



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:33 PM UTC

PDB ID : 1TYF / pdb_00001tyf
Title : THE STRUCTURE OF CLPP AT 2.3 ANGSTROM RESOLUTION SUGGESTS A MODEL FOR ATP-DEPENDENT PROTEOLYSIS
Authors : Wang, J.; Hartling, J.A.; Flanagan, J.M.
Deposited on : 1997-10-13
Resolution : 2.30 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:

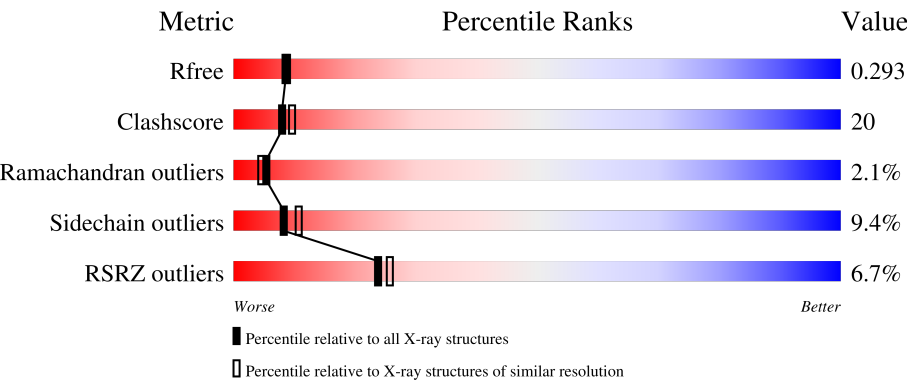
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	193	6% 55%33%6%• 5%
1	B	193	6% 51%35%8%• 5%
1	C	193	8% 53%34%7%• 5%
1	D	193	8% 50%36%9%5%
1	E	193	7% 54%32%8%• 5%

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Mol	Chain	Length	Quality of chain
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21308 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 CLP PEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	B	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	C	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	D	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	E	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	F	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	G	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	H	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	I	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	J	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	K	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	L	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	M	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			
1	N	183	Total	C	N	O	S	0	0	0
			1433	901	251	270	11			

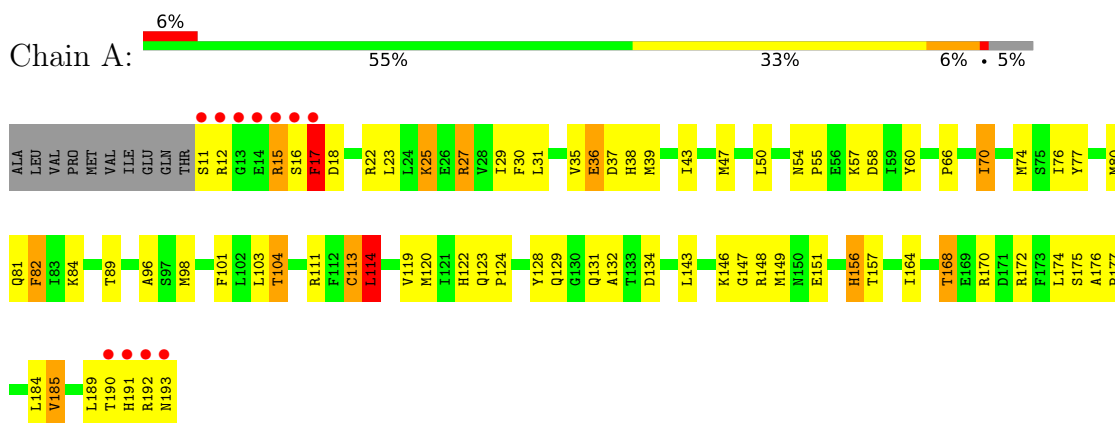
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	89	Total	O	0	0
			89	89		
2	C	94	Total	O	0	0
			94	94		
2	D	89	Total	O	0	0
			89	89		
2	E	82	Total	O	0	0
			82	82		
2	F	91	Total	O	0	0
			91	91		
2	G	90	Total	O	0	0
			90	90		
2	H	86	Total	O	0	0
			86	86		
2	I	88	Total	O	0	0
			88	88		
2	J	86	Total	O	0	0
			86	86		
2	K	92	Total	O	0	0
			92	92		
2	L	92	Total	O	0	0
			92	92		
2	M	84	Total	O	0	0
			84	84		
2	N	94	Total	O	0	0
			94	94		

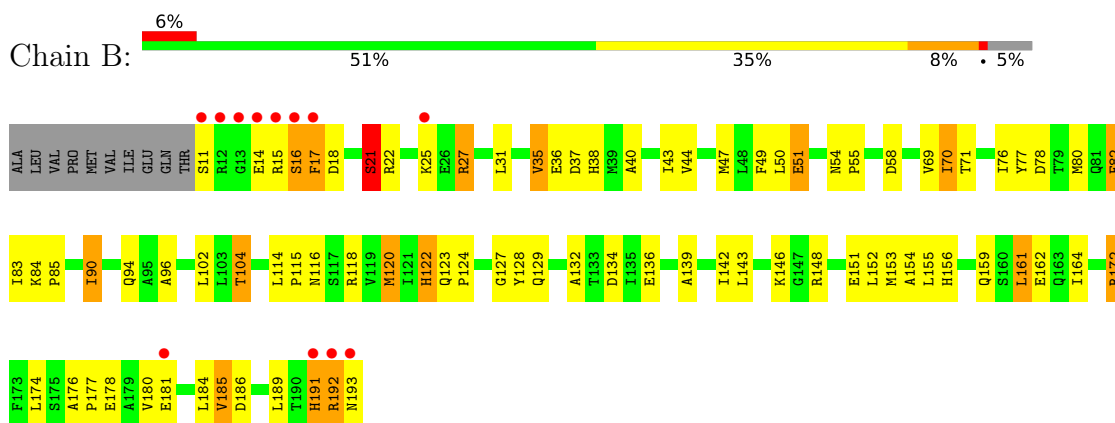
3 Residue-property plots

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.

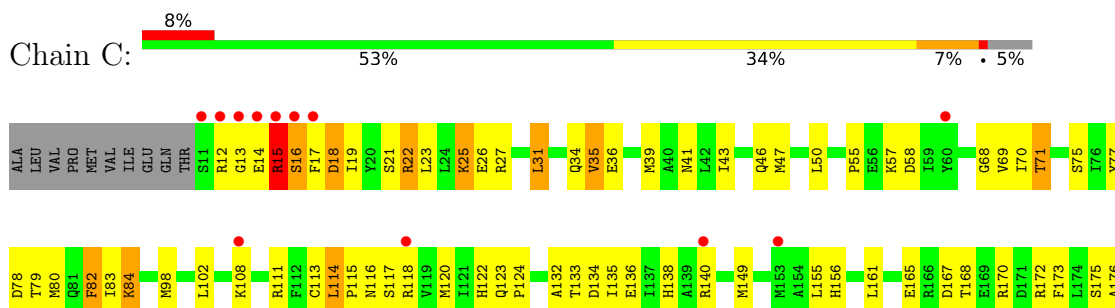
• Molecule 1: CLP PEPTIDASE



• Molecule 1: CLP PEPTIDASE

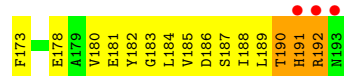
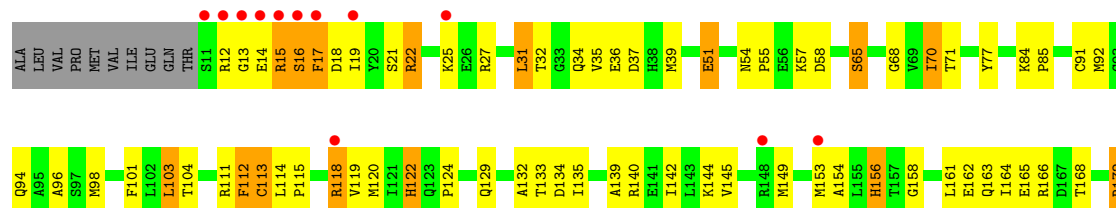


• Molecule 1: CLP PEPTIDASE

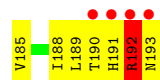
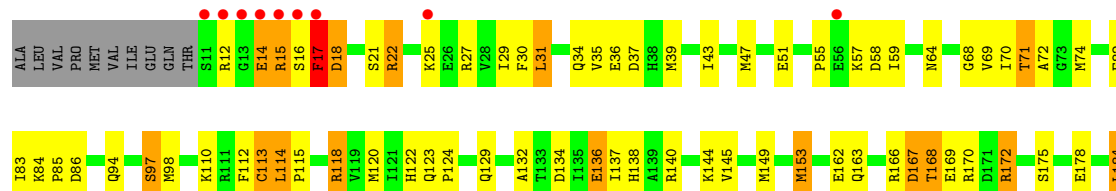




