



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2017 – 01:19 AM EDT

PDB ID : 1PD5  
Title : Crystal structure of E.coli chloramphenicol acetyltransferase type I at 2.5 Angstrom resolution  
Authors : Roidis, A.; Kokkinidis, M.  
Deposited on : unknown  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

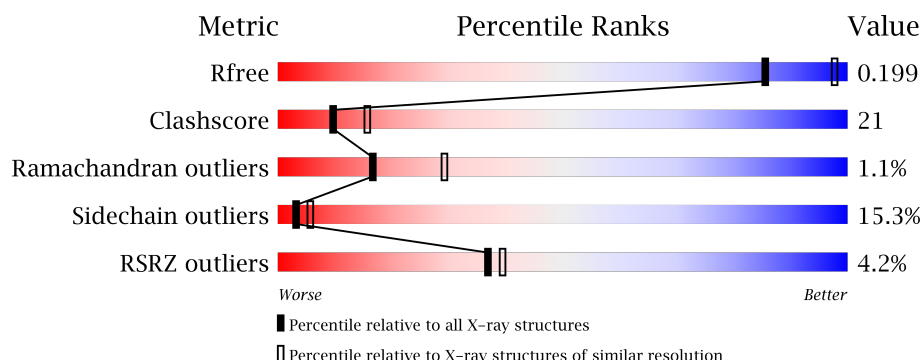
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	219	
1	B	219	
1	C	219	
1	D	219	
1	E	219	

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Mol	Chain	Length	Quality of chain
1	F	219	<div><div>2%</div><div><div></div><div>48%</div><div>38%</div><div>10%</div><div></div></div><div></div></div>
1	G	219	<div><div>2%</div><div><div></div><div>51%</div><div>35%</div><div>8%</div><div></div></div><div></div></div>
1	H	219	<div><div>3%</div><div><div></div><div>49%</div><div>40%</div><div>8%</div><div></div></div><div></div></div>
1	I	219	<div><div>%</div><div><div></div><div>44%</div><div>41%</div><div>10%</div><div></div></div><div></div></div>
1	J	219	<div><div>12%</div><div><div></div><div>43%</div><div>36%</div><div>13%</div><div></div></div><div></div></div>
1	K	219	<div><div>11%</div><div><div></div><div>47%</div><div>39%</div><div>10%</div><div></div></div><div></div></div>
1	L	219	<div><div>13%</div><div><div></div><div>41%</div><div>39%</div><div>16%</div><div></div></div><div></div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 21418 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 Chloramphenicol acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	B	216	Total	C	N	O	S	0	0	0
			1789	1162	295	319	13			
1	C	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	D	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	E	215	Total	C	N	O	S	0	0	0
			1785	1160	294	318	13			
1	F	212	Total	C	N	O	S	0	0	0
			1759	1142	289	315	13			
1	G	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	H	216	Total	C	N	O	S	0	0	0
			1785	1159	294	319	13			
1	I	214	Total	C	N	O	S	0	0	0
			1776	1154	292	317	13			
1	J	211	Total	C	N	O	S	0	0	0
			1755	1140	288	314	13			
1	K	212	Total	C	N	O	S	0	0	0
			1763	1147	289	314	13			
1	L	210	Total	C	N	O	S	0	0	0
			1746	1135	286	312	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	22	Total	O	0	0
			22	22		

