57	0.63
1:G:242:ILE:CD1	1:I:50:GLU:OE1[1_565]	1.60	0.60
1:G:50:GLU:OE1	1:I:242:ILE:CD1[1_665]	1.65	0.55
1:D:318:ARG:NH1	1:K:99:GLN:O[1_544]	1.78	0.42
1:D:248:GLU:OE2	1:G:96:ARG:NH2[1_444]	1.93	0.27
1:B:67:ASP:CG	1:K:243:LYS:NZ[1_454]	2.03	0.17
1:C:67:ASP:OD1	1:E:243:LYS:NZ[1_445]	2.06	0.14
1:C:67:ASP:CB	1:E:243:LYS:NZ[1_445]	2.09	0.11
1:C:67:ASP:CG	1:E:243:LYS:NZ[1_445]	2.10	0.10
1:G:50:GLU:CD	1:I:242:ILE:CG2[1_665]	2.11	0.09
1:G:50:GLU:OE2	1:I:242:ILE:CG2[1_665]	2.19	0.01

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	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	C	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	D	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	E	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	F	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	G	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	H	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	I	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	J	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	K	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
1	L	340/365 (93%)	313 (92%)	24 (7%)	3 (1%)	14	48
All	All	4080/4380 (93%)	3756 (92%)	288 (7%)	36 (1%)	14	48

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	B	49	VAL
1	C	49	VAL
1	D	49	VAL
1	E	49	VAL
1	F	49	VAL
1	G	49	VAL
1	H	49	VAL
1	I	49	VAL
1	J	49	VAL
1	K	49	VAL
1	L	49	VAL
1	A	6	PRO
1	B	6	PRO
1	C	6	PRO
1	D	6	PRO
1	E	6	PRO
1	F	6	PRO
1	G	6	PRO
1	H	6	PRO
1	I	6	PRO
1	J	6	PRO

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Mol	Chain	Res	Type
1	K	6	PRO
1	L	6	PRO
1	A	158	THR
1	B	158	THR
1	C	158	THR
1	D	158	THR
1	E	158	THR
1	F	158	THR
1	G	158	THR
1	H	158	THR
1	I	158	THR
1	J	158	THR
1	K	158	THR
1	L	158	THR

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	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	B	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	C	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	D	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	E	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	F	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	G	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	H	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	I	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	J	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	K	277/291 (95%)	260 (94%)	17 (6%)	17	49
1	L	277/291 (95%)	260 (94%)	17 (6%)	17	49
All	All	3324/3492 (95%)	3120 (94%)	204 (6%)	17	49

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	6	PRO
1	A	11	GLU
1	A	37	VAL
1	A	50	GLU
1	A	70	VAL
1	A	96	ARG
1	A	107	ILE
1	A	137	GLN
1	A	165	LEU
1	A	234	VAL
1	A	245	THR
1	A	299	THR
1	A	319	ASP
1	A	327	GLU
1	A	331	ARG
1	A	334	VAL
1	B	3	HIS
1	B	6	PRO
1	B	11	GLU
1	B	37	VAL
1	B	50	GLU
1	B	70	VAL
1	B	96	ARG
1	B	107	ILE
1	B	137	GLN
1	B	165	LEU
1	B	234	VAL
1	B	245	THR
1	B	299	THR
1	B	319	ASP
1	B	327	GLU
1	B	331	ARG
1	B	334	VAL
1	C	3	HIS
1	C	6	PRO
1	C	11	GLU
1	C	37	VAL
1	C	50	GLU
1	C	70	VAL
1	C	96	ARG
1	C	107	ILE

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Mol	Chain	Res	Type
1	C	137	GLN
1	C	165	LEU
1	C	234	VAL
1	C	245	THR
1	C	299	THR
1	C	319	ASP
1	C	327	GLU
1	C	331	ARG
1	C	334	VAL
1	D	3	HIS
1	D	6	PRO
1	D	11	GLU
1	D	37	VAL
1	D	50	GLU
1	D	70	VAL
1	D	96	ARG
1	D	107	ILE
1	D	137	GLN
1	D	165	LEU
1	D	234	VAL
1	D	245	THR
1	D	299	THR
1	D	319	ASP
1	D	327	GLU
1	D	331	ARG
1	D	334	VAL
1	E	3	HIS
1	E	6	PRO
1	E	11	GLU
1	E	37	VAL
1	E	50	GLU
1	E	70	VAL
1	E	96	ARG
1	E	107	ILE
1	E	137	GLN
1	E	165	LEU
1	E	234	VAL
1	E	245	THR
1	E	299	THR
1	E	319	ASP
1	E	327	GLU
1	E	331	ARG