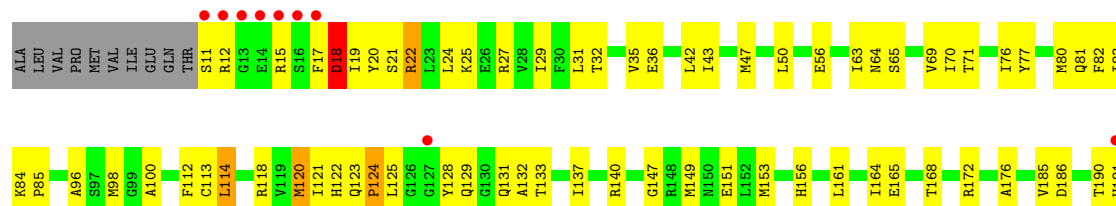
• Molecule 1: CLP PEPTIDASE



• Molecule 1: CLP PEPTIDASE

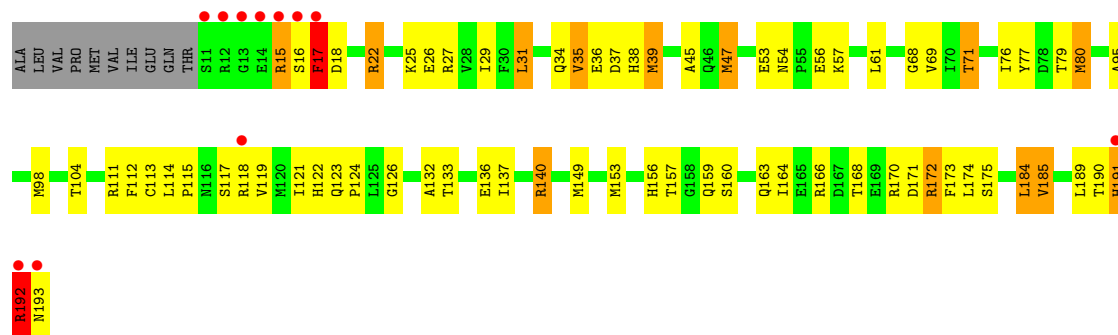


• Molecule 1: CLP PEPTIDASE

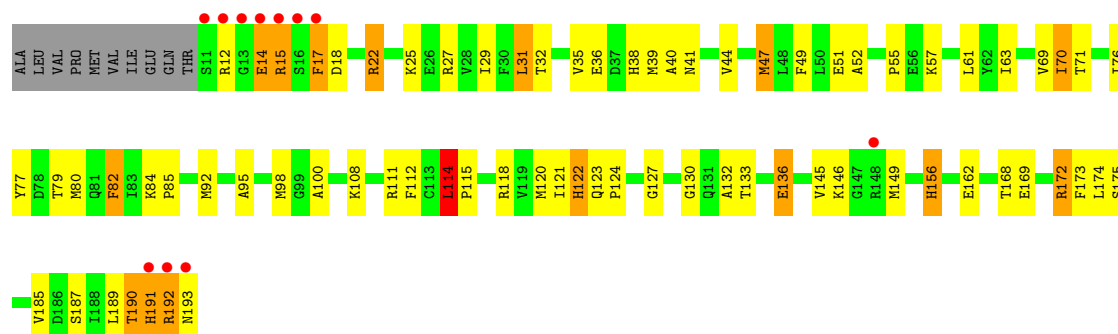


• Molecule 1: CLP PEPTIDASE

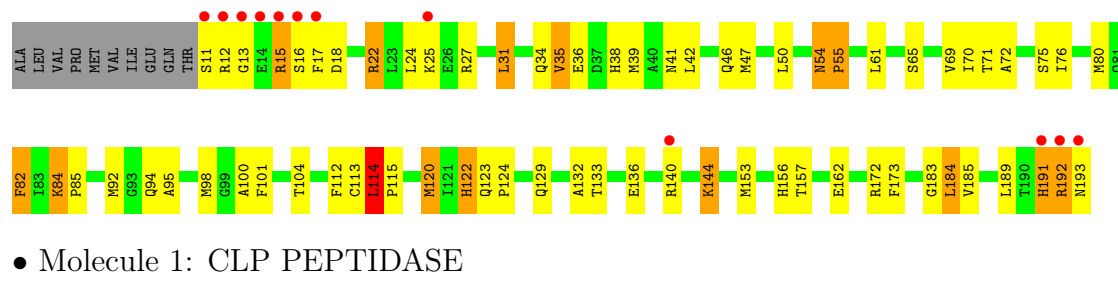




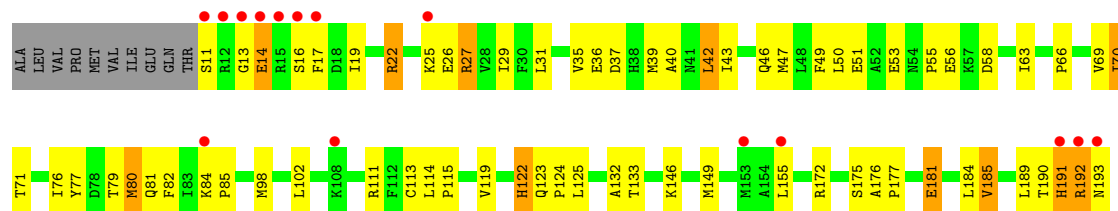
- Molecule 1: CLP PEPTIDASE



- Molecule 1: CLP PEPTIDASE

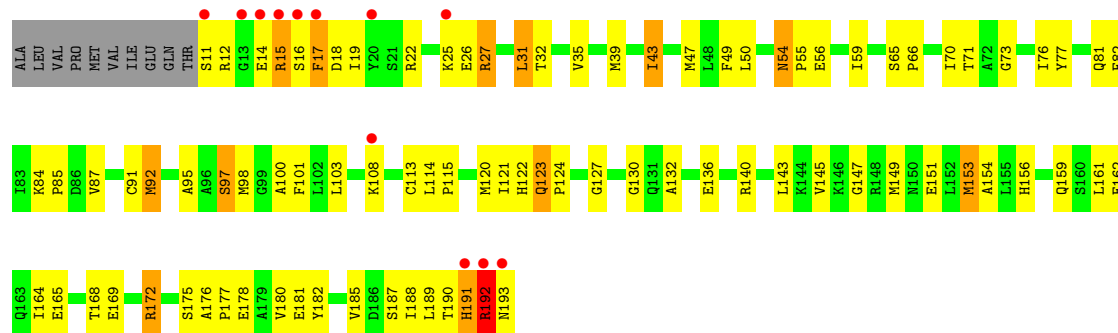


- Molecule 1: CLP PEPTIDASE

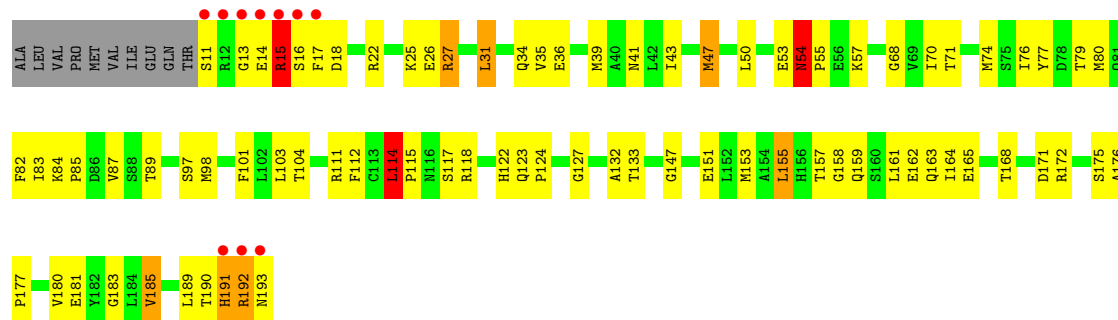


- Molecule 1: CLP PEPTIDASE

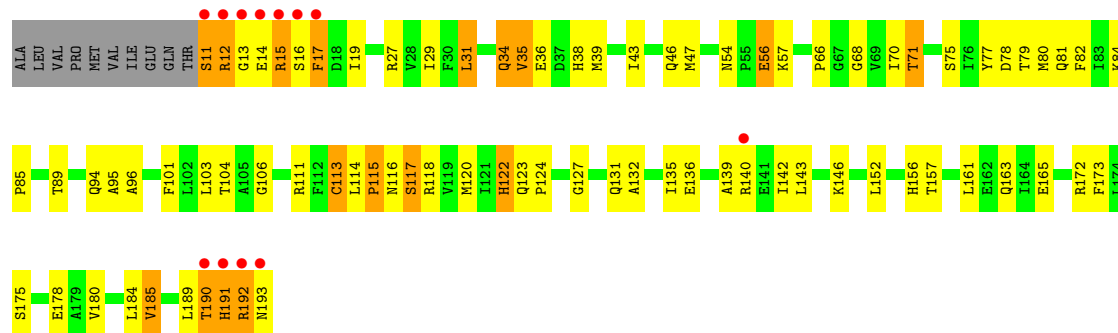




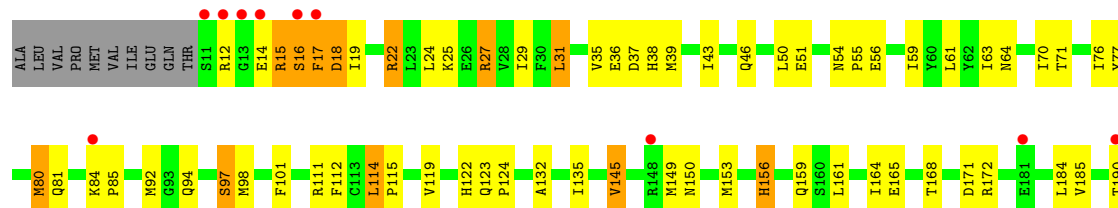
• Molecule 1: CLP PEPTIDASE



• Molecule 1: CLP PEPTIDASE



• Molecule 1: CLP PEPTIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.32Å 102.46Å 157.08Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	80.00 – 2.30 80.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (80.00-2.30) 92.2 (80.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.20Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.219 , 0.292 0.217 , 0.293	Depositor DCC
R_{free} test set	6924 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21308	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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	0.82	0/1456	1.20	11/1960 (0.6%)
1	B	0.81	0/1456	1.20	13/1960 (0.7%)
1	C	0.74	0/1456	1.16	11/1960 (0.6%)
1	D	0.77	1/1456 (0.1%)	1.24	16/1960 (0.8%)
1	E	0.77	1/1456 (0.1%)	1.23	13/1960 (0.7%)
1	F	0.80	0/1456	1.18	13/1960 (0.7%)
1	G	0.87	2/1456 (0.1%)	1.26	14/1960 (0.7%)
1	H	0.81	1/1456 (0.1%)	1.14	9/1960 (0.5%)
1	I	0.80	1/1456 (0.1%)	1.17	14/1960 (0.7%)
1	J	0.80	1/1456 (0.1%)	1.10	7/1960 (0.4%)
1	K	0.76	1/1456 (0.1%)	1.13	9/1960 (0.5%)
1	L	0.82	1/1456 (0.1%)	1.17	9/1960 (0.5%)
1	M	0.78	1/1456 (0.1%)	1.21	13/1960 (0.7%)
1	N	0.79	1/1456 (0.1%)	1.20	11/1960 (0.6%)
All	All	0.80	11/20384 (0.1%)	1.19	163/27440 (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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	47	MET	SD-CE	-6.62	1.63	1.79
1	G	80	MET	SD-CE	-6.31	1.63	1.79
1	K	92	MET	SD-CE	6.14	1.95	1.79
1	I	47	MET	SD-CE	-6.07	1.64	1.79
1	L	47	MET	SD-CE	-6.06	1.64	1.79
1	D	92	MET	SD-CE	5.83	1.94	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	80	MET	SD-CE	-5.75	1.65	1.79
1	E	21	SER	CB-OG	-5.68	1.30	1.42
1	H	47	MET	SD-CE	-5.41	1.66	1.79
1	J	80	MET	SD-CE	-5.21	1.66	1.79
1	M	117	SER	CB-OG	-5.01	1.32	1.42