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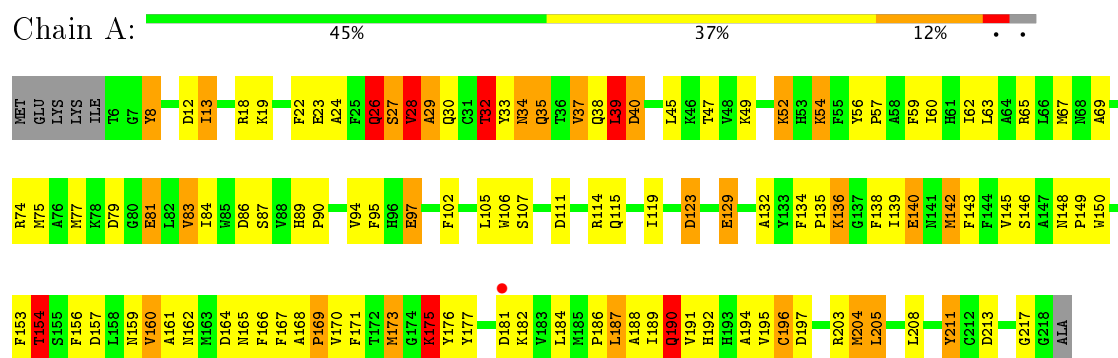
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	19	Total 19	O 19	0	0
2	D	21	Total 21	O 21	0	0
2	E	15	Total 15	O 15	0	0
2	F	16	Total 16	O 16	0	0
2	G	20	Total 20	O 20	0	0
2	H	36	Total 36	O 36	0	0
2	I	17	Total 17	O 17	0	0
2	J	11	Total 11	O 11	0	0
2	K	4	Total 4	O 4	0	0
2	L	8	Total 8	O 8	0	0

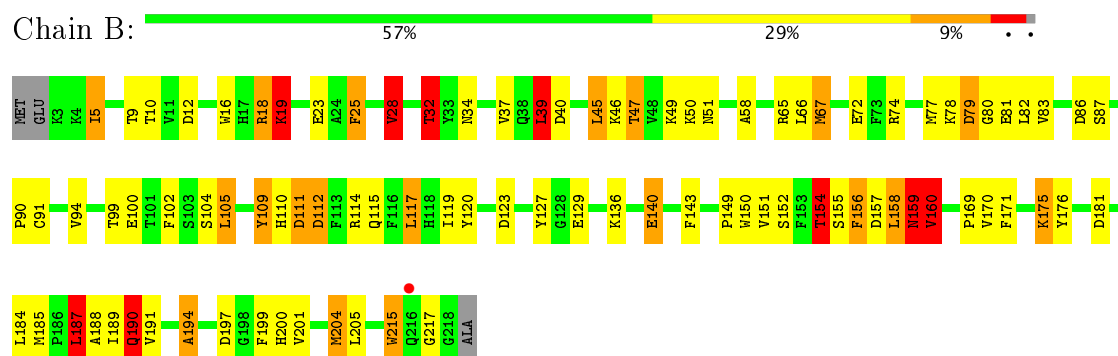
### 3 Residue-property plots

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

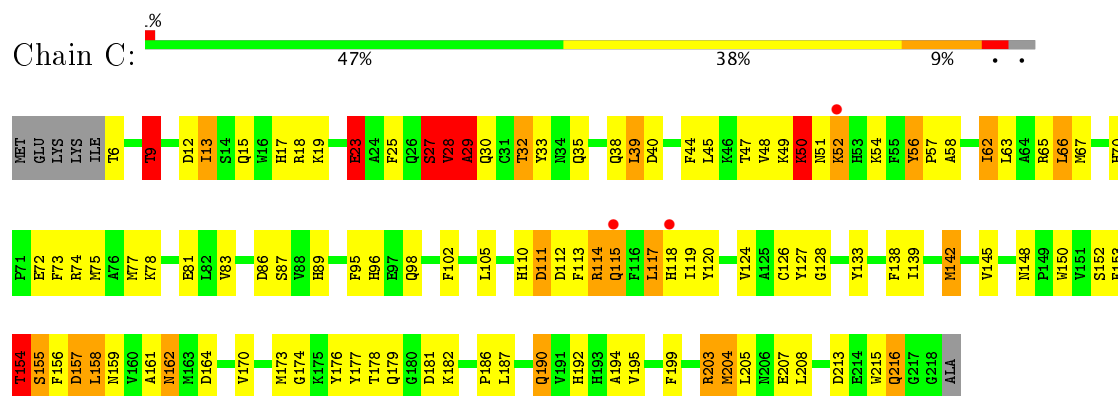
#### • Molecule 1: Chloramphenicol acetyltransferase