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Mol	Chain	Res	Type
1	E	334	VAL
1	F	3	HIS
1	F	6	PRO
1	F	11	GLU
1	F	37	VAL
1	F	50	GLU
1	F	70	VAL
1	F	96	ARG
1	F	107	ILE
1	F	137	GLN
1	F	165	LEU
1	F	234	VAL
1	F	245	THR
1	F	299	THR
1	F	319	ASP
1	F	327	GLU
1	F	331	ARG
1	F	334	VAL
1	G	3	HIS
1	G	6	PRO
1	G	11	GLU
1	G	37	VAL
1	G	50	GLU
1	G	70	VAL
1	G	96	ARG
1	G	107	ILE
1	G	137	GLN
1	G	165	LEU
1	G	234	VAL
1	G	245	THR
1	G	299	THR
1	G	319	ASP
1	G	327	GLU
1	G	331	ARG
1	G	334	VAL
1	H	3	HIS
1	H	6	PRO
1	H	11	GLU
1	H	37	VAL
1	H	50	GLU
1	H	70	VAL
1	H	96	ARG

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Mol	Chain	Res	Type
1	H	107	ILE
1	H	137	GLN
1	H	165	LEU
1	H	234	VAL
1	H	245	THR
1	H	299	THR
1	H	319	ASP
1	H	327	GLU
1	H	331	ARG
1	H	334	VAL
1	I	3	HIS
1	I	6	PRO
1	I	11	GLU
1	I	37	VAL
1	I	50	GLU
1	I	70	VAL
1	I	96	ARG
1	I	107	ILE
1	I	137	GLN
1	I	165	LEU
1	I	234	VAL
1	I	245	THR
1	I	299	THR
1	I	319	ASP
1	I	327	GLU
1	I	331	ARG
1	I	334	VAL
1	J	3	HIS
1	J	6	PRO
1	J	11	GLU
1	J	37	VAL
1	J	50	GLU
1	J	70	VAL
1	J	96	ARG
1	J	107	ILE
1	J	137	GLN
1	J	165	LEU
1	J	234	VAL
1	J	245	THR
1	J	299	THR
1	J	319	ASP
1	J	327	GLU

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Mol	Chain	Res	Type
1	J	331	ARG
1	J	334	VAL
1	K	3	HIS
1	K	6	PRO
1	K	11	GLU
1	K	37	VAL
1	K	50	GLU
1	K	70	VAL
1	K	96	ARG
1	K	107	ILE
1	K	137	GLN
1	K	165	LEU
1	K	234	VAL
1	K	245	THR
1	K	299	THR
1	K	319	ASP
1	K	327	GLU
1	K	331	ARG
1	K	334	VAL
1	L	3	HIS
1	L	6	PRO
1	L	11	GLU
1	L	37	VAL
1	L	50	GLU
1	L	70	VAL
1	L	96	ARG
1	L	107	ILE
1	L	137	GLN
1	L	165	LEU
1	L	234	VAL
1	L	245	THR
1	L	299	THR
1	L	319	ASP
1	L	327	GLU
1	L	331	ARG
1	L	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	99	GLN
1	A	180	GLN
1	A	232	ASN
1	A	283	ASN
1	A	317	GLN
1	A	320	ASN
1	B	46	GLN
1	B	61	GLN
1	B	99	GLN
1	B	180	GLN
1	B	232	ASN
1	B	283	ASN
1	B	320	ASN
1	C	46	GLN
1	C	61	GLN
1	C	99	GLN
1	C	180	GLN
1	C	232	ASN
1	C	283	ASN
1	C	320	ASN
1	D	46	GLN
1	D	61	GLN
1	D	99	GLN
1	D	180	GLN
1	D	232	ASN
1	D	283	ASN
1	D	320	ASN
1	E	46	GLN
1	E	61	GLN
1	E	99	GLN
1	E	180	GLN
1	E	232	ASN
1	E	283	ASN
1	E	320	ASN
1	F	46	GLN
1	F	61	GLN
1	F	99	GLN
1	F	180	GLN
1	F	181	ASN
1	F	232	ASN
1	F	283	ASN
1	F	320	ASN