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	SER	N-CA-C	-11.55	97.77	112.90
1	E	16	SER	N-CA-C	-11.48	99.27	113.28
1	D	16	SER	N-CA-C	-11.08	96.27	111.56
1	B	16	SER	N-CA-C	-10.66	100.39	113.50
1	C	16	SER	N-CA-C	-8.92	102.41	113.38
1	M	56	GLU	N-CA-C	8.72	124.60	112.04
1	G	54	ASN	CA-C-N	8.67	128.89	119.87
1	G	54	ASN	C-N-CA	8.67	128.89	119.87
1	J	16	SER	N-CA-C	-8.33	103.12	113.28
1	E	15	ARG	N-CA-C	8.04	123.17	107.57
1	A	82	PHE	N-CA-C	8.04	121.57	111.69
1	B	15	ARG	N-CA-C	7.99	122.69	108.24
1	M	54	ASN	CA-C-N	7.95	129.78	119.84
1	M	54	ASN	C-N-CA	7.95	129.78	119.84
1	D	15	ARG	N-CA-C	7.89	121.69	108.20
1	D	182	TYR	N-CA-C	-7.87	103.47	113.23
1	M	70	ILE	N-CA-C	7.81	117.87	110.53
1	I	15	ARG	N-CA-C	7.79	122.77	110.70
1	N	37	ASP	N-CA-C	7.77	120.43	111.11
1	H	114	LEU	N-CA-C	-7.63	99.11	110.24
1	M	15	ARG	N-CA-C	7.63	122.79	111.81
1	L	114	LEU	N-CA-C	-7.46	100.36	110.36
1	F	15	ARG	N-CA-C	7.29	126.32	110.80
1	M	66	PRO	N-CA-C	-7.23	104.43	114.98
1	A	54	ASN	CA-C-N	7.21	126.89	119.82
1	A	54	ASN	C-N-CA	7.21	126.89	119.82
1	G	16	SER	N-CA-C	-7.21	104.63	113.50
1	A	15	ARG	N-CA-C	7.16	121.87	107.41
1	G	15	ARG	N-CA-C	7.14	121.43	107.57
1	A	168	THR	N-CA-C	7.13	122.00	113.16
1	K	114	LEU	N-CA-C	-7.09	100.29	110.08
1	A	30	PHE	N-CA-C	7.08	120.46	109.07
1	D	51	GLU	N-CA-C	-7.07	103.50	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	54	ASN	CA-C-N	6.99	126.69	119.56
1	N	54	ASN	C-N-CA	6.99	126.69	119.56
1	I	38	HIS	N-CA-C	6.93	118.62	111.14
1	F	114	LEU	N-CA-C	-6.88	101.15	110.36
1	I	82	PHE	N-CA-C	6.88	118.85	111.36
1	B	37	ASP	N-CA-C	6.86	119.38	111.02
1	D	190	THR	N-CA-C	-6.79	102.39	111.96
1	F	65	SER	N-CA-C	6.78	116.86	108.11
1	L	158	GLY	N-CA-C	-6.78	105.96	115.32
1	L	54	ASN	CA-C-N	6.77	126.91	119.87
1	L	54	ASN	C-N-CA	6.77	126.91	119.87
1	D	158	GLY	N-CA-C	-6.76	106.64	114.69
1	I	65	SER	CA-C-N	6.76	127.34	120.04
1	I	65	SER	C-N-CA	6.76	127.34	120.04
1	N	16	SER	N-CA-C	-6.52	105.62	112.93
1	I	114	LEU	N-CA-C	-6.48	100.67	110.39
1	J	37	ASP	N-CA-C	6.45	122.00	111.37
1	F	186	ASP	N-CA-C	6.41	119.22	111.40
1	N	70	ILE	N-CA-C	6.41	117.08	110.36
1	H	82	PHE	N-CA-C	6.39	119.19	111.40
1	B	186	ASP	N-CA-C	6.36	118.00	111.14
1	H	63	ILE	N-CA-C	6.35	117.03	107.75
1	F	18	ASP	N-CA-C	-6.32	97.34	110.80
1	I	75	SER	N-CA-C	-6.31	104.32	111.07
1	N	56	GLU	N-CA-C	6.27	121.06	113.41
1	H	41	ASN	N-CA-C	-6.24	104.48	111.28
1	A	70	ILE	N-CA-C	6.18	116.93	110.62
1	G	37	ASP	N-CA-C	6.17	118.80	111.33
1	G	114	LEU	N-CA-C	-6.15	101.26	110.24
1	A	37	ASP	N-CA-C	6.15	121.45	111.37
1	G	175	SER	N-CA-C	-6.10	102.67	110.53
1	L	112	PHE	N-CA-C	6.07	118.41	109.24
1	K	26	GLU	N-CA-C	-6.07	104.52	112.41
1	B	154	ALA	N-CA-C	-6.06	104.75	111.36
1	K	70	ILE	N-CA-C	6.04	116.78	110.62
1	B	82	PHE	N-CA-C	6.03	119.82	112.23
1	I	156	HIS	N-CA-C	6.03	118.81	111.82
1	D	70	ILE	N-CA-C	6.02	116.14	110.30
1	D	37	ASP	N-CA-C	6.01	121.22	111.37
1	K	123	GLN	CA-C-N	6.00	125.96	119.78
1	K	123	GLN	C-N-CA	6.00	125.96	119.78
1	D	154	ALA	N-CA-C	-5.98	104.67	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	130	GLY	N-CA-C	5.96	118.20	110.45
1	N	156	HIS	N-CA-C	5.96	118.73	111.82
1	I	84	LYS	CA-C-N	-5.89	113.90	119.85
1	I	84	LYS	C-N-CA	-5.89	113.90	119.85
1	I	54	ASN	CA-C-N	5.89	125.57	119.56
1	I	54	ASN	C-N-CA	5.89	125.57	119.56
1	G	112	PHE	N-CA-C	5.86	119.11	109.85
1	C	82	PHE	N-CA-C	5.85	118.44	111.71
1	E	17	PHE	N-CA-C	-5.85	98.35	110.80
1	F	82	PHE	N-CA-C	5.84	118.87	111.69
1	G	192	ARG	N-CA-C	5.84	123.23	110.80
1	D	112	PHE	N-CA-C	5.77	119.09	110.14
1	H	156	HIS	N-CA-C	5.74	117.62	111.36
1	M	75	SER	N-CA-C	-5.73	104.94	111.07
1	K	192	ARG	N-CA-C	5.71	122.97	110.80
1	H	175	SER	N-CA-C	-5.70	103.17	110.53
1	A	156	HIS	N-CA-C	5.70	117.49	111.28
1	E	168	THR	N-CA-C	5.68	120.91	113.30
1	G	35	VAL	N-CA-CB	5.68	116.91	110.72
1	L	155	LEU	N-CA-C	5.66	117.44	111.28
1	C	84	LYS	CA-C-N	-5.65	113.94	119.76
1	C	84	LYS	C-N-CA	-5.65	113.94	119.76
1	N	97	SER	CB-CA-C	-5.63	110.06	116.54
1	H	130	GLY	N-CA-C	5.63	118.02	110.43
1	B	35	VAL	N-CA-CB	5.62	116.65	110.53
1	E	86	ASP	N-CA-C	-5.60	102.00	110.28
1	C	15	ARG	N-CA-C	5.59	122.71	110.80
1	F	100	ALA	N-CA-C	-5.58	105.28	111.36
1	J	175	SER	N-CA-C	-5.56	102.67	110.35
1	B	38	HIS	N-CA-C	5.55	117.01	111.07
1	B	70	ILE	N-CA-C	5.48	116.11	110.36
1	M	95	ALA	N-CA-C	-5.46	98.31	107.32
1	F	112	PHE	N-CA-C	5.46	117.98	109.52
1	L	15	ARG	N-CA-C	5.45	122.42	110.80
1	N	63	ILE	N-CA-C	5.45	115.71	107.75
1	M	13	GLY	N-CA-C	-5.45	104.13	111.54
1	F	24	LEU	N-CA-C	-5.44	105.45	111.71
1	G	39	MET	N-CA-C	-5.43	105.52	111.82
1	B	21	SER	N-CA-C	-5.41	105.46	111.36
1	E	97	SER	CB-CA-C	-5.38	110.35	116.54
1	K	54	ASN	CA-C-N	5.37	125.84	120.04
1	K	54	ASN	C-N-CA	5.37	125.84	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	ARG	N-CA-C	5.36	122.22	110.80
1	B	51	GLU	N-CA-C	-5.36	104.87	111.40
1	I	112	PHE	N-CA-C	5.35	117.82	109.52
1	M	34	GLN	N-CA-C	5.35	118.32	110.30
1	F	176	ALA	CA-C-N	-5.35	113.12	119.05
1	F	176	ALA	C-N-CA	-5.35	113.12	119.05
1	D	192	ARG	N-CA-C	5.32	122.13	110.80
1	E	184	LEU	N-CA-C	-5.31	105.53	112.23
1	J	63	ILE	N-CA-C	5.30	115.62	107.77
1	D	54	ASN	CA-C-N	5.30	126.46	119.84
1	D	54	ASN	C-N-CA	5.30	126.46	119.84
1	L	180	VAL	N-CA-C	-5.29	105.55	110.53
1	M	35	VAL	N-CA-CB	5.29	116.29	110.53
1	G	26	GLU	N-CA-C	-5.28	106.70	112.72
1	G	17	PHE	N-CA-C	-5.27	99.58	110.80
1	D	156	HIS	N-CA-C	5.26	117.92	111.82
1	E	112	PHE	N-CA-C	5.23	117.77	109.50
1	J	70	ILE	N-CA-C	5.22	115.43	110.53
1	C	18	ASP	N-CA-C	-5.21	99.70	110.80
1	F	63	ILE	N-CA-C	5.21	115.46	108.17
1	F	70	ILE	N-CA-C	5.21	115.42	110.42
1	M	116	ASN	N-CA-C	5.20	118.65	112.72
1	A	114	LEU	N-CA-C	-5.19	103.40	110.36
1	H	70	ILE	N-CA-C	5.18	115.40	110.42
1	H	15	ARG	N-CA-C	5.17	121.82	110.80
1	M	82	PHE	N-CA-C	5.17	116.61	110.97
1	N	112	PHE	N-CA-C	5.17	117.53	109.52
1	I	55	PRO	N-CA-C	5.13	120.51	113.84
1	J	26	GLU	N-CA-C	-5.12	106.89	112.72
1	B	54	ASN	CA-C-N	5.12	124.78	119.56
1	B	54	ASN	C-N-CA	5.12	124.78	119.56
1	G	140	ARG	N-CA-C	-5.11	105.79	111.36
1	D	65	SER	N-CA-C	5.09	116.48	108.23
1	E	14	GLU	N-CA-C	5.09	117.68	110.10
1	C	175	SER	N-CA-C	-5.08	103.97	110.53
1	C	186	ASP	N-CA-C	5.08	118.64	112.23
1	C	75	SER	N-CA-C	-5.08	105.93	111.82
1	D	13	GLY	N-CA-C	-5.07	101.18	113.18
1	C	167	ASP	N-CA-C	5.06	118.71	112.54
1	L	175	SER	N-CA-C	-5.04	104.03	110.53
1	E	82	PHE	N-CA-C	5.04	117.55	111.40
1	J	114	LEU	N-CA-C	-5.03	103.35	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	145	VAL	N-CA-C	-5.03	105.49	110.62
1	E	30	PHE	N-CA-C	5.02	117.15	109.07
1	E	167	ASP	N-CA-C	5.01	118.50	112.38
1	C	83	ILE	N-CA-C	5.00	117.03	109.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	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	1433	0	1436	59	0
1	B	1433	0	1436	73	0
1	C	1433	0	1436	79	0
1	D	1433	0	1436	68	0
1	E	1433	0	1436	67	0
1	F	1433	0	1436	50	0
1	G	1433	0	1436	56	0
1	H	1433	0	1436	65	0
1	I	1433	0	1436	59	0
1	J	1433	0	1436	57	0
1	K	1433	0	1436	72	0
1	L	1433	0	1436	72	0
1	M	1433	0	1436	61	0
1	N	1433	0	1436	56	0
2	A	89	0	0	11	0
2	B	89	0	0	11	0
2	C	94	0	0	7	0
2	D	89	0	0	10	0
2	E	82	0	0	7	0
2	F	91	0	0	8	0
2	G	90	0	0	8	0
2	H	86	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	88	0	0	7	0
2	J	86	0	0	5	0
2	K	92	0	0	11	0
2	L	92	0	0	10	0
2	M	84	0	0	12	0
2	N	94	0	0	13	0
All	All	21308	0	20104	787	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (787) 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:L:55:PRO:HB3	1:L:84:LYS:HD3	1.35	1.06
1:F:84:LYS:HA	1:G:193:ASN:HB2	1.47	0.97
1:C:136:GLU:HG2	1:C:140:ARG:HH11	1.32	0.95
1:C:78:ASP:HB3	1:D:114:LEU:HD12	1.50	0.93
1:L:15:ARG:HG3	1:M:15:ARG:HH22	1.34	0.92
1:J:76:ILE:HG22	1:J:80:MET:HE2	1.49	0.92
1:F:76:ILE:HG22	1:F:80:MET:HE3	1.52	0.92
1:I:31:LEU:HD13	1:I:39:MET:HE1	1.55	0.89
1:E:55:PRO:HB3	1:E:84:LYS:HD2	1.53	0.89
1:D:55:PRO:HB3	1:D:84:LYS:HD3	1.53	0.89
1:B:76:ILE:HG22	1:B:80:MET:HE2	1.54	0.88
1:K:43:ILE:HG22	1:K:47:MET:HE2	1.53	0.87
2:A:221:HOH:O	1:G:71:THR:HG23	1.76	0.86
1:B:55:PRO:HB3	1:B:84:LYS:HD2	1.56	0.85
1:J:77:TYR:HA	1:J:80:MET:HE3	1.58	0.85
1:L:193:ASN:HB2	1:M:84:LYS:HA	1.57	0.85
1:N:76:ILE:HG22	1:N:80:MET:HE3	1.57	0.85
1:I:76:ILE:HG22	1:I:80:MET:HE3	1.60	0.83
1:D:22:ARG:O	1:D:25:LYS:HG2	1.77	0.83
1:J:80:MET:HE1	1:J:102:LEU:HD22	1.60	0.83
1:D:84:LYS:HA	1:E:193:ASN:HB2	1.60	0.83
1:N:29:ILE:HG23	2:N:1212:HOH:O	1.79	0.82
1:J:55:PRO:HB3	1:J:84:LYS:HD2	1.62	0.82
1:M:161:LEU:O	1:M:165:GLU:HG3	1.80	0.81
1:C:133:THR:H	1:J:123:GLN:HE22	1.28	0.80
1:M:34:GLN:NE2	1:M:68:GLY:HA2	1.97	0.80
1:I:70:ILE:HA	1:I:98:MET:HE3	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:ILE:HG22	1:G:80:MET:HE3	1.64	0.80
1:K:172:ARG:HB2	1:K:172:ARG:HH11	1.48	0.79
1:I:104:THR:HB	1:I:184:LEU:HD23	1.65	0.79
1:L:15:ARG:HG3	1:M:15:ARG:NH2	1.98	0.79
1:I:140:ARG:HG2	1:I:144:LYS:NZ	1.98	0.78
1:B:80:MET:HE1	1:B:102:LEU:HD22	1.63	0.78
1:A:29:ILE:HG23	2:A:238:HOH:O	1.85	0.77
1:K:136:GLU:HG2	1:K:140:ARG:HH12	1.50	0.77
1:B:43:ILE:HG22	1:B:47:MET:HE2	1.68	0.76
1:E:136:GLU:HG2	2:E:402:HOH:O	1.86	0.76
1:K:136:GLU:HG2	1:K:140:ARG:NH1	2.01	0.76
1:K:122:HIS:HA	2:K:903:HOH:O	1.86	0.75
1:J:31:LEU:CD1	1:J:39:MET:HE1	2.15	0.75
1:F:22:ARG:O	1:F:25:LYS:HB3	1.86	0.74
1:C:13:GLY:H	1:D:12:ARG:HH21	1.35	0.74
1:K:172:ARG:HB2	1:K:172:ARG:NH1	2.03	0.74
1:C:77:TYR:HA	1:C:80:MET:HE3	1.69	0.74
1:K:189:LEU:HD22	1:L:82:PHE:HE2	1.53	0.74
1:E:31:LEU:HD13	1:E:39:MET:HE1	1.68	0.74
1:G:29:ILE:HG23	2:G:250:HOH:O	1.88	0.73
1:N:124:PRO:HD2	2:N:1242:HOH:O	1.86	0.73
1:B:84:LYS:HA	1:C:193:ASN:CB	2.18	0.73
1:J:122:HIS:HA	2:J:212:HOH:O	1.88	0.73
1:L:161:LEU:O	1:L:165:GLU:HG3	1.88	0.73
1:K:59:ILE:HB	1:K:87:VAL:HG22	1.69	0.73
1:N:98:MET:HE1	1:N:149:MET:HE1	1.71	0.73
1:C:82:PHE:CE2	1:D:191:HIS:HB3	2.24	0.73
1:J:31:LEU:HD12	1:J:39:MET:HE1	1.71	0.73
1:C:70:ILE:HA	1:C:98:MET:HE2	1.72	0.72
1:F:43:ILE:HG22	1:F:47:MET:HE2	1.72	0.72
1:L:54:ASN:ND2	1:L:57:LYS:HG3	2.04	0.72
1:G:31:LEU:HD13	1:G:39:MET:HE1	1.69	0.71
1:J:14:GLU:HB2	1:J:19:ILE:HB	1.72	0.71
1:L:153:MET:SD	2:L:986:HOH:O	2.48	0.71
1:H:193:ASN:HB2	1:I:84:LYS:HA	1.71	0.71
1:A:123:GLN:HB2	2:A:262:HOH:O	1.89	0.71
1:A:76:ILE:HG22	1:A:80:MET:HE3	1.71	0.71
1:A:124:PRO:HD2	2:A:262:HOH:O	1.89	0.71
1:K:189:LEU:HD22	1:L:82:PHE:CE2	2.25	0.71
1:A:43:ILE:HG22	1:A:47:MET:HE2	1.72	0.71
1:E:124:PRO:HD2	2:E:441:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:PHE:HA	2:K:897:HOH:O	1.90	0.70
1:J:191:HIS:HB3	1:K:82:PHE:CE1	2.27	0.69
1:H:124:PRO:HD2	2:H:266:HOH:O	1.91	0.69
1:E:162:GLU:H	1:E:162:GLU:CD	1.99	0.69
1:E:29:ILE:HG22	2:E:411:HOH:O	1.93	0.69
1:A:82:PHE:CD1	1:B:191:HIS:HB3	2.27	0.69
1:E:175:SER:OG	1:E:178:GLU:HG3	1.93	0.69
1:L:115:PRO:HD3	1:L:189:LEU:O	1.92	0.69
1:L:74:MET:HB3	2:L:898:HOH:O	1.92	0.69
2:I:230:HOH:O	1:J:71:THR:HG23	1.91	0.69
1:A:132:ALA:HB3	2:H:266:HOH:O	1.92	0.69
1:F:84:LYS:HA	1:G:193:ASN:CB	2.21	0.68
1:M:34:GLN:HE22	1:M:68:GLY:HA2	1.58	0.68
1:D:153:MET:SD	2:D:202:HOH:O	2.51	0.68
1:H:22:ARG:O	1:H:25:LYS:HG2	1.92	0.68
1:L:54:ASN:CG	1:L:57:LYS:HG3	2.18	0.68
1:L:171:ASP:HB2	2:M:1046:HOH:O	1.94	0.68
1:D:153:MET:HE1	1:D:168:THR:HG21	1.76	0.68
1:G:172:ARG:HH11	1:G:172:ARG:HB2	1.59	0.68
1:C:69:VAL:HG12	1:C:71:THR:HG22	1.74	0.68
1:M:77:TYR:HA	1:M:80:MET:HE3	1.76	0.68
1:G:168:THR:HA	2:G:214:HOH:O	1.94	0.68
1:B:76:ILE:HG22	1:B:80:MET:CE	2.23	0.67
1:A:192:ARG:O	1:A:193:ASN:HB2	1.95	0.67
1:E:43:ILE:HG22	1:E:47:MET:HE2	1.75	0.67
1:M:122:HIS:HA	2:M:1081:HOH:O	1.95	0.67
1:N:98:MET:HE1	1:N:149:MET:CE	2.24	0.67
1:D:168:THR:HA	2:D:208:HOH:O	1.93	0.67
1:D:113:CYS:HB2	1:D:185:VAL:HG11	1.77	0.67
1:G:124:PRO:HD2	2:G:274:HOH:O	1.94	0.67
1:A:143:LEU:HD11	1:H:136:GLU:HG3	1.76	0.66
1:D:133:THR:H	1:K:123:GLN:HE22	1.40	0.66
1:H:82:PHE:CE1	1:N:191:HIS:HB3	2.30	0.66
1:M:31:LEU:HD13	1:M:39:MET:HE1	1.76	0.66
1:I:140:ARG:HG2	1:I:144:LYS:HZ1	1.59	0.66
1:L:70:ILE:HG12	1:L:98:MET:HE2	1.77	0.66
1:A:77:TYR:OH	1:A:156:HIS:HE1	1.79	0.66
1:B:27:ARG:NH2	1:B:50:LEU:O	2.28	0.66
1:M:124:PRO:HD2	2:M:1153:HOH:O	1.95	0.66
1:L:27:ARG:NH2	1:L:50:LEU:O	2.27	0.66
1:B:172:ARG:HB2	1:B:172:ARG:HH11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:MET:HE1	1:C:102:LEU:HD22	1.76	0.66
1:N:119:VAL:HG11	1:N:184:LEU:HD13	1.77	0.66
1:A:23:LEU:HD11	1:G:45:ALA:HB1	1.78	0.66
1:G:132:ALA:HB3	2:N:1242:HOH:O	1.96	0.66
1:D:153:MET:HE3	1:D:164:ILE:HG23	1.77	0.65
1:H:31:LEU:HD13	1:H:39:MET:HE1	1.78	0.65
1:I:76:ILE:CG2	1:I:80:MET:HE3	2.27	0.65
1:L:47:MET:HE3	1:L:79:THR:HG22	1.76	0.65
1:I:157:THR:HA	1:I:183:GLY:O	1.96	0.65
1:N:14:GLU:HB2	1:N:19:ILE:HB	1.78	0.65
1:E:43:ILE:HG12	2:E:411:HOH:O	1.95	0.65
1:H:76:ILE:HG22	1:H:80:MET:HE3	1.78	0.65
1:L:77:TYR:HA	1:L:80:MET:HE3	1.78	0.65
1:C:47:MET:HE3	1:C:79:THR:CG2	2.27	0.65
1:F:27:ARG:NH2	1:F:50:LEU:O	2.30	0.65
1:I:122:HIS:HA	2:I:211:HOH:O	1.95	0.65
1:C:47:MET:HE3	1:C:79:THR:HG22	1.78	0.65
1:F:153:MET:SD	2:F:452:HOH:O	2.55	0.65
1:B:153:MET:SD	2:B:205:HOH:O	2.54	0.64
1:D:16:SER:O	1:D:17:PHE:HB3	1.97	0.64
1:C:27:ARG:NH2	1:C:50:LEU:O	2.30	0.64
1:D:124:PRO:HD2	2:D:270:HOH:O	1.98	0.64
1:E:120:MET:HG2	1:E:172:ARG:O	1.97	0.64
1:F:77:TYR:OH	1:F:156:HIS:HE1	1.80	0.64
1:G:77:TYR:OH	1:G:156:HIS:HE1	1.80	0.64
1:F:132:ALA:HB3	2:M:1153:HOH:O	1.96	0.64
1:M:106:GLY:O	1:M:111:ARG:HD3	1.98	0.64
1:C:55:PRO:HB3	1:C:84:LYS:HD2	1.80	0.64
1:L:47:MET:HE3	1:L:79:THR:CG2	2.27	0.64
1:E:129:GLN:NE2	1:L:127:GLY:HA3	2.13	0.64
1:G:123:GLN:HB2	2:G:274:HOH:O	1.98	0.64
1:B:84:LYS:O	1:C:193:ASN:HB3	1.98	0.64
1:C:12:ARG:CD	1:D:12:ARG:HH22	2.10	0.64
1:J:69:VAL:HG12	1:J:71:THR:HG22	1.80	0.64
1:D:98:MET:HE1	1:D:149:MET:HE2	1.80	0.64
1:C:27:ARG:HD3	1:C:58:ASP:O	1.98	0.63
1:L:176:ALA:HB3	1:L:177:PRO:HD3	1.80	0.63
1:D:191:HIS:HB2	2:D:264:HOH:O	1.98	0.63
1:M:43:ILE:HG12	2:M:1123:HOH:O	1.97	0.63
1:L:22:ARG:O	1:L:25:LYS:HG2	1.99	0.63
1:N:111:ARG:O	1:N:185:VAL:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:29:ILE:HG22	2:M:1123:HOH:O	1.99	0.63