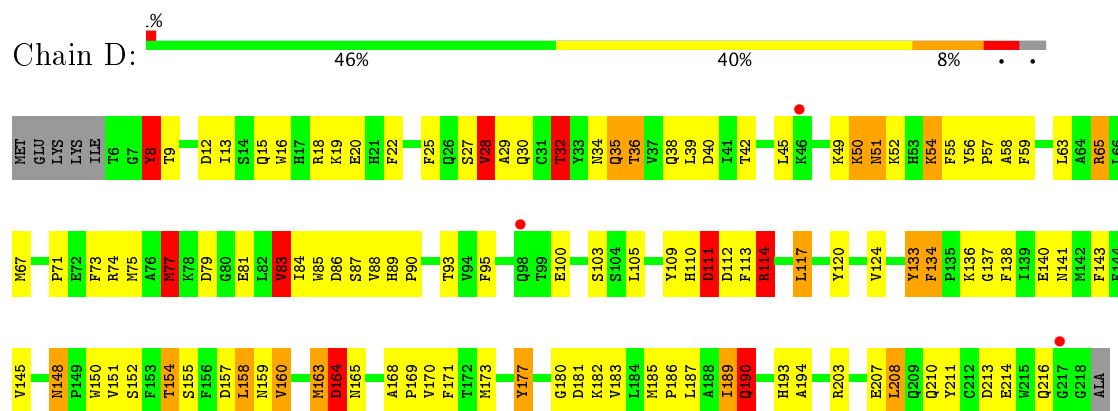
#### • Molecule 1: Chloramphenicol acetyltransferase



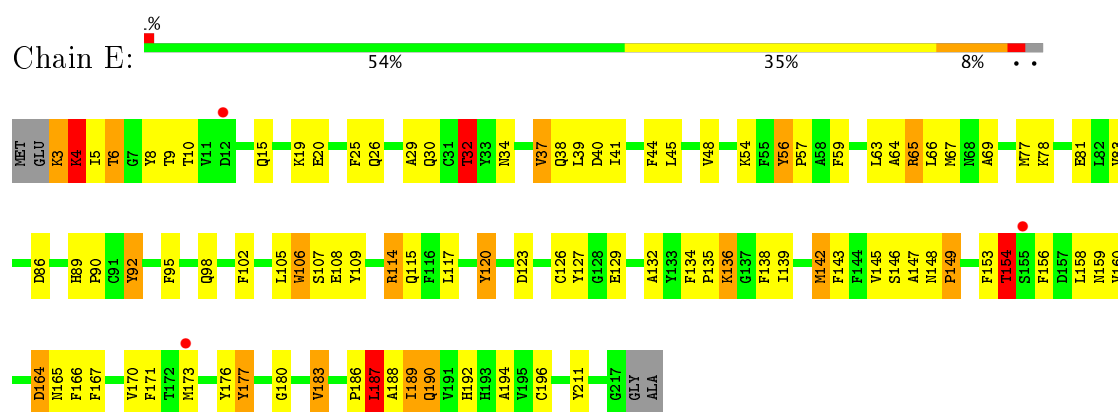
#### • Molecule 1: Chloramphenicol acetyltransferase



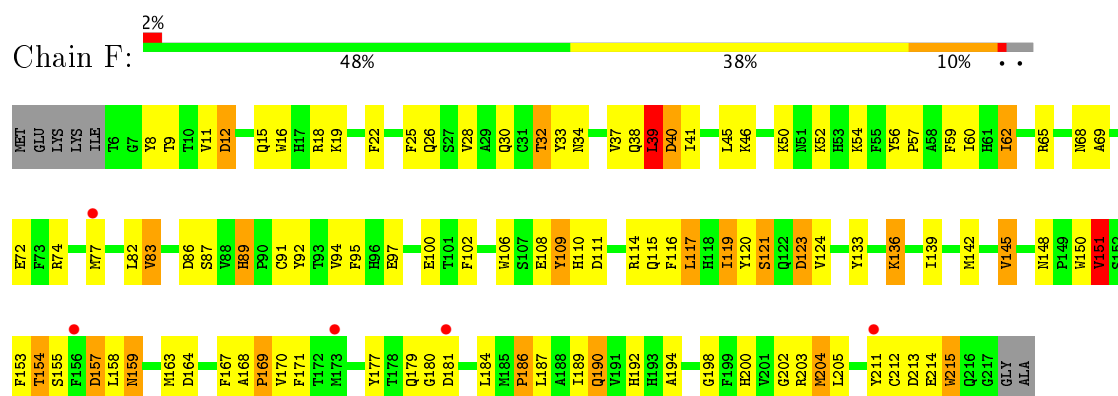
- Molecule 1: Chloramphenicol acetyltransferase