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Mol	Chain	Res	Type
1	G	3	HIS
1	G	46	GLN
1	G	61	GLN
1	G	99	GLN
1	G	180	GLN
1	G	232	ASN
1	G	283	ASN
1	G	320	ASN
1	H	3	HIS
1	H	46	GLN
1	H	61	GLN
1	H	99	GLN
1	H	180	GLN
1	H	232	ASN
1	H	283	ASN
1	H	320	ASN
1	I	46	GLN
1	I	61	GLN
1	I	180	GLN
1	I	232	ASN
1	I	283	ASN
1	I	320	ASN
1	J	3	HIS
1	J	46	GLN
1	J	61	GLN
1	J	99	GLN
1	J	180	GLN
1	J	232	ASN
1	J	283	ASN
1	J	320	ASN
1	K	46	GLN
1	K	61	GLN
1	K	99	GLN
1	K	180	GLN
1	K	232	ASN
1	K	283	ASN
1	K	320	ASN
1	L	46	GLN
1	L	61	GLN
1	L	99	GLN
1	L	180	GLN
1	L	181	ASN

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Mol	Chain	Res	Type
1	L	232	ASN
1	L	283	ASN
1	L	320	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 oligosaccharides 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	342/365 (93%)	0.57	26 (7%)	20 10	8, 30, 70, 94	0
1	B	342/365 (93%)	0.50	21 (6%)	27 14	8, 30, 70, 94	0
1	C	342/365 (93%)	0.42	21 (6%)	27 14	8, 30, 70, 94	0
1	D	342/365 (93%)	0.46	19 (5%)	30 15	8, 30, 70, 94	0
1	E	342/365 (93%)	0.35	18 (5%)	32 16	8, 30, 70, 94	0
1	F	342/365 (93%)	0.44	21 (6%)	27 14	8, 30, 70, 94	0
1	G	342/365 (93%)	0.70	41 (11%)	9 5	8, 30, 70, 94	0
1	H	342/365 (93%)	0.50	21 (6%)	27 14	8, 30, 70, 94	0
1	I	342/365 (93%)	0.91	63 (18%)	3 2	8, 30, 70, 94	0
1	J	342/365 (93%)	0.42	19 (5%)	30 15	8, 30, 70, 94	0
1	K	342/365 (93%)	0.39	22 (6%)	25 13	8, 30, 70, 94	0
1	L	342/365 (93%)	0.53	30 (8%)	15 8	8, 30, 70, 94	0
All	All	4104/4380 (93%)	0.52	322 (7%)	19 10	8, 30, 72, 94	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	50	GLU	8.0
1	I	50	GLU	7.1
1	J	48	GLY	6.3
1	D	3	HIS	5.5
1	I	53	GLU	5.1
1	G	180	GLN	5.1
1	I	46	GLN	5.0
1	G	53	GLU	4.8
1	H	4	SER	4.8
1	H	180	GLN	4.8
1	B	241	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	J	180	GLN	4.5
1	I	242	ILE	4.5
1	C	158	THR	4.4
1	L	3	HIS	4.4
1	H	48	GLY	4.4
1	J	53	GLU	4.4
1	F	180	GLN	4.3
1	D	180	GLN	4.3
1	L	180	GLN	4.2
1	I	241	PRO	4.2
1	G	4	SER	4.2
1	G	278	GLU	4.1
1	F	3	HIS	4.1
1	I	180	GLN	4.1
1	I	96	ARG	4.1
1	E	180	GLN	4.1
1	H	3	HIS	4.1
1	I	156	GLU	4.0
1	I	47	ILE	4.0
1	F	4	SER	4.0
1	I	52	THR	4.0
1	C	180	GLN	3.9
1	I	3	HIS	3.9
1	I	200	LYS	3.9
1	I	43	ARG	3.8
1	K	3	HIS	3.8
1	E	3	HIS	3.8
1	I	278	GLU	3.7
1	B	158	THR	3.7
1	D	4	SER	3.7
1	G	52	THR	3.7
1	I	243	LYS	3.7
1	L	4	SER	3.7
1	L	53	GLU	3.7
1	D	344	GLU	3.6
1	I	49	VAL	3.6
1	K	158	THR	3.6
1	A	180	GLN	3.6