1:E:84:LYS:O	1:F:193:ASN:HB3	1.98	0.63
1:A:148:ARG:HD2	1:B:116:ASN:ND2	2.14	0.62
1:N:101:PHE:HA	2:N:1164:HOH:O	1.99	0.62
1:I:153:MET:SD	2:I:206:HOH:O	2.56	0.62
1:B:191:HIS:HB2	2:B:264:HOH:O	1.99	0.62
1:H:168:THR:HA	2:H:205:HOH:O	2.00	0.62
1:I:124:PRO:HD2	2:I:270:HOH:O	2.00	0.62
1:C:31:LEU:HD22	1:C:43:ILE:HD13	1.82	0.62
1:H:98:MET:HE1	1:H:149:MET:HE1	1.81	0.62
1:C:69:VAL:CG1	1:C:71:THR:HG22	2.29	0.62
1:B:71:THR:HG23	2:B:274:HOH:O	2.00	0.61
1:G:104:THR:HB	1:G:184:LEU:HD23	1.82	0.61
1:J:43:ILE:HG22	1:J:47:MET:HE2	1.81	0.61
1:E:27:ARG:HD3	1:E:58:ASP:O	2.00	0.61
1:K:98:MET:HE1	1:K:149:MET:HE1	1.82	0.61
1:I:69:VAL:HG12	1:I:71:THR:HG22	1.82	0.61
1:K:191:HIS:HB2	2:K:969:HOH:O	2.01	0.61
1:B:143:LEU:HD11	1:I:136:GLU:HG3	1.82	0.61
1:D:139:ALA:O	1:D:142:ILE:HG22	2.00	0.61
1:F:71:THR:HG23	2:G:233:HOH:O	2.00	0.61
1:N:150:ASN:HD22	1:N:165:GLU:HG2	1.65	0.61
1:C:41:ASN:ND2	1:D:32:THR:OG1	2.34	0.61
1:F:168:THR:HA	2:F:458:HOH:O	1.99	0.61
1:N:98:MET:HA	1:N:98:MET:HE2	1.83	0.61
2:A:262:HOH:O	1:H:132:ALA:HB3	2.00	0.61
1:E:114:LEU:HD12	1:E:189:LEU:HB2	1.82	0.61
1:E:132:ALA:HB3	2:L:1064:HOH:O	2.00	0.61
1:G:22:ARG:O	1:G:25:LYS:HG2	2.01	0.61
1:C:136:GLU:CG	1:C:140:ARG:HH11	2.12	0.60
1:K:161:LEU:O	1:K:165:GLU:HG3	2.00	0.60
1:I:120:MET:HE3	1:I:173:PHE:CZ	2.36	0.60
1:L:147:GLY:O	1:L:151:GLU:HG3	2.00	0.60
1:M:29:ILE:HG23	1:M:46:GLN:OE1	2.00	0.60
1:L:192:ARG:HA	1:M:81:GLN:O	2.01	0.60
1:B:122:HIS:HA	2:B:210:HOH:O	2.00	0.60
1:H:61:LEU:HD22	1:H:80:MET:HE2	1.82	0.60
1:B:124:PRO:HD2	2:B:269:HOH:O	2.01	0.60
1:J:27:ARG:NH2	1:J:50:LEU:O	2.34	0.60
2:C:273:HOH:O	1:J:132:ALA:HB3	2.02	0.60
1:A:17:PHE:CG	1:A:17:PHE:O	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:HG23	2:C:280:HOH:O	2.01	0.59
1:G:98:MET:HE1	1:G:149:MET:HE2	1.84	0.59
1:N:17:PHE:CG	1:N:17:PHE:O	2.55	0.59
1:C:133:THR:H	1:J:123:GLN:NE2	1.99	0.59
1:A:81:GLN:O	1:B:192:ARG:HA	2.02	0.59
1:C:14:GLU:HB2	1:C:19:ILE:HB	1.82	0.59
1:I:55:PRO:HB3	1:I:84:LYS:HD2	1.84	0.59
1:A:74:MET:HB3	2:A:267:HOH:O	2.02	0.59
1:G:172:ARG:HB2	1:G:172:ARG:NH1	2.18	0.59
1:L:165:GLU:HB3	2:L:1033:HOH:O	2.02	0.59
1:C:132:ALA:HB3	2:J:272:HOH:O	2.03	0.59
1:B:82:PHE:CE1	1:C:191:HIS:HB3	2.37	0.59
1:C:136:GLU:HG2	1:C:140:ARG:NH1	2.10	0.59
1:H:47:MET:HE2	1:H:79:THR:HG22	1.83	0.59
1:B:115:PRO:HD3	1:B:189:LEU:O	2.02	0.59
1:K:14:GLU:HB2	1:K:19:ILE:HB	1.83	0.58
1:F:129:GLN:NE2	1:M:127:GLY:HA3	2.18	0.58
1:I:16:SER:O	1:I:17:PHE:HB3	2.02	0.58
1:M:115:PRO:HD3	1:M:189:LEU:O	2.03	0.58
1:F:83:ILE:HD12	1:F:85:PRO:HG2	1.84	0.58
1:N:38:HIS:HD2	2:N:1127:HOH:O	1.85	0.58
1:C:82:PHE:CE2	1:D:189:LEU:HB3	2.38	0.58
1:H:69:VAL:HG12	1:H:71:THR:HG22	1.83	0.58
1:G:38:HIS:HD2	2:G:198:HOH:O	1.86	0.58
1:L:89:THR:HB	1:L:103:LEU:HD12	1.85	0.58
1:I:140:ARG:HG2	1:I:144:LYS:HZ2	1.69	0.58
1:B:132:ALA:HB3	2:I:270:HOH:O	2.02	0.58
1:E:17:PHE:CG	1:E:17:PHE:O	2.57	0.58
1:C:134:ASP:O	1:C:138:HIS:HD2	1.87	0.58
1:F:133:THR:H	1:M:123:GLN:HE22	1.52	0.58
1:C:176:ALA:HB3	1:C:177:PRO:HD3	1.86	0.58
1:H:192:ARG:NH1	1:H:192:ARG:HG2	2.18	0.58
1:D:183:GLY:HA2	2:D:200:HOH:O	2.03	0.57
1:J:49:PHE:O	1:J:53:GLU:HG2	2.04	0.57
1:K:91:CYS:SG	1:K:95:ALA:HB2	2.43	0.57
1:N:77:TYR:OH	1:N:156:HIS:HE1	1.88	0.57
1:B:70:ILE:HD11	2:B:252:HOH:O	2.04	0.57
1:K:92:MET:O	1:K:92:MET:HG3	2.05	0.57
1:D:163:GLN:HE22	1:D:166:ARG:NH1	2.03	0.57
1:H:172:ARG:NH1	1:H:172:ARG:HB2	2.19	0.57
1:D:17:PHE:O	1:D:17:PHE:CG	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:PRO:HD2	2:C:273:HOH:O	2.05	0.57
1:E:192:ARG:HH11	1:E:192:ARG:HG2	1.69	0.57
1:J:51:GLU:HG3	1:J:85:PRO:CD	2.34	0.57
1:B:192:ARG:O	1:B:193:ASN:HB2	2.05	0.57
2:F:601:HOH:O	1:G:171:ASP:HB2	2.04	0.57
1:H:70:ILE:HA	1:H:98:MET:HE3	1.86	0.57
1:A:66:PRO:HA	1:A:96:ALA:HB3	1.86	0.57
1:B:161:LEU:HD21	2:B:257:HOH:O	2.04	0.57
1:H:29:ILE:HG23	2:H:239:HOH:O	2.03	0.56
1:C:133:THR:N	1:J:123:GLN:HE22	2.01	0.56
1:H:76:ILE:CG2	1:H:80:MET:HE3	2.35	0.56
1:M:139:ALA:O	1:M:142:ILE:HG22	2.04	0.56
1:I:61:LEU:CD2	1:I:80:MET:HE2	2.36	0.56
1:I:192:ARG:HA	1:J:81:GLN:O	2.05	0.56
1:I:27:ARG:NH2	1:I:54:ASN:HB3	2.20	0.56
1:L:111:ARG:C	1:L:185:VAL:HG22	2.31	0.56
1:G:98:MET:HE1	1:G:149:MET:CE	2.36	0.56
1:H:162:GLU:H	1:H:162:GLU:CD	2.13	0.56
1:C:80:MET:CE	1:C:102:LEU:HD22	2.35	0.56
1:B:77:TYR:OH	1:B:156:HIS:HE1	1.86	0.56
1:E:115:PRO:HD3	1:E:189:LEU:O	2.06	0.56
1:E:98:MET:HE1	1:E:149:MET:HE2	1.88	0.56
1:J:29:ILE:HG23	2:J:248:HOH:O	2.06	0.56
1:J:47:MET:HE3	1:J:79:THR:HG21	1.88	0.56
1:K:84:LYS:N	1:K:85:PRO:HD2	2.21	0.56
1:E:136:GLU:HG3	1:E:137:ILE:N	2.21	0.55
1:F:76:ILE:CG2	1:F:80:MET:HE3	2.31	0.55
1:N:159:GLN:HB2	1:N:164:ILE:HD11	1.87	0.55
2:E:441:HOH:O	1:L:132:ALA:HB3	2.06	0.55
1:F:124:PRO:HD2	2:F:530:HOH:O	2.07	0.55
1:H:112:PHE:HB3	1:H:189:LEU:HG	1.87	0.55
1:B:44:VAL:HA	1:B:47:MET:HE3	1.89	0.55
1:K:121:ILE:HD12	1:K:168:THR:HG22	1.87	0.55
1:N:51:GLU:HG3	1:N:85:PRO:CD	2.37	0.55
1:B:123:GLN:HE22	1:I:133:THR:H	1.54	0.55
1:J:193:ASN:HB2	1:K:84:LYS:HA	1.89	0.55
1:N:145:VAL:O	1:N:149:MET:HG2	2.06	0.55
1:C:22:ARG:NH1	1:C:25:LYS:HD3	2.22	0.55
1:D:84:LYS:HE3	2:D:265:HOH:O	2.06	0.55
1:N:192:ARG:O	1:N:193:ASN:HB2	2.06	0.55
1:A:12:ARG:HH12	1:A:15:ARG:HH21	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:ARG:NH1	1:G:57:LYS:O	2.40	0.55
1:N:29:ILE:HG22	1:N:61:LEU:CD1	2.37	0.55
1:B:90:ILE:HD12	1:B:90:ILE:N	2.21	0.55
1:N:29:ILE:HG22	1:N:61:LEU:HD12	1.88	0.55
1:K:115:PRO:HD3	1:K:189:LEU:O	2.06	0.55
1:G:115:PRO:HD3	1:G:189:LEU:O	2.06	0.55
1:J:66:PRO:HD3	2:K:890:HOH:O	2.05	0.55
1:L:34:GLN:NE2	1:L:68:GLY:HA2	2.21	0.55
1:A:84:LYS:O	1:B:193:ASN:HB3	2.07	0.55
1:I:27:ARG:NH2	1:I:50:LEU:O	2.40	0.55
1:H:17:PHE:CG	1:H:17:PHE:O	2.60	0.54
1:D:111:ARG:O	1:D:185:VAL:HG13	2.06	0.54
1:H:32:THR:OG1	1:I:41:ASN:ND2	2.40	0.54
1:K:32:THR:OG1	1:L:41:ASN:ND2	2.40	0.54
1:A:82:PHE:HA	1:B:191:HIS:O	2.08	0.54
1:D:180:VAL:HG21	1:D:188:ILE:CD1	2.38	0.54
1:H:47:MET:HE2	1:H:79:THR:CG2	2.36	0.54
1:D:70:ILE:HA	1:D:98:MET:HE3	1.88	0.54
1:N:51:GLU:HG3	1:N:85:PRO:HD2	1.90	0.54
1:A:146:LYS:HD2	2:A:262:HOH:O	2.08	0.54
2:A:267:HOH:O	1:B:116:ASN:HB2	2.07	0.54
1:J:124:PRO:HD2	2:J:272:HOH:O	2.07	0.54
1:D:71:THR:HG23	2:D:276:HOH:O	2.07	0.54
1:D:115:PRO:HD3	1:D:189:LEU:O	2.06	0.54
1:I:94:GLN:HB3	1:J:71:THR:OG1	2.08	0.54
1:A:17:PHE:O	1:A:18:ASP:HB3	2.06	0.54
1:E:22:ARG:O	1:E:25:LYS:HG2	2.08	0.54
1:E:113:CYS:O	1:E:188:ILE:HA	2.08	0.54
1:J:181:GLU:HG3	1:J:181:GLU:O	2.08	0.54
1:N:84:LYS:N	1:N:85:PRO:HD2	2.22	0.54
1:A:123:GLN:HE22	1:H:133:THR:H	1.55	0.54
1:C:31:LEU:HD22	1:C:43:ILE:CD1	2.38	0.54
1:C:123:GLN:HE22	1:J:133:THR:H	1.54	0.54
1:G:153:MET:HA	2:G:210:HOH:O	2.08	0.54
1:H:51:GLU:OE2	1:H:84:LYS:HE3	2.08	0.54
1:B:51:GLU:HG3	1:B:85:PRO:HD2	1.90	0.53
1:K:153:MET:SD	2:K:897:HOH:O	2.59	0.53
2:B:269:HOH:O	1:I:132:ALA:HB3	2.07	0.53
1:G:133:THR:H	1:N:123:GLN:HE22	1.55	0.53
1:I:162:GLU:CD	1:I:162:GLU:H	2.16	0.53
1:E:192:ARG:O	1:E:193:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:274:HOH:O	1:N:132:ALA:HB3	2.07	0.53
1:L:26:GLU:OE1	1:L:26:GLU:HA	2.07	0.53
1:B:84:LYS:HA	1:C:193:ASN:HB3	1.91	0.53
1:H:172:ARG:HB2	1:H:172:ARG:HH11	1.73	0.53
1:B:22:ARG:HD3	1:B:25:LYS:HD3	1.91	0.53
1:G:47:MET:HE2	1:G:79:THR:HG22	1.91	0.53
1:K:193:ASN:HB2	1:L:84:LYS:HA	1.91	0.53
1:G:34:GLN:HE21	1:G:68:GLY:HA2	1.74	0.53
1:J:98:MET:HE1	1:J:149:MET:HE1	1.89	0.53
1:F:29:ILE:HG23	2:F:500:HOH:O	2.08	0.53
1:I:22:ARG:O	1:I:25:LYS:HG2	2.09	0.53
1:M:27:ARG:NH1	1:M:57:LYS:O	2.42	0.52
1:C:168:THR:HA	2:C:211:HOH:O	2.09	0.52
1:D:133:THR:H	1:K:123:GLN:NE2	2.07	0.52
1:C:161:LEU:O	1:C:165:GLU:HG3	2.10	0.52
1:J:40:ALA:HA	1:J:76:ILE:HD11	1.92	0.52
1:A:123:GLN:NE2	1:H:133:THR:H	2.08	0.52
1:D:77:TYR:OH	1:D:156:HIS:HE1	1.92	0.52
1:H:40:ALA:O	1:H:44:VAL:HG23	2.10	0.52
1:K:77:TYR:OH	1:K:156:HIS:HE1	1.93	0.52
1:D:51:GLU:HG3	1:D:85:PRO:HD2	1.92	0.52
2:D:270:HOH:O	1:K:132:ALA:HB3	2.09	0.52
1:H:192:ARG:O	1:H:193:ASN:HB2	2.09	0.52
1:J:31:LEU:HD11	1:J:39:MET:HE1	1.92	0.52
1:D:122:HIS:C	1:D:122:HIS:CD2	2.88	0.52
1:D:134:ASP:CG	1:E:170:ARG:HH21	2.17	0.52
1:E:98:MET:HE1	1:E:149:MET:CE	2.40	0.52
1:K:175:SER:OG	1:K:178:GLU:HG3	2.10	0.52
1:A:101:PHE:O	1:A:104:THR:HG22	2.10	0.52
1:K:17:PHE:CD2	1:K:17:PHE:O	2.63	0.52
1:M:47:MET:HE3	1:M:79:THR:CG2	2.39	0.52
1:B:174:LEU:HD23	1:B:178:GLU:HB3	1.90	0.52
1:K:16:SER:O	1:K:17:PHE:HB3	2.10	0.52
1:L:168:THR:HA	2:L:992:HOH:O	2.09	0.52
1:M:77:TYR:OH	1:M:156:HIS:HE1	1.92	0.52
1:M:131:GLN:O	1:M:135:ILE:HG13	2.10	0.52
1:N:115:PRO:HG2	2:N:639:HOH:O	2.10	0.52
1:J:51:GLU:HG3	1:J:85:PRO:HD2	1.92	0.51
1:H:108:LYS:NZ	1:H:111:ARG:HH22	2.09	0.51
1:K:123:GLN:HB2	2:K:975:HOH:O	2.11	0.51
2:B:214:HOH:O	1:C:173:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLN:OE1	1:D:14:GLU:HG3	2.10	0.51
1:C:192:ARG:O	1:C:193:ASN:HB2	2.11	0.51
1:E:122:HIS:C	1:E:122:HIS:CD2	2.87	0.51
1:L:101:PHE:O	1:L:104:THR:HG22	2.10	0.51
1:B:77:TYR:OH	1:B:156:HIS:CE1	2.62	0.51
1:H:123:GLN:HB2	2:H:266:HOH:O	2.10	0.51
1:F:98:MET:HE1	1:F:149:MET:HE2	1.92	0.51
1:G:157:THR:HG22	1:G:184:LEU:HA	1.92	0.51
1:N:50:LEU:HD12	1:N:59:ILE:HG23	1.92	0.51
1:N:161:LEU:O	1:N:165:GLU:HG3	2.11	0.51
1:H:120:MET:HG3	1:H:173:PHE:CE1	2.45	0.51
1:L:53:GLU:O	1:L:54:ASN:HB2	2.11	0.51
1:B:17:PHE:O	1:B:17:PHE:CD1	2.64	0.51
1:D:178:GLU:HA	1:D:181:GLU:HG2	1.91	0.51
1:G:31:LEU:C	1:G:31:LEU:HD12	2.36	0.51
1:J:42:LEU:HD23	1:J:46:GLN:NE2	2.26	0.51
1:M:84:LYS:HE3	2:M:1148:HOH:O	2.10	0.51
1:N:64:ASN:HA	1:N:94:GLN:O	2.11	0.51
1:C:13:GLY:N	1:D:12:ARG:HH21	2.06	0.51
1:E:94:GLN:HA	1:E:118:ARG:O	2.11	0.51
1:L:162:GLU:HA	1:L:165:GLU:OE1	2.11	0.51
1:B:40:ALA:HA	1:B:76:ILE:HD11	1.93	0.51
1:F:69:VAL:HG12	1:F:71:THR:HG22	1.91	0.51
1:B:17:PHE:O	1:B:18:ASP:HB3	2.10	0.50
1:B:84:LYS:HA	1:C:193:ASN:HB2	1.93	0.50
1:F:161:LEU:O	1:F:165:GLU:HG3	2.11	0.50
1:H:69:VAL:CG1	1:H:71:THR:HG22	2.41	0.50
1:A:70:ILE:HG12	1:A:98:MET:HE2	1.92	0.50
1:K:159:GLN:HB2	1:K:164:ILE:HD11	1.93	0.50
1:B:77:TYR:HA	1:B:80:MET:HE3	1.93	0.50
1:D:17:PHE:O	1:D:17:PHE:CD1	2.65	0.50
1:H:190:THR:O	1:H:191:HIS:C	2.54	0.50
1:I:61:LEU:HD22	1:I:80:MET:HE2	1.94	0.50
1:L:76:ILE:HG22	1:L:80:MET:HE2	1.93	0.50
1:L:17:PHE:CG	1:L:17:PHE:O	2.64	0.50
1:M:136:GLU:HG2	1:M:140:ARG:HD3	1.92	0.50
1:F:147:GLY:O	1:F:151:GLU:HG3	2.12	0.50
1:L:31:LEU:HD22	1:L:43:ILE:CD1	2.42	0.50
1:L:124:PRO:HD2	2:L:1064:HOH:O	2.10	0.50
1:C:111:ARG:HB3	1:C:185:VAL:HG22	1.94	0.50
1:E:84:LYS:HA	1:F:193:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:84:LYS:N	1:M:85:PRO:HD2	2.27	0.50
1:J:146:LYS:HD2	2:J:272:HOH:O	2.10	0.50
1:J:190:THR:HG23	2:K:906:HOH:O	2.11	0.50
1:L:97:SER:HG	1:L:122:HIS:CE1	2.29	0.50
1:B:139:ALA:O	1:B:142:ILE:HG22	2.12	0.50
1:B:151:GLU:HG2	1:B:161:LEU:HD11	1.94	0.50
1:F:125:LEU:HD21	2:M:492:HOH:O	2.11	0.50
1:K:16:SER:HA	1:L:17:PHE:HE1	1.77	0.50
1:L:123:GLN:HB2	2:L:1064:HOH:O	2.11	0.50
1:D:162:GLU:HA	1:D:165:GLU:OE1	2.12	0.49
1:E:15:ARG:HH21	1:F:12:ARG:NH2	2.09	0.49
1:G:17:PHE:O	1:G:17:PHE:CD2	2.64	0.49
1:M:122:HIS:C	1:M:122:HIS:CD2	2.89	0.49
1:A:36:GLU:O	1:A:39:MET:HG3	2.11	0.49
1:E:145:VAL:O	1:E:149:MET:HG2	2.13	0.49
1:L:34:GLN:HE22	1:L:68:GLY:HA2	1.77	0.49
1:A:119:VAL:HG11	1:A:184:LEU:HD13	1.95	0.49
1:D:91:CYS:HB2	1:D:103:LEU:HD13	1.93	0.49
1:K:77:TYR:OH	1:K:156:HIS:CE1	2.66	0.49
1:L:83:ILE:HD12	1:L:85:PRO:HG2	1.93	0.49
1:M:16:SER:O	1:M:17:PHE:HB2	2.11	0.49
1:M:192:ARG:HB3	1:N:81:GLN:O	2.13	0.49
1:N:190:THR:HG23	2:N:639:HOH:O	2.11	0.49
1:D:27:ARG:HD3	1:D:58:ASP:O	2.12	0.49
1:E:134:ASP:O	1:E:138:HIS:HD2	1.95	0.49
1:F:19:ILE:HG23	1:F:20:TYR:N	2.28	0.49
1:H:77:TYR:OH	1:H:156:HIS:HE1	1.95	0.49
1:K:95:ALA:O	1:K:100:ALA:HB2	2.11	0.49
1:C:115:PRO:HD3	1:C:189:LEU:O	2.13	0.49
1:L:159:GLN:HB2	1:L:164:ILE:HD11	1.93	0.49
1:N:123:GLN:HB2	2:N:1242:HOH:O	2.12	0.49
1:A:168:THR:HA	2:A:203:HOH:O	2.12	0.49
1:H:38:HIS:HD2	2:H:277:HOH:O	1.94	0.49
1:I:189:LEU:HB3	1:J:82:PHE:CE1	2.48	0.49
1:L:193:ASN:CB	1:M:84:LYS:HA	2.36	0.49
1:L:16:SER:O	1:L:17:PHE:HB3	2.13	0.49
1:B:17:PHE:O	1:B:17:PHE:CG	2.65	0.48
1:G:122:HIS:C	1:G:122:HIS:CD2	2.90	0.48
1:I:115:PRO:HD3	1:I:189:LEU:O	2.13	0.48
1:N:15:ARG:C	1:N:17:PHE:H	2.20	0.48
1:E:34:GLN:HE21	1:E:68:GLY:HA2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:31:LEU:HD13	1:L:39:MET:HE1	1.94	0.48
1:C:122:HIS:C	1:C:122:HIS:CD2	2.92	0.48
1:F:122:HIS:C	1:F:122:HIS:CD2	2.91	0.48
1:K:124:PRO:HD2	2:K:975:HOH:O	2.14	0.48
1:L:192:ARG:O	1:L:193:ASN:HB2	2.13	0.48
1:M:14:GLU:HB2	1:M:19:ILE:HB	1.96	0.48
1:B:18:ASP:HB3	1:B:21:SER:OG	2.14	0.48
1:E:69:VAL:HG12	1:E:71:THR:CG2	2.43	0.48
1:H:61:LEU:CD2	1:H:80:MET:HE2	2.44	0.48
1:C:190:THR:O	1:C:191:HIS:C	2.57	0.48
1:E:70:ILE:HD11	1:E:124:PRO:HB3	1.96	0.48
1:E:192:ARG:HG2	1:E:192:ARG:NH1	2.27	0.48
1:H:22:ARG:HH11	1:H:25:LYS:HD3	1.79	0.48
1:H:191:HIS:HB2	2:H:261:HOH:O	2.12	0.48
1:A:113:CYS:HB2	1:A:185:VAL:HG11	1.95	0.48
1:A:148:ARG:HD2	1:B:116:ASN:HD22	1.78	0.48
1:C:31:LEU:HD13	1:C:39:MET:HE1	1.95	0.48
1:J:31:LEU:HD13	1:J:43:ILE:CD1	2.44	0.48
1:K:27:ARG:NH2	1:K:50:LEU:O	2.47	0.48
1:F:84:LYS:N	1:F:85:PRO:HD2	2.29	0.48
1:F:192:ARG:O	1:F:193:ASN:HB2	2.12	0.48
1:H:192:ARG:HG2	1:H:192:ARG:HH11	1.79	0.48
1:A:122:HIS:C	1:A:122:HIS:CD2	2.92	0.48
1:I:71:THR:HG23	1:I:72:ALA:N	2.29	0.48
1:K:22:ARG:O	1:K:25:LYS:HG2	2.14	0.48
1:M:175:SER:OG	1:M:178:GLU:HG3	2.14	0.48
1:E:123:GLN:HE22	1:L:133:THR:H	1.60	0.47
2:F:530:HOH:O	1:M:132:ALA:HB3	2.12	0.47
1:H:47:MET:CE	1:H:79:THR:HG22	2.43	0.47
1:A:15:ARG:HG2	1:A:18:ASP:H	1.79	0.47
1:C:35:VAL:HG13	1:C:68:GLY:HA3	1.96	0.47
1:J:115:PRO:HD3	1:J:189:LEU:O	2.14	0.47
1:L:84:LYS:N	1:L:85:PRO:HD2	2.28	0.47
1:M:190:THR:O	1:M:191:HIS:C	2.56	0.47
1:A:76:ILE:HG22	1:A:80:MET:CE	2.42	0.47
1:A:174:LEU:HD23	1:A:184:LEU:HD12	1.95	0.47
1:C:12:ARG:HD2	1:D:12:ARG:HH22	1.78	0.47
1:D:172:ARG:HA	2:D:252:HOH:O	2.12	0.47
1:G:191:HIS:O	1:G:191:HIS:ND1	2.47	0.47
1:B:27:ARG:HD3	1:B:58:ASP:O	2.15	0.47
1:B:69:VAL:HG12	1:B:71:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:THR:HA	2:E:369:HOH:O	2.14	0.47