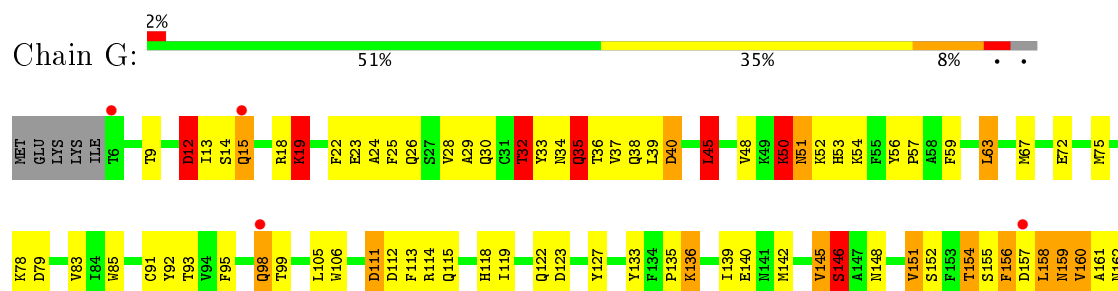
- Molecule 1: Chloramphenicol acetyltransferase



- Molecule 1: Chloramphenicol acetyltransferase

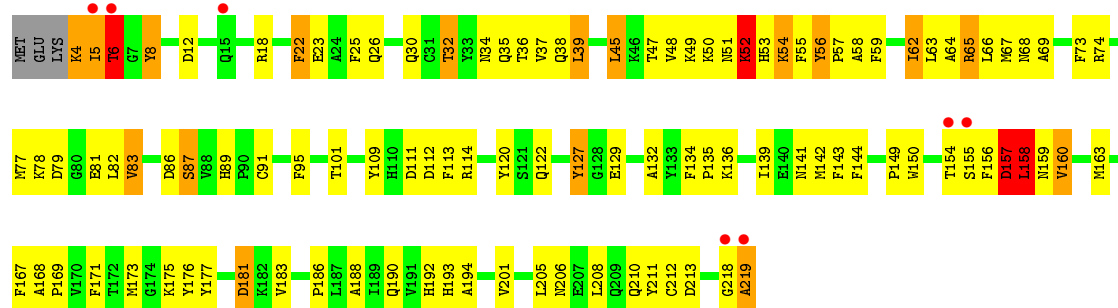


- Molecule 1: Chloramphenicol acetyltransferase

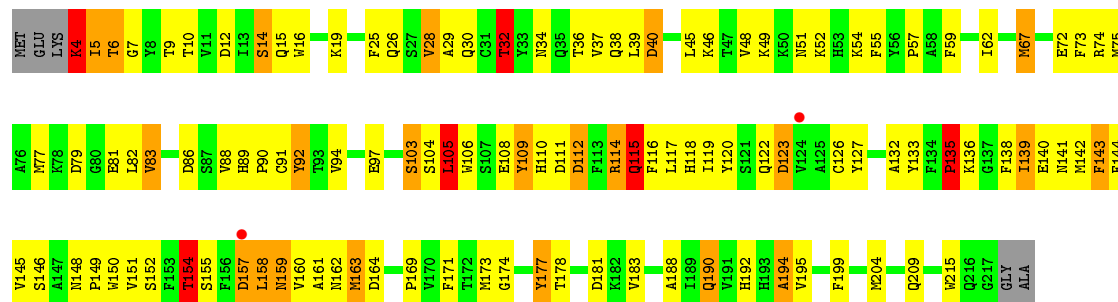
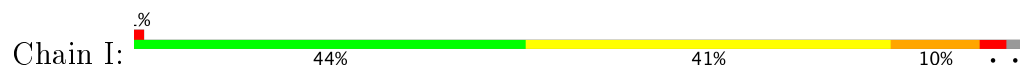