1	G	344	GLU	3.6
1	A	4	SER	3.6
1	I	45	SER	3.6
1	J	158	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	315	ARG	3.5
1	I	319	ASP	3.5
1	G	96	ARG	3.5
1	B	3	HIS	3.5
1	A	50	GLU	3.5
1	J	3	HIS	3.5
1	A	3	HIS	3.4
1	I	157	ARG	3.4
1	G	3	HIS	3.4
1	J	4	SER	3.4
1	K	4	SER	3.4
1	B	180	GLN	3.4
1	F	156	GLU	3.4
1	G	157	ARG	3.4
1	D	96	ARG	3.4
1	G	48	GLY	3.4
1	G	158	THR	3.4
1	K	180	GLN	3.4
1	B	243	LYS	3.3
1	B	317	GLN	3.3
1	I	99	GLN	3.3
1	H	315	ARG	3.3
1	F	243	LYS	3.3
1	I	4	SER	3.3
1	D	241	PRO	3.3
1	L	90	ASN	3.3
1	J	50	GLU	3.3
1	L	5	TYR	3.2
1	G	5	TYR	3.2
1	L	37	VAL	3.2
1	I	55	ASN	3.2
1	G	46	GLN	3.2
1	G	312	ASN	3.2
1	E	200	LYS	3.1
1	G	243	LYS	3.1
1	H	158	THR	3.1
1	F	5	TYR	3.1
1	D	243	LYS	3.1
1	F	344	GLU	3.1
1	F	158	THR	3.1
1	I	48	GLY	3.1
1	F	50	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	156	GLU	3.1
1	F	90	ASN	3.1
1	E	344	GLU	3.1
1	I	304	ARG	3.0
1	E	4	SER	3.0
1	I	196	ASP	3.0
1	J	5	TYR	3.0
1	G	55	ASN	3.0
1	G	99	GLN	3.0
1	I	245	THR	3.0
1	C	48	GLY	3.0
1	G	47	ILE	3.0
1	C	317	GLN	3.0
1	B	315	ARG	2.9
1	I	5	TYR	2.9
1	E	158	THR	2.9
1	E	53	GLU	2.9
1	K	156	GLU	2.9
1	A	49	VAL	2.9
1	B	48	GLY	2.9
1	C	3	HIS	2.9
1	E	304	ARG	2.9
1	E	278	GLU	2.9
1	H	5	TYR	2.9
1	I	238	HIS	2.9
1	H	319	ASP	2.9
1	E	156	GLU	2.9
1	F	53	GLU	2.9
1	F	319	ASP	2.9
1	F	238	HIS	2.8
1	F	89	ASP	2.8
1	G	245	THR	2.8
1	G	319	ASP	2.8
1	I	37	VAL	2.8
1	K	344	GLU	2.8
1	L	11	GLU	2.8
1	L	156	GLU	2.8
1	H	320	ASN	2.8
1	I	42	LYS	2.8
1	I	54	GLU	2.8
1	J	243	LYS	2.8
1	L	319	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	304	ARG	2.8
1	L	50	GLU	2.8
1	A	319	ASP	2.8
1	B	319	ASP	2.8
1	L	318	ARG	2.8
1	F	318	ARG	2.7
1	D	48	GLY	2.7
1	G	38	GLY	2.7
1	A	37	VAL	2.7
1	J	238	HIS	2.7
1	G	289	ARG	2.7
1	B	278	GLU	2.7
1	A	47	ILE	2.6
1	G	317	GLN	2.6
1	I	315	ARG	2.6
1	G	11	GLU	2.6
1	I	39	SER	2.6
1	I	40	MET	2.6
1	I	158	THR	2.6
1	F	48	GLY	2.6
1	I	38	GLY	2.6
1	C	156	GLU	2.6
1	H	278	GLU	2.6
1	K	304	ARG	2.6
1	C	238	HIS	2.6
1	C	344	GLU	2.6
1	A	238	HIS	2.6
1	D	317	GLN	2.6
1	C	319	ASP	2.6
1	A	344	GLU	2.6
1	D	314	TRP	2.5
1	I	344	GLU	2.5
1	L	344	GLU	2.5
1	I	97	THR	2.5
1	L	6	PRO	2.5
1	A	200	LYS	2.5
1	B	43	ARG	2.5
1	I	312	ASN	2.5
1	I	311	LEU	2.5
1	H	53	GLU	2.5
1	G	45	SER	2.5
1	C	278	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	133	GLU	2.5
1	D	158	THR	2.5
1	E	5	TYR	2.5
1	I	309	SER	2.4
1	G	43	ARG	2.4
1	J	320	ASN	2.4
1	J	282	PHE	2.4
1	E	43	ARG	2.4
1	K	157	ARG	2.4