1:F:81:GLN:OE1	1:F:81:GLN:HA	2.14	0.47
1:H:22:ARG:NH1	1:H:25:LYS:HD3	2.29	0.47
1:I:192:ARG:HG2	1:I:192:ARG:NH1	2.30	0.47
1:L:191:HIS:CG	1:L:191:HIS:O	2.67	0.47
1:A:27:ARG:NH1	1:A:57:LYS:O	2.48	0.47
1:A:27:ARG:NH2	1:A:50:LEU:O	2.47	0.47
1:E:123:GLN:NE2	1:L:133:THR:H	2.13	0.47
1:F:153:MET:HG2	1:F:164:ILE:HD12	1.96	0.47
1:J:111:ARG:O	1:J:185:VAL:HG22	2.15	0.47
1:N:16:SER:O	1:N:17:PHE:HB3	2.14	0.47
1:A:12:ARG:NH1	1:A:15:ARG:HH21	2.12	0.47
1:B:22:ARG:O	1:B:25:LYS:HG2	2.15	0.47
1:E:110:LYS:HG2	2:E:409:HOH:O	2.14	0.47
1:E:114:LEU:CD1	1:E:189:LEU:HB2	2.44	0.47
1:H:191:HIS:O	1:I:82:PHE:O	2.32	0.47
1:I:193:ASN:HB2	1:J:84:LYS:HA	1.97	0.47
1:N:122:HIS:C	1:N:122:HIS:CD2	2.93	0.47
1:D:119:VAL:HG11	1:D:184:LEU:CD1	2.45	0.47
1:D:161:LEU:O	1:D:164:ILE:HB	2.15	0.47
1:G:191:HIS:O	1:G:191:HIS:CG	2.66	0.47
1:I:12:ARG:HH11	1:I:15:ARG:HG3	1.80	0.47
1:A:27:ARG:HD3	1:A:58:ASP:O	2.15	0.47
1:C:22:ARG:O	1:C:22:ARG:HD3	2.15	0.47
1:E:27:ARG:NH1	1:E:57:LYS:O	2.48	0.47
1:A:114:LEU:HD12	1:A:189:LEU:HB2	1.96	0.47
1:E:84:LYS:HA	1:F:193:ASN:CB	2.44	0.47
1:F:18:ASP:HB3	1:F:21:SER:OG	2.14	0.47
1:K:101:PHE:HD1	1:K:153:MET:HE2	1.80	0.47
1:B:134:ASP:CG	1:C:170:ARG:HH21	2.23	0.46
1:L:77:TYR:HA	1:L:80:MET:CE	2.44	0.46
1:C:55:PRO:HB3	1:C:84:LYS:CD	2.43	0.46
1:D:31:LEU:HD13	1:D:39:MET:HE1	1.95	0.46
1:D:145:VAL:O	1:D:149:MET:HG2	2.15	0.46
1:E:15:ARG:HD3	1:E:18:ASP:HA	1.97	0.46
1:E:27:ARG:NH1	1:E:59:ILE:HG13	2.30	0.46
1:G:126:GLY:O	1:N:135:ILE:HD11	2.15	0.46
1:F:19:ILE:CG2	1:F:20:TYR:N	2.78	0.46
1:I:84:LYS:N	1:I:85:PRO:HD2	2.30	0.46
1:I:192:ARG:HG2	1:I:192:ARG:HH11	1.80	0.46
1:K:17:PHE:O	1:K:17:PHE:CG	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:LEU:CD1	1:K:31:LEU:C	2.89	0.46
1:L:157:THR:HA	1:L:183:GLY:O	2.15	0.46
1:D:27:ARG:NH1	1:D:57:LYS:O	2.48	0.46
1:D:132:ALA:HB3	2:K:975:HOH:O	2.15	0.46
1:E:15:ARG:HH21	1:F:12:ARG:HH22	1.64	0.46
1:H:115:PRO:HD3	1:H:189:LEU:O	2.15	0.46
1:K:180:VAL:HG21	1:K:188:ILE:HD12	1.96	0.46
1:E:22:ARG:O	1:E:22:ARG:HD3	2.15	0.46
1:G:95:ALA:HB3	1:G:119:VAL:HG22	1.98	0.46
1:G:173:PHE:C	1:G:174:LEU:HD12	2.40	0.46
1:H:15:ARG:NH2	1:N:12:ARG:HH12	2.13	0.46
1:I:123:GLN:HB2	2:I:270:HOH:O	2.14	0.46
1:K:176:ALA:N	1:K:177:PRO:HD2	2.30	0.46
1:E:162:GLU:CD	1:E:162:GLU:N	2.69	0.46
1:K:15:ARG:C	1:K:17:PHE:H	2.23	0.46
1:N:92:MET:HB3	1:N:114:LEU:HD22	1.96	0.46
1:A:147:GLY:O	1:A:151:GLU:HG3	2.16	0.46
1:C:21:SER:HB3	1:D:15:ARG:O	2.16	0.46
1:H:17:PHE:O	1:H:18:ASP:HB3	2.15	0.46
1:L:122:HIS:CD2	1:L:122:HIS:C	2.93	0.46
1:M:94:GLN:HA	1:M:118:ARG:O	2.16	0.46
1:N:55:PRO:HB3	1:N:84:LYS:HD2	1.98	0.46
1:D:96:ALA:HA	1:D:120:MET:O	2.16	0.46
1:E:167:ASP:HA	1:E:172:ARG:NH2	2.31	0.46
1:F:76:ILE:HG22	1:F:80:MET:CE	2.36	0.46
1:G:47:MET:HE1	1:G:80:MET:N	2.31	0.45
1:A:23:LEU:CD1	1:G:45:ALA:HB1	2.46	0.45
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.62	0.45
1:B:152:LEU:O	1:B:155:LEU:HB3	2.16	0.45
1:G:192:ARG:HG2	1:G:192:ARG:HH11	1.81	0.45
1:H:14:GLU:OE1	1:I:24:LEU:HD22	2.16	0.45
1:L:17:PHE:O	1:L:18:ASP:HB3	2.16	0.45
1:H:27:ARG:NH1	1:H:57:LYS:C	2.74	0.45
1:K:12:ARG:HH21	1:L:13:GLY:H	1.64	0.45
1:K:175:SER:HG	1:K:178:GLU:HG3	1.81	0.45
1:M:77:TYR:HA	1:M:80:MET:CE	2.44	0.45
1:C:12:ARG:HD3	1:D:12:ARG:HH22	1.82	0.45
1:E:69:VAL:HG12	1:E:71:THR:HG22	1.98	0.45
1:H:15:ARG:HH21	1:N:12:ARG:HH12	1.63	0.45
1:I:42:LEU:HG	1:I:46:GLN:NE2	2.31	0.45
1:J:22:ARG:O	1:J:25:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLN:NE2	1:I:133:THR:H	2.14	0.45
1:C:123:GLN:HB2	2:C:273:HOH:O	2.15	0.45
1:L:117:SER:O	1:L:118:ARG:HD2	2.16	0.45
1:A:101:PHE:HD1	2:A:198:HOH:O	2.00	0.45
1:E:37:ASP:OD1	1:E:72:ALA:HB2	2.17	0.45
1:C:31:LEU:CD2	1:C:43:ILE:HD13	2.45	0.45
1:E:163:GLN:CD	1:E:166:ARG:HH12	2.24	0.45
1:F:32:THR:HA	1:F:64:ASN:O	2.16	0.45
1:M:89:THR:HB	1:M:103:LEU:HD12	1.98	0.45
1:C:12:ARG:HG3	1:C:13:GLY:N	2.32	0.45
1:G:159:GLN:HB2	1:G:164:ILE:HD11	1.99	0.45
1:B:122:HIS:C	1:B:122:HIS:CD2	2.95	0.45
1:G:111:ARG:C	1:G:185:VAL:HG22	2.42	0.45
1:H:49:PHE:O	1:H:52:ALA:HB3	2.16	0.45
1:M:14:GLU:HG3	1:N:46:GLN:CD	2.41	0.45
1:B:180:VAL:HA	1:B:185:VAL:O	2.16	0.45
1:K:16:SER:HA	1:L:17:PHE:CE1	2.51	0.45
1:L:159:GLN:OE1	1:L:163:GLN:HG2	2.17	0.45
1:N:31:LEU:HD22	1:N:43:ILE:HD13	1.98	0.45
1:A:38:HIS:CD2	2:A:270:HOH:O	2.69	0.44
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.70	0.44
1:D:162:GLU:CD	1:D:162:GLU:H	2.25	0.44
1:I:13:GLY:HA2	1:J:42:LEU:HD11	1.98	0.44
1:J:122:HIS:C	1:J:122:HIS:CD2	2.95	0.44
1:N:191:HIS:HB2	2:N:1236:HOH:O	2.16	0.44
1:C:77:TYR:OH	1:C:156:HIS:HE1	2.00	0.44
1:D:101:PHE:O	1:D:104:THR:HG22	2.17	0.44
1:A:157:THR:HG22	1:A:184:LEU:HA	1.99	0.44
1:I:31:LEU:C	1:I:31:LEU:HD12	2.42	0.44
1:L:101:PHE:HD1	2:L:986:HOH:O	2.00	0.44
1:M:101:PHE:O	1:M:104:THR:HG22	2.17	0.44
1:C:71:THR:OG1	1:D:94:GLN:HB3	2.17	0.44
1:D:191:HIS:O	1:D:191:HIS:ND1	2.51	0.44
1:J:19:ILE:HD11	1:K:49:PHE:HB2	1.99	0.44
1:J:70:ILE:HA	1:J:98:MET:HE3	1.99	0.44
1:H:108:LYS:NZ	1:H:111:ARG:NH2	2.65	0.44
1:I:191:HIS:O	1:J:82:PHE:O	2.35	0.44
1:K:91:CYS:HB2	1:K:103:LEU:HD22	1.99	0.44
1:K:122:HIS:C	1:K:122:HIS:CD2	2.95	0.44
1:L:43:ILE:HG12	2:L:1034:HOH:O	2.18	0.44
1:B:127:GLY:HA3	1:I:129:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:GLN:CD	1:M:127:GLY:HA3	2.43	0.44
1:G:53:GLU:OE1	1:G:53:GLU:HA	2.17	0.44
1:J:190:THR:O	1:J:191:HIS:C	2.61	0.44
1:M:146:LYS:HD2	2:M:1153:HOH:O	2.17	0.44
1:N:31:LEU:HB2	1:N:61:LEU:HD11	2.00	0.44
1:E:51:GLU:OE2	1:E:83:ILE:HA	2.18	0.44
1:F:121:ILE:HG13	2:F:458:HOH:O	2.18	0.44
1:A:17:PHE:CE2	1:A:25:LYS:HD3	2.53	0.44
1:A:82:PHE:CE1	1:B:191:HIS:HB3	2.53	0.44
1:C:22:ARG:HD3	1:C:22:ARG:C	2.42	0.43
1:H:122:HIS:C	1:H:122:HIS:CD2	2.96	0.43
1:I:17:PHE:O	1:I:18:ASP:HB3	2.17	0.43
1:F:131:GLN:OE1	1:G:170:ARG:NH2	2.47	0.43
1:G:117:SER:O	1:G:118:ARG:HD2	2.19	0.43
1:I:17:PHE:O	1:I:17:PHE:CG	2.71	0.43
1:I:42:LEU:HG	1:I:46:GLN:HE21	1.83	0.43
1:D:140:ARG:O	1:D:144:LYS:HG3	2.17	0.43
1:A:17:PHE:HE2	1:A:25:LYS:HD3	1.83	0.43
1:A:131:GLN:O	1:A:134:ASP:HB2	2.18	0.43
1:B:55:PRO:HA	1:B:85:PRO:HD3	2.00	0.43
1:F:123:GLN:HE21	1:M:132:ALA:HB3	1.83	0.43
1:H:12:ARG:NH1	1:I:15:ARG:HH21	2.16	0.43
1:H:121:ILE:HG13	1:H:172:ARG:HB3	2.00	0.43
1:J:19:ILE:HD11	1:K:49:PHE:CB	2.48	0.43
1:J:69:VAL:CG1	1:J:71:THR:HG22	2.47	0.43
1:N:168:THR:HA	2:N:1170:HOH:O	2.17	0.43
1:B:139:ALA:O	1:B:143:LEU:HG	2.18	0.43
1:D:84:LYS:HA	1:E:193:ASN:CB	2.40	0.43
1:E:163:GLN:OE1	1:E:166:ARG:NH1	2.51	0.43
1:G:163:GLN:HE22	1:G:166:ARG:HH12	1.66	0.43
1:I:191:HIS:O	1:I:191:HIS:CG	2.71	0.43
1:K:181:GLU:O	1:K:181:GLU:HG2	2.19	0.43
1:M:173:PHE:HE2	2:N:1135:HOH:O	2.01	0.43
1:B:49:PHE:CD1	1:C:22:ARG:HD2	2.54	0.43
1:B:96:ALA:HA	1:B:120:MET:O	2.19	0.43
1:B:104:THR:HB	1:B:184:LEU:HD23	2.01	0.43
1:D:34:GLN:HE21	1:D:68:GLY:HA2	1.84	0.43
1:F:98:MET:HE1	1:F:149:MET:CE	2.48	0.43
1:L:114:LEU:HB3	1:M:78:ASP:OD2	2.19	0.43
1:M:71:THR:HG23	2:M:1013:HOH:O	2.18	0.43
1:N:24:LEU:O	1:N:27:ARG:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:SER:OG	1:N:122:HIS:CE1	2.72	0.43
2:H:278:HOH:O	1:N:171:ASP:HB2	2.18	0.43
1:I:92:MET:HA	2:I:278:HOH:O	2.19	0.43
1:K:39:MET:O	1:K:43:ILE:HG13	2.18	0.43
1:K:192:ARG:O	1:K:193:ASN:HB2	2.18	0.43
1:E:120:MET:HA	1:E:172:ARG:O	2.18	0.43
1:F:19:ILE:HD12	1:F:19:ILE:HA	1.86	0.43
1:H:145:VAL:O	1:H:149:MET:HG2	2.19	0.43
1:J:191:HIS:O	1:J:191:HIS:ND1	2.52	0.43
1:L:76:ILE:O	1:L:80:MET:HG3	2.19	0.43
1:M:117:SER:O	1:M:118:ARG:HD2	2.19	0.43
1:B:83:ILE:O	1:C:193:ASN:HB2	2.19	0.43
1:B:159:GLN:HB2	1:B:164:ILE:HD11	2.01	0.43
1:B:176:ALA:N	1:B:177:PRO:HD2	2.34	0.43
1:B:123:GLN:HB2	2:B:269:HOH:O	2.18	0.43
1:E:118:ARG:HD2	1:E:118:ARG:HA	1.80	0.43
1:F:118:ARG:HA	1:F:118:ARG:HD2	1.80	0.43
1:F:137:ILE:HG12	1:F:140:ARG:HH22	1.84	0.43
1:H:92:MET:HB3	1:H:114:LEU:HD23	2.01	0.43
1:H:191:HIS:HB3	1:I:82:PHE:CE2	2.54	0.43
1:M:47:MET:HE3	1:M:79:THR:HG21	2.00	0.43
1:C:123:GLN:NE2	1:J:133:THR:H	2.16	0.42
1:G:61:LEU:CD2	1:G:80:MET:HE2	2.49	0.42
1:H:57:LYS:O	1:H:85:PRO:HB3	2.19	0.42
1:C:111:ARG:O	1:C:185:VAL:HG13	2.19	0.42
1:D:173:PHE:HD1	2:D:252:HOH:O	2.01	0.42
1:G:133:THR:H	1:N:123:GLN:NE2	2.16	0.42
1:K:66:PRO:HD3	2:K:979:HOH:O	2.19	0.42
1:N:71:THR:HG23	2:N:1102:HOH:O	2.19	0.42
1:C:98:MET:HE1	1:C:149:MET:HE1	2.02	0.42
1:K:54:ASN:HA	1:K:55:PRO:HD3	1.83	0.42
1:A:176:ALA:N	1:A:177:PRO:HD2	2.34	0.42
1:B:146:LYS:HD2	2:B:269:HOH:O	2.19	0.42
1:B:148:ARG:HD2	1:C:116:ASN:ND2	2.34	0.42
1:C:15:ARG:NH1	2:C:276:HOH:O	2.52	0.42
1:D:118:ARG:HA	1:D:118:ARG:HD2	1.76	0.42
1:I:120:MET:CE	1:I:173:PHE:CZ	3.01	0.42
1:K:178:GLU:O	1:K:182:TYR:HB2	2.20	0.42
1:L:83:ILE:HB	1:L:85:PRO:HD2	2.02	0.42
1:D:21:SER:HA	1:E:14:GLU:OE1	2.19	0.42
1:F:123:GLN:NE2	1:M:132:ALA:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:PHE:O	1:I:104:THR:HG22	2.19	0.42
1:L:191:HIS:O	1:L:191:HIS:ND1	2.52	0.42
1:M:152:LEU:HA	1:M:152:LEU:HD23	1.71	0.42
1:M:192:ARG:HB2	1:M:193:ASN:H	1.55	0.42
1:N:27:ARG:NH2	1:N:50:LEU:O	2.52	0.42
1:D:129:GLN:NE2	1:K:127:GLY:HA3	2.35	0.42
1:E:14:GLU:OE2	1:E:14:GLU:HA	2.19	0.42
1:G:61:LEU:HD22	1:G:80:MET:HE2	2.01	0.42
1:H:95:ALA:O	1:H:100:ALA:HB2	2.19	0.42
1:M:157:THR:CG2	1:M:184:LEU:HD23	2.49	0.42
1:M:180:VAL:HG22	1:M:185:VAL:HG12	2.02	0.42
1:E:153:MET:HE2	1:E:153:MET:HB2	1.96	0.42
1:G:160:SER:O	1:G:164:ILE:HG12	2.19	0.42
1:D:180:VAL:HG13	1:D:186:ASP:O	2.19	0.42
1:H:192:ARG:HH11	1:H:192:ARG:CG	2.33	0.42
1:K:147:GLY:O	1:K:151:GLU:HG3	2.19	0.42
1:A:111:ARG:C	1:A:185:VAL:HG22	2.45	0.42
1:C:108:LYS:NZ	1:C:111:ARG:NH2	2.67	0.42
1:F:96:ALA:HA	1:F:120:MET:O	2.19	0.42
1:H:55:PRO:HB3	1:H:84:LYS:HD2	2.02	0.42
1:B:94:GLN:HA	1:B:118:ARG:O	2.20	0.42
1:C:136:GLU:HG2	1:C:140:ARG:HD3	2.01	0.42
1:E:64:ASN:HA	1:E:94:GLN:O	2.20	0.42
1:K:154:ALA:HB1	1:K:159:GLN:O	2.20	0.42
1:M:11:SER:O	1:M:12:ARG:HB3	2.19	0.42
1:B:51:GLU:HG3	1:B:85:PRO:CD	2.50	0.41
1:C:14:GLU:O	1:C:16:SER:N	2.48	0.41
1:E:57:LYS:O	1:E:85:PRO:HB3	2.19	0.41
1:F:81:GLN:O	1:G:192:ARG:HA	2.19	0.41
1:F:151:GLU:HG2	2:F:513:HOH:O	2.20	0.41
1:G:69:VAL:HG12	1:G:71:THR:HG22	2.02	0.41
1:G:136:GLU:OE1	1:G:140:ARG:NH1	2.53	0.41
1:J:13:GLY:O	1:J:14:GLU:C	2.63	0.41
1:J:176:ALA:N	1:J:177:PRO:HD2	2.35	0.41
1:L:190:THR:O	1:L:191:HIS:C	2.63	0.41
1:M:113:CYS:HB2	1:M:185:VAL:HG11	2.02	0.41
1:A:55:PRO:HB3	1:A:84:LYS:HD2	2.00	0.41
1:K:180:VAL:HG21	1:K:187:SER:HA	2.02	0.41
1:L:114:LEU:HD13	1:L:114:LEU:HA	1.95	0.41
1:N:31:LEU:HD13	1:N:39:MET:HE1	2.02	0.41
1:C:25:LYS:HG3	1:C:26:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:MET:HE1	1:D:149:MET:CE	2.48	0.41
1:H:71:THR:HG23	2:N:1191:HOH:O	2.19	0.41
1:J:27:ARG:HD3	1:J:58:ASP:O	2.21	0.41
1:K:108:LYS:NZ	2:K:954:HOH:O	2.51	0.41
1:L:83:ILE:HD11	1:L:87:VAL:CG2	2.50	0.41
1:M:191:HIS:ND1	1:M:191:HIS:O	2.53	0.41
1:G:192:ARG:O	1:G:193:ASN:HB2	2.20	0.41
1:I:69:VAL:CG1	1:I:71:THR:HG22	2.48	0.41
1:E:167:ASP:HA	1:E:172:ARG:HH22	1.84	0.41
1:H:146:LYS:HD2	2:H:266:HOH:O	2.19	0.41
1:J:119:VAL:HG11	1:J:184:LEU:HD13	2.01	0.41
2:L:1038:HOH:O	1:M:38:HIS:HD2	2.03	0.41
1:N:190:THR:HG22	1:N:192:ARG:HG3	2.02	0.41
1:G:192:ARG:HG2	1:G:192:ARG:NH1	2.34	0.41
1:J:111:ARG:C	1:J:185:VAL:HG22	2.46	0.41
1:L:22:ARG:NH1	1:L:25:LYS:HD3	2.36	0.41
1:A:164:ILE:HD13	1:A:164:ILE:HA	1.88	0.41
1:E:97:SER:OG	1:E:122:HIS:CE1	2.73	0.41
1:E:140:ARG:O	1:E:144:LYS:HG3	2.21	0.41
1:E:192:ARG:O	1:E:193:ASN:CB	2.68	0.41
1:K:31:LEU:CD1	1:K:65:SER:HB2	2.51	0.41
1:K:31:LEU:C	1:K:31:LEU:HD13	2.46	0.41
1:C:27:ARG:NH1	1:C:57:LYS:O	2.54	0.41
1:K:97:SER:HB3	1:K:122:HIS:NE2	2.36	0.41
1:N:76:ILE:CG2	1:N:80:MET:HE3	2.41	0.41
1:A:89:THR:HB	1:A:103:LEU:HD12	2.02	0.41
1:A:128:TYR:O	1:H:127:GLY:CA	2.69	0.41
1:A:175:SER:OG	1:A:177:PRO:HG2	2.21	0.41
1:C:192:ARG:O	1:C:193:ASN:CB	2.69	0.41
1:I:35:VAL:HA	1:I:39:MET:SD	2.61	0.41
1:I:95:ALA:O	1:I:100:ALA:HB2	2.20	0.41
1:K:153:MET:HE2	1:K:153:MET:HB2	1.92	0.41
1:L:122:HIS:HD2	1:L:122:HIS:O	2.03	0.41
1:M:34:GLN:NE2	1:M:68:GLY:CA	2.75	0.41
1:M:123:GLN:HB2	2:M:1153:HOH:O	2.20	0.41
1:N:17:PHE:O	1:N:18:ASP:HB3	2.20	0.41
1:B:21:SER:HB3	1:C:16:SER:HB3	2.02	0.41
1:E:70:ILE:O	1:E:74:MET:HG2	2.20	0.41
1:F:128:TYR:CG	1:F:129:GLN:N	2.89	0.41
1:G:190:THR:O	1:G:191:HIS:C	2.63	0.41
1:J:192:ARG:HA	1:K:81:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:CG	1:A:129:GLN:N	2.89	0.40
1:K:143:LEU:HA	1:K:143:LEU:HD23	1.89	0.40
1:K:190:THR:O	1:K:191:HIS:C	2.64	0.40
1:C:84:LYS:HE3	2:C:268:HOH:O	2.21	0.40
1:D:112:PHE:HA	1:D:185:VAL:HG13	2.03	0.40
1:D:119:VAL:HG11	1:D:184:LEU:HD13	2.03	0.40
1:M:31:LEU:C	1:M:31:LEU:HD12	2.45	0.40
1:A:174:LEU:CD2	1:A:184:LEU:HD12	2.51	0.40
1:G:121:ILE:HD12	1:G:168:THR:HG22	2.03	0.40
1:I:114:LEU:HD13	1:I:114:LEU:HA	1.86	0.40
1:M:143:LEU:HD23	1:M:143:LEU:HA	1.86	0.40
1:B:78:ASP:CB	1:C:114:LEU:HD23	2.51	0.40
1:C:34:GLN:HE21	1:C:68:GLY:HA2	1.86	0.40
1:G:133:THR:O	1:G:137:ILE:HG13	2.21	0.40
1:K:73:GLY:O	1:K:76:ILE:HB	2.21	0.40
1:M:96:ALA:HB2	2:M:1139:HOH:O	2.20	0.40
1:A:98:MET:HE1	1:A:149:MET:HE2	2.04	0.40
1:B:128:TYR:CG	1:B:129:GLN:N	2.89	0.40
1:D:163:GLN:NE2	1:D:166:ARG:CZ	2.84	0.40
1:H:114:LEU:HD13	1:H:114:LEU:HA	1.91	0.40
1:K:145:VAL:O	1:K:149:MET:HG2	2.21	0.40
1:N:22:ARG:NH1	1:N:25:LYS:HD3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/193 (94%)	171 (94%)	8 (4%)	2 (1%)	11	13
1	B	181/193 (94%)	168 (93%)	10 (6%)	3 (2%)	7	7
1	C	181/193 (94%)	164 (91%)	12 (7%)	5 (3%)	4	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	181/193 (94%)	166 (92%)	11 (6%)	4 (2%)	5	4
1	E	181/193 (94%)	166 (92%)	11 (6%)	4 (2%)	5	4
1	F	181/193 (94%)	171 (94%)	7 (4%)	3 (2%)	7	7
1	G	181/193 (94%)	173 (96%)	4 (2%)	4 (2%)	5	4
1	H	181/193 (94%)	171 (94%)	7 (4%)	3 (2%)	7	7
1	I	181/193 (94%)	167 (92%)	12 (7%)	2 (1%)	11	13
1	J	181/193 (94%)	169 (93%)	8 (4%)	4 (2%)	5	4
1	K	181/193 (94%)	167 (92%)	9 (5%)	5 (3%)	4	2
1	L	181/193 (94%)	167 (92%)	9 (5%)	5 (3%)	4	2
1	M	181/193 (94%)	165 (91%)	13 (7%)	3 (2%)	7	7
1	N	181/193 (94%)	170 (94%)	6 (3%)	5 (3%)	4	2
All	All	2534/2702 (94%)	2355 (93%)	127 (5%)	52 (2%)	5	4