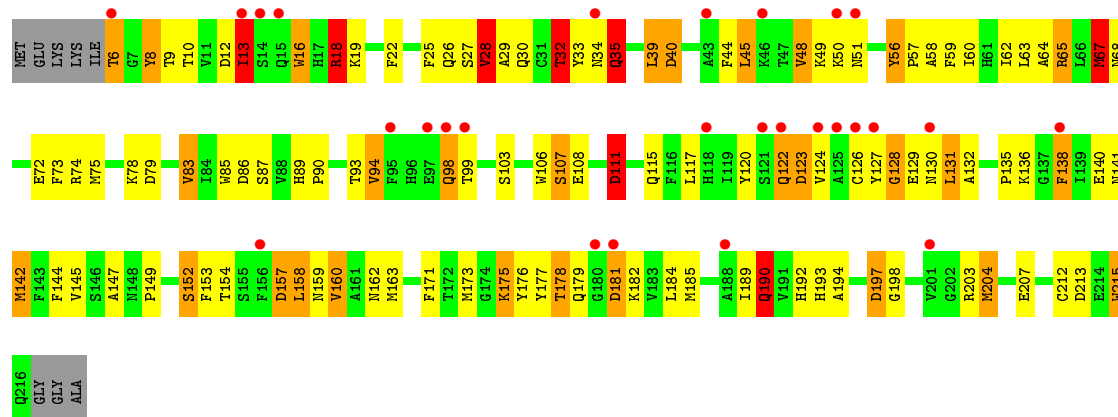
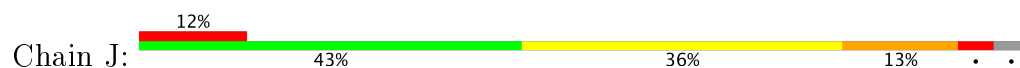
• Molecule 1: Chloramphenicol acetyltransferase



• Molecule 1: Chloramphenicol acetyltransferase



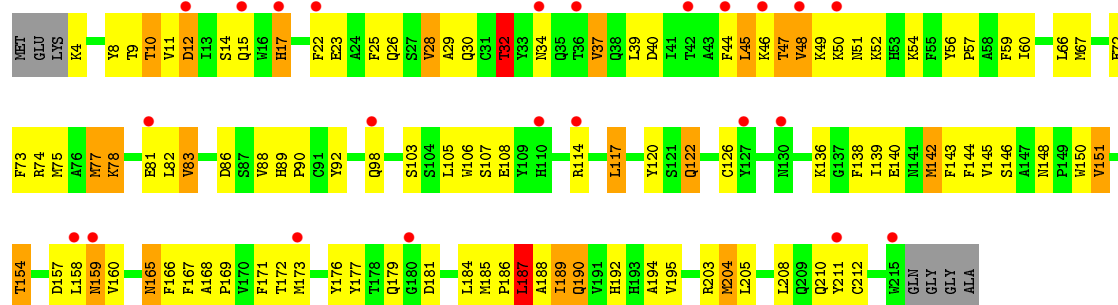
• Molecule 1: Chloramphenicol acetyltransferase



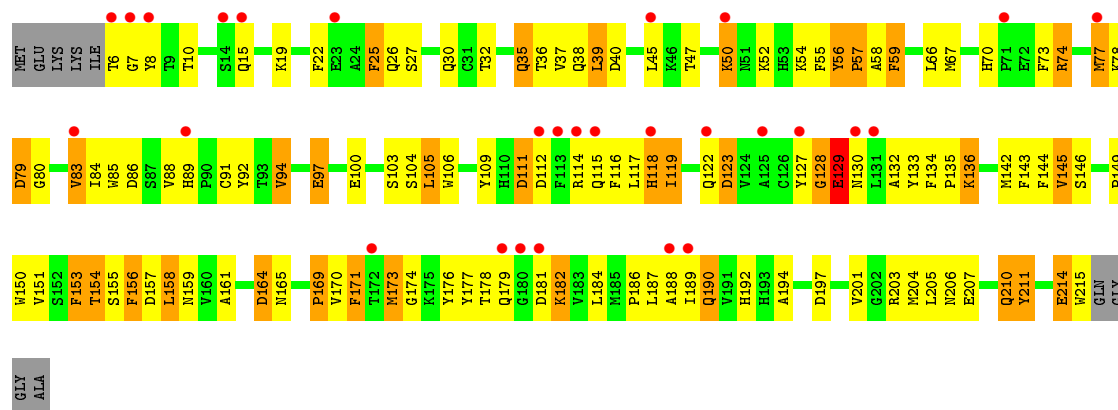
• Molecule 1: Chloramphenicol acetyltransferase