1	K	200	LYS	2.4
1	B	238	HIS	2.4
1	G	49	VAL	2.4
1	I	91	GLY	2.4
1	A	282	PHE	2.4
1	E	157	ARG	2.4
1	H	11	GLU	2.4
1	H	344	GLU	2.4
1	G	241	PRO	2.4
1	J	52	THR	2.4
1	A	5	TYR	2.4
1	B	5	TYR	2.4
1	A	322	GLY	2.4
1	C	200	LYS	2.4
1	L	243	LYS	2.4
1	G	315	ARG	2.4
1	L	96	ARG	2.4
1	A	311	LEU	2.4
1	L	311	LEU	2.4
1	D	330	LYS	2.3
1	G	242	ILE	2.3
1	I	41	ALA	2.3
1	D	319	ASP	2.3
1	E	50	GLU	2.3
1	G	200	LYS	2.3
1	C	43	ARG	2.3
1	I	316	GLY	2.3
1	C	242	ILE	2.3
1	L	47	ILE	2.3
1	L	158	THR	2.3
1	G	51	ASN	2.3
1	I	320	ASN	2.3
1	L	133	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	243	LYS	2.3
1	G	42	LYS	2.3
1	J	315	ARG	2.3
1	J	55	ASN	2.3
1	F	46	GLN	2.3
1	L	46	GLN	2.3
1	F	11	GLU	2.3
1	K	278	GLU	2.3
1	A	243	LYS	2.3
1	D	49	VAL	2.3
1	J	312	ASN	2.3
1	I	317	GLN	2.3
1	B	200	LYS	2.3
1	I	11	GLU	2.3
1	C	241	PRO	2.3
1	H	121	GLY	2.3
1	B	157	ARG	2.3
1	H	157	ARG	2.3
1	L	89	ASP	2.3
1	J	156	GLU	2.2
1	K	5	TYR	2.2
1	I	289	ARG	2.2
1	I	90	ASN	2.2
1	A	53	GLU	2.2
1	C	50	GLU	2.2
1	H	50	GLU	2.2
1	K	50	GLU	2.2
1	L	49	VAL	2.2
1	F	312	ASN	2.2
1	I	6	PRO	2.2
1	L	91	GLY	2.2
1	K	42	LYS	2.2
1	B	52	THR	2.2
1	L	52	THR	2.2
1	A	62	VAL	2.2
1	L	312	ASN	2.2
1	B	41	ALA	2.2
1	K	66	ALA	2.2
1	C	157	ARG	2.2
1	K	43	ARG	2.2
1	A	317	GLN	2.2
1	A	51	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	48	GLY	2.2
1	I	93	PRO	2.2
1	K	48	GLY	2.2
1	I	60	ARG	2.2
1	I	318	ARG	2.2
1	E	52	THR	2.1
1	G	311	LEU	2.1
1	C	330	LYS	2.1
1	A	327	GLU	2.1
1	B	133	GLU	2.1
1	G	239	ALA	2.1
1	I	155	SER	2.1
1	L	321	ALA	2.1
1	D	157	ARG	2.1
1	H	43	ARG	2.1
1	A	55	ASN	2.1
1	I	51	ASN	2.1
1	E	296	TRP	2.1
1	K	49	VAL	2.1
1	E	317	GLN	2.1
1	J	317	GLN	2.1
1	B	45	SER	2.1
1	D	50	GLU	2.1
1	C	51	ASN	2.1
1	G	90	ASN	2.1
1	A	314	TRP	2.1
1	H	52	THR	2.1
1	I	44	LEU	2.1
1	I	330	LYS	2.1
1	I	239	ALA	2.1
1	I	118	GLY	2.1
1	B	282	PHE	2.1
1	H	282	PHE	2.1
1	G	37	VAL	2.1
1	G	238	HIS	2.1
1	H	311	LEU	2.1
1	J	319	ASP	2.1
1	A	158	THR	2.1
1	D	6	PRO	2.1
1	K	53	GLU	2.1
1	H	289	ARG	2.1
1	F	241	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	45	SER	2.0
1	A	320	ASN	2.0
1	K	318	ARG	2.0
1	C	5	TYR	2.0
1	I	142	GLY	2.0
1	I	282	PHE	2.0
1	L	48	GLY	2.0
1	L	99	GLN	2.0
1	I	58	LEU	2.0
1	L	289	ARG	2.0
1	K	36	SER	2.0
1	K	309	SER	2.0
1	I	314	TRP	2.0
1	D	324	ALA	2.0
1	F	68	ASP	2.0
1	B	50	GLU	2.0
1	D	53	GLU	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 oligosaccharides 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.