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	B	17	PHE
1	B	192	ARG
1	C	15	ARG
1	C	17	PHE
1	C	18	ASP
1	C	192	ARG
1	D	17	PHE
1	D	192	ARG
1	E	17	PHE
1	E	191	HIS
1	E	192	ARG
1	F	17	PHE
1	F	18	ASP
1	F	191	HIS
1	G	17	PHE
1	G	18	ASP
1	G	191	HIS
1	G	192	ARG
1	H	17	PHE
1	I	191	HIS
1	J	17	PHE

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Mol	Chain	Res	Type
1	J	192	ARG
1	K	15	ARG
1	K	17	PHE
1	K	191	HIS
1	K	192	ARG
1	L	191	HIS
1	L	192	ARG
1	M	17	PHE
1	M	191	HIS
1	N	17	PHE
1	A	191	HIS
1	C	191	HIS
1	D	191	HIS
1	E	18	ASP
1	H	191	HIS
1	I	192	ARG
1	J	191	HIS
1	K	18	ASP
1	L	15	ARG
1	M	12	ARG
1	J	14	GLU
1	L	14	GLU
1	N	15	ARG
1	N	192	ARG
1	B	191	HIS
1	D	18	ASP
1	H	14	GLU
1	N	18	ASP
1	N	191	HIS
1	L	54	ASN