• Molecule 1: Chloramphenicol acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.74Å 129.70Å 117.98Å 90.00° 108.38° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 39.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (10.00-2.50) 98.7 (39.33-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.195 , 0.281 0.207 , 0.199	Depositor DCC
$R_{free}$ test set	5598 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.31 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.2096e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	2.04	58/1822 (3.2%)	1.62	38/2473 (1.5%)
1	B	1.76	22/1848 (1.2%)	1.59	34/2506 (1.4%)
1	C	1.84	35/1822 (1.9%)	1.58	36/2473 (1.5%)
1	D	1.83	38/1822 (2.1%)	1.52	25/2473 (1.0%)
1	E	1.67	20/1844 (1.1%)	1.39	14/2501 (0.6%)
1	F	1.76	26/1818 (1.4%)	1.53	31/2468 (1.3%)
1	G	1.71	18/1822 (1.0%)	1.53	30/2473 (1.2%)
1	H	1.85	33/1844 (1.8%)	1.55	30/2502 (1.2%)
1	I	1.85	38/1835 (2.1%)	1.50	23/2490 (0.9%)
1	J	1.57	15/1814 (0.8%)	1.47	26/2463 (1.1%)
1	K	1.55	14/1822 (0.8%)	1.35	9/2473 (0.4%)
1	L	1.67	21/1805 (1.2%)	1.41	19/2451 (0.8%)
All	All	1.76	338/21918 (1.5%)	1.51	315/29746 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	G	0	1
1	I	0	1
1	J	0	3
1	K	0	1
1	L	0	1
All	All	0	10