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	154/163 (94%)	138 (90%)	16 (10%)	7 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	154/163 (94%)	135 (88%)	19 (12%)	4	5
1	C	154/163 (94%)	137 (89%)	17 (11%)	6	7
1	D	154/163 (94%)	140 (91%)	14 (9%)	9	11
1	E	154/163 (94%)	136 (88%)	18 (12%)	5	6
1	F	154/163 (94%)	140 (91%)	14 (9%)	9	11
1	G	154/163 (94%)	143 (93%)	11 (7%)	13	19
1	H	154/163 (94%)	139 (90%)	15 (10%)	8	10
1	I	154/163 (94%)	140 (91%)	14 (9%)	9	11
1	J	154/163 (94%)	140 (91%)	14 (9%)	9	11
1	K	154/163 (94%)	139 (90%)	15 (10%)	8	10
1	L	154/163 (94%)	143 (93%)	11 (7%)	13	19
1	M	154/163 (94%)	138 (90%)	16 (10%)	7	8
1	N	154/163 (94%)	146 (95%)	8 (5%)	21	31
All	All	2156/2282 (94%)	1954 (91%)	202 (9%)	8	11

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	17	PHE
1	A	22	ARG
1	A	25	LYS
1	A	27	ARG
1	A	31	LEU
1	A	35	VAL
1	A	36	GLU
1	A	104	THR
1	A	113	CYS
1	A	114	LEU
1	A	120	MET
1	A	170	ARG
1	A	172	ARG
1	A	185	VAL
1	A	190	THR
1	B	11	SER
1	B	14	GLU
1	B	16	SER