All (338) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	TRP	CE3-CZ3	10.79	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	PHE	CE2-CZ	10.43	1.57	1.37
1	A	87	SER	CB-OG	-10.09	1.29	1.42
1	I	127	TYR	CD1-CE1	10.07	1.54	1.39
1	I	140	GLU	CD-OE1	9.99	1.36	1.25
1	E	146	SER	CB-OG	9.66	1.54	1.42
1	G	151	VAL	CB-CG2	9.36	1.72	1.52
1	I	28	VAL	CB-CG2	9.03	1.71	1.52
1	I	183	VAL	CB-CG1	9.00	1.71	1.52
1	F	171	PHE	CE2-CZ	8.93	1.54	1.37
1	A	28	VAL	CB-CG1	8.76	1.71	1.52
1	F	145	VAL	CB-CG1	8.62	1.71	1.52
1	K	151	VAL	CB-CG2	8.49	1.70	1.52
1	C	95	PHE	CE1-CZ	8.35	1.53	1.37
1	C	28	VAL	CB-CG2	8.33	1.70	1.52
1	F	116	PHE	CE2-CZ	8.24	1.53	1.37
1	I	144	PHE	CD1-CE1	8.23	1.55	1.39
1	A	35	GLN	CB-CG	-8.21	1.30	1.52
1	J	94	VAL	CB-CG2	8.21	1.70	1.52
1	A	177	TYR	CE1-CZ	8.19	1.49	1.38
1	J	177	TYR	CD2-CE2	-8.13	1.27	1.39
1	H	69	ALA	CA-CB	8.12	1.69	1.52
1	B	159	ASN	CB-CG	8.07	1.69	1.51
1	F	211	TYR	CD2-CE2	8.05	1.51	1.39
1	D	58	ALA	CA-CB	8.04	1.69	1.52
1	A	33	TYR	CD1-CE1	8.03	1.51	1.39
1	D	35	GLN	CB-CG	-7.99	1.30	1.52
1	A	162	ASN	CB-CG	7.94	1.69	1.51
1	A	129	GLU	CD-OE1	7.81	1.34	1.25
1	J	198	GLY	C-O	7.71	1.35	1.23
1	E	160	VAL	CB-CG1	-7.67	1.36	1.52
1	L	143	PHE	CE1-CZ	7.66	1.51	1.37
1	A	24	ALA	C-O	7.63	1.37	1.23
1	A	86	ASP	CB-CG	7.62	1.67	1.51
1	A	156	PHE	CE2-CZ	7.62	1.51	1.37
1	F	211	TYR	CD1-CE1	7.61	1.50	1.39
1	I	109	TYR	CB-CG	-7.59	1.40	1.51
1	C	162	ASN	CB-CG	-7.49	1.33	1.51
1	F	170	VAL	CB-CG2	7.47	1.68	1.52
1	C	98	GLN	CG-CD	7.45	1.68	1.51
1	C	195	VAL	CB-CG1	7.44	1.68	1.52
1	J	160	VAL	CB-CG2	7.42	1.68	1.52
1	B	160	VAL	CB-CG1	-7.39	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	157	ASP	CB-CG	-7.38	1.36	1.51
1	B	28	VAL	CB-CG2	7.38	1.68	1.52
1	I	111	ASP	CB-CG	7.38	1.67	1.51
1	F	150	TRP	CB-CG	-7.26	1.37	1.50
1	C	87	SER	CB-OG	-7.22	1.32	1.42
1	B	102	PHE	CE2-CZ	7.17	1.50	1.37
1	E	166	PHE	CD1-CE1	7.16	1.53	1.39
1	A	69	ALA	CA-CB	7.14	1.67	1.52
1	A	81	GLU	CG-CD	7.14	1.62	1.51
1	K	211	TYR	CD1-CE1	7.13	1.50	1.39
1	I	162	ASN	C-O	-7.12	1.09	1.23
1	H	81	GLU	CD-OE2	7.11	1.33	1.25
1	A	195	VAL	CB-CG1	7.11	1.67	1.52
1	I	152	SER	CB-OG	7.10	1.51	1.42
1	B	199	PHE	CE1-CZ	7.08	1.50	1.37
1	F	102	PHE	CD1-CE1	7.08	1.53	1.39
1	G	176	TYR	CD1-CE1	7.08	1.50	1.39
1	I	55	PHE	CE2-CZ	7.07	1.50	1.37
1	F	167	PHE	CG-CD2	7.06	1.49	1.38
1	A	8	TYR	CD1-CE1	-7.04	1.28	1.39
1	A	95	PHE	CE2-CZ	7.02	1.50	1.37
1	A	161	ALA	CA-CB	-6.97	1.37	1.52
1	C	156	PHE	CE2-CZ	6.96	1.50	1.37
1	I	116	PHE	CE1-CZ	6.92	1.50	1.37
1	H	134	PHE	CD1-CE1	6.91	1.53	1.39
1	L	174	GLY	C-O	6.90	1.34	1.23
1	K	98	GLN	CG-CD	6.89	1.66	1.51
1	I	103	SER	C-O	6.88	1.36	1.23
1	L	176	TYR	CG-CD1	6.86	1.48	1.39
1	K	144	PHE	CD1-CE1	6.85	1.52	1.39
1	I	106	TRP	CB-CG	6.84	1.62	1.50
1	I	199	PHE	CE1-CZ	6.80	1.50	1.37
1	H	22	PHE	CE1-CZ	6.79	1.50	1.37
1	I	6	THR	CB-CG2	6.79	1.74	1.52
1	H	143	PHE	CE2-CZ	6.78	1.50	1.37
1	D	190	GLN	CB-CG	-6.75	1.34	1.52
1	G	159	ASN	CB-CG	6.74	1.66	1.51
1	B	215	TRP	CG-CD1	6.71	1.46	1.36
1	L	171	PHE	CE2-CZ	6.71	1.50	1.37
1	C	176	TYR