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Mol	Chain	Res	Type
1	B	21	SER
1	B	27	ARG
1	B	31	LEU
1	B	35	VAL
1	B	36	GLU
1	B	90	ILE
1	B	104	THR
1	B	114	LEU
1	B	120	MET
1	B	122	HIS
1	B	136	GLU
1	B	161	LEU
1	B	162	GLU
1	B	172	ARG
1	B	181	GLU
1	B	185	VAL
1	C	22	ARG
1	C	23	LEU
1	C	25	LYS
1	C	31	LEU
1	C	35	VAL
1	C	36	GLU
1	C	71	THR
1	C	113	CYS
1	C	114	LEU
1	C	117	SER
1	C	118	ARG
1	C	120	MET
1	C	135	ILE
1	C	155	LEU
1	C	172	ARG
1	C	185	VAL
1	C	190	THR
1	D	19	ILE
1	D	22	ARG
1	D	31	LEU
1	D	35	VAL
1	D	36	GLU
1	D	65	SER
1	D	103	LEU
1	D	113	CYS
1	D	118	ARG

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Mol	Chain	Res	Type
1	D	122	HIS
1	D	135	ILE
1	D	172	ARG
1	D	187	SER
1	D	190	THR
1	E	12	ARG
1	E	17	PHE
1	E	22	ARG
1	E	31	LEU
1	E	35	VAL
1	E	36	GLU
1	E	71	THR
1	E	113	CYS
1	E	114	LEU
1	E	118	ARG
1	E	136	GLU
1	E	153	MET
1	E	169	GLU
1	E	172	ARG
1	E	184	LEU
1	E	185	VAL
1	E	190	THR
1	E	192	ARG
1	F	11	SER
1	F	22	ARG
1	F	31	LEU
1	F	35	VAL
1	F	36	GLU
1	F	42	LEU
1	F	56	GLU
1	F	113	CYS
1	F	114	LEU
1	F	120	MET
1	F	124	PRO
1	F	172	ARG
1	F	185	VAL
1	F	190	THR
1	G	15	ARG
1	G	22	ARG
1	G	31	LEU
1	G	35	VAL
1	G	36	GLU

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Mol	Chain	Res	Type
1	G	56	GLU
1	G	71	THR
1	G	113	CYS
1	G	172	ARG
1	G	184	LEU
1	G	185	VAL
1	H	22	ARG
1	H	31	LEU
1	H	35	VAL
1	H	36	GLU
1	H	114	LEU
1	H	118	ARG
1	H	122	HIS
1	H	136	GLU
1	H	169	GLU
1	H	172	ARG
1	H	174	LEU
1	H	185	VAL
1	H	187	SER
1	H	190	THR
1	H	192	ARG
1	I	11	SER
1	I	22	ARG
1	I	31	LEU
1	I	34	GLN
1	I	35	VAL
1	I	36	GLU
1	I	113	CYS
1	I	114	LEU
1	I	120	MET
1	I	122	HIS
1	I	144	LYS
1	I	172	ARG
1	I	184	LEU
1	I	185	VAL
1	J	11	SER
1	J	22	ARG
1	J	27	ARG
1	J	35	VAL
1	J	36	GLU
1	J	42	LEU
1	J	56	GLU

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Mol	Chain	Res	Type
1	J	113	CYS
1	J	122	HIS
1	J	125	LEU
1	J	155	LEU
1	J	172	ARG
1	J	181	GLU
1	J	185	VAL
1	K	11	SER
1	K	27	ARG
1	K	31	LEU
1	K	35	VAL
1	K	43	ILE
1	K	56	GLU
1	K	71	THR
1	K	97	SER
1	K	113	CYS
1	K	120	MET
1	K	153	MET
1	K	162	GLU
1	K	169	GLU
1	K	172	ARG
1	K	185	VAL
1	L	11	SER
1	L	27	ARG
1	L	31	LEU
1	L	35	VAL
1	L	36	GLU
1	L	71	THR
1	L	114	LEU
1	L	155	LEU
1	L	172	ARG
1	L	181	GLU
1	L	185	VAL
1	M	11	SER
1	M	31	LEU
1	M	35	VAL
1	M	36	GLU
1	M	56	GLU
1	M	71	THR
1	M	113	CYS
1	M	114	LEU
1	M	115	PRO

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Mol	Chain	Res	Type
1	M	120	MET
1	M	122	HIS
1	M	163	GLN
1	M	172	ARG
1	M	185	VAL
1	M	190	THR
1	M	192	ARG
1	N	22	ARG
1	N	27	ARG
1	N	31	LEU
1	N	35	VAL
1	N	36	GLU
1	N	114	LEU
1	N	153	MET
1	N	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	41	ASN
1	A	123	GLN
1	A	156	HIS
1	B	38	HIS
1	B	41	ASN
1	B	116	ASN
1	B	123	GLN
1	B	150	ASN
1	B	156	HIS
1	C	34	GLN
1	C	41	ASN
1	C	116	ASN
1	C	123	GLN
1	C	138	HIS
1	C	156	HIS
1	D	38	HIS
1	D	41	ASN
1	D	122	HIS
1	D	129	GLN
1	D	156	HIS
1	D	163	GLN
1	E	34	GLN

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Mol	Chain	Res	Type
1	E	38	HIS
1	E	41	ASN
1	E	123	GLN
1	E	129	GLN
1	E	156	HIS
1	E	163	GLN
1	F	123	GLN
1	F	156	HIS
1	F	163	GLN
1	G	34	GLN
1	G	38	HIS
1	G	116	ASN
1	G	122	HIS
1	G	123	GLN
1	G	129	GLN
1	G	156	HIS
1	G	163	GLN
1	H	38	HIS
1	H	41	ASN
1	H	123	GLN
1	H	129	GLN
1	H	156	HIS
1	H	163	GLN
1	I	41	ASN
1	I	46	GLN
1	I	123	GLN
1	I	156	HIS
1	I	163	GLN
1	I	193	ASN
1	J	122	HIS
1	J	123	GLN
1	J	156	HIS
1	J	163	GLN
1	J	191	HIS
1	K	41	ASN
1	K	46	GLN
1	K	123	GLN
1	K	156	HIS
1	K	163	GLN
1	L	38	HIS
1	L	41	ASN
1	L	116	ASN

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Mol	Chain	Res	Type
1	L	123	GLN
1	L	156	HIS
1	L	163	GLN
1	M	34	GLN
1	M	41	ASN
1	M	122	HIS
1	M	123	GLN
1	M	156	HIS
1	M	163	GLN
1	M	193	ASN
1	N	38	HIS
1	N	122	HIS
1	N	123	GLN
1	N	150	ASN
1	N	156	HIS
1	N	193	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 ⓘ

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	183/193 (94%)	0.31	11 (6%)	27	29	16, 27, 68, 93	0
1	B	183/193 (94%)	0.37	12 (6%)	24	26	16, 28, 55, 91	0
1	C	183/193 (94%)	0.53	15 (8%)	17	19	20, 32, 58, 99	0
1	D	183/193 (94%)	0.54	15 (8%)	17	19	17, 33, 62, 92	0
1	E	183/193 (94%)	0.39	13 (7%)	22	24	17, 30, 63, 98	0
1	F	183/193 (94%)	0.08	11 (6%)	27	29	10, 21, 55, 100	0
1	G	183/193 (94%)	0.06	11 (6%)	27	29	13, 21, 49, 98	0
1	H	183/193 (94%)	0.30	11 (6%)	27	29	16, 28, 59, 100	0
1	I	183/193 (94%)	0.25	12 (6%)	24	26	13, 27, 58, 100	0
1	J	183/193 (94%)	0.29	15 (8%)	17	19	17, 29, 60, 99	0
1	K	183/193 (94%)	0.44	12 (6%)	24	26	18, 32, 65, 90	0
1	L	183/193 (94%)	0.22	10 (5%)	30	32	16, 27, 59, 99	0
1	M	183/193 (94%)	0.13	12 (6%)	24	26	15, 24, 54, 97	0
1	N	183/193 (94%)	0.21	12 (6%)	24	26	13, 26, 58, 100	0
All	All	2562/2702 (94%)	0.29	172 (6%)	24	26	10, 28, 66, 100	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	16	SER	6.3
1	L	16	SER	6.3
1	F	14	GLU	6.2
1	B	14	GLU	5.9
1	G	193	ASN	5.9
1	H	11	SER	5.9
1	H	13	GLY	5.8
1	M	17	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	11	SER	5.7
1	L	193	ASN	5.6
1	J	11	SER	5.6
1	B	17	PHE	5.6
1	L	192	ARG	5.5
1	E	14	GLU	5.3
1	M	14	GLU	5.3
1	F	11	SER	5.3
1	J	193	ASN	5.3
1	K	193	ASN	5.2
1	E	17	PHE	5.2
1	I	13	GLY	5.2
1	A	14	GLU	5.2
1	D	17	PHE	5.1
1	B	193	ASN	5.1
1	H	17	PHE	5.1
1	A	192	ARG	5.0
1	J	17	PHE	5.0
1	L	11	SER	4.9
1	C	13	GLY	4.9
1	F	192	ARG	4.9
1	A	193	ASN	4.9
1	H	192	ARG	4.8
1	C	193	ASN	4.8
1	N	193	ASN	4.8
1	N	17	PHE	4.8
1	L	17	PHE	4.8
1	K	11	SER	4.7
1	G	11	SER	4.6
1	M	193	ASN	4.6
1	N	11	SER	4.5
1	I	14	GLU	4.5
1	J	13	GLY	4.4
1	F	13	GLY	4.4
1	M	16	SER	4.4
1	D	14	GLU	4.4
1	F	17	PHE	4.4
1	I	193	ASN	4.4
1	M	11	SER	4.4
1	H	193	ASN	4.4
1	A	13	GLY	4.3
1	E	11	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	14	GLU	4.3
1	J	14	GLU	4.2
1	I	11	SER	4.2
1	K	17	PHE	4.2
1	G	14	GLU	4.2
1	C	12	ARG	4.2
1	L	13	GLY	4.2
1	G	16	SER	4.2
1	I	192	ARG	4.1
1	G	17	PHE	4.1
1	E	13	GLY	4.1
1	A	191	HIS	4.0
1	D	11	SER	4.0
1	G	13	GLY	4.0
1	G	192	ARG	4.0
1	E	190	THR	4.0
1	F	193	ASN	4.0
1	H	12	ARG	3.9
1	N	13	GLY	3.9
1	F	16	SER	3.9
1	B	15	ARG	3.9
1	A	190	THR	3.9
1	H	14	GLU	3.8
1	J	153	MET	3.8
1	F	191	HIS	3.8
1	A	17	PHE	3.8
1	D	15	ARG	3.8
1	B	13	GLY	3.8
1	E	193	ASN	3.7
1	A	15	ARG	3.7
1	M	192	ARG	3.7
1	G	15	ARG	3.7
1	M	13	GLY	3.6
1	B	11	SER	3.5
1	B	191	HIS	3.5
1	E	12	ARG	3.5
1	N	192	ARG	3.5
1	H	16	SER	3.4
1	C	14	GLU	3.4
1	K	13	GLY	3.4
1	A	11	SER	3.4
1	N	14	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	17	PHE	3.4
1	I	12	ARG	3.4
1	K	15	ARG	3.4
1	K	16	SER	3.4
1	C	192	ARG	3.3
1	E	15	ARG	3.3
1	N	12	ARG	3.3
1	D	16	SER	3.3
1	J	12	ARG	3.3
1	G	191	HIS	3.3
1	N	16	SER	3.3
1	E	191	HIS	3.3
1	D	191	HIS	3.2
1	K	192	ARG	3.2
1	A	16	SER	3.1
1	F	12	ARG	3.1
1	M	12	ARG	3.1
1	D	193	ASN	3.1
1	G	12	ARG	3.1
1	D	13	GLY	3.0
1	J	191	HIS	3.0
1	C	15	ARG	2.9
1	F	15	ARG	2.9
1	J	192	ARG	2.9
1	M	15	ARG	2.9
1	A	12	ARG	2.9
1	I	17	PHE	2.9
1	B	16	SER	2.8
1	B	192	ARG	2.8
1	B	12	ARG	2.8
1	J	15	ARG	2.8
1	L	12	ARG	2.8
1	L	191	HIS	2.8
1	I	16	SER	2.7
1	C	191	HIS	2.7
1	E	25	LYS	2.7
1	C	153	MET	2.7
1	H	191	HIS	2.7
1	E	192	ARG	2.6
1	G	118	ARG	2.6
1	D	192	ARG	2.6
1	D	118	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	148	ARG	2.5
1	I	15	ARG	2.5
1	I	191	HIS	2.5
1	E	16	SER	2.5
1	H	15	ARG	2.5
1	F	127	GLY	2.5
1	D	25	LYS	2.4
1	M	140	ARG	2.4
1	J	16	SER	2.3
1	D	153	MET	2.3
1	D	12	ARG	2.3
1	K	191	HIS	2.3
1	C	118	ARG	2.3
1	C	108	LYS	2.3
1	K	14	GLU	2.2
1	N	190	THR	2.2
1	J	84	LYS	2.2
1	J	108	LYS	2.2
1	C	140	ARG	2.2
1	M	191	HIS	2.2
1	K	20	TYR	2.2
1	D	19	ILE	2.2
1	B	25	LYS	2.2
1	I	25	LYS	2.2
1	K	108	LYS	2.2
1	D	148	ARG	2.1
1	N	148	ARG	2.1
1	I	140	ARG	2.1
1	N	84	LYS	2.1
1	N	181	GLU	2.1
1	C	60	TYR	2.1
1	B	181	GLU	2.1
1	L	15	ARG	2.1
1	K	25	LYS	2.0
1	E	56	GLU	2.0
1	M	190	THR	2.0
1	J	155	LEU	2.0
1	J	25	LYS	2.0

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

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

6.3 Carbohydrates [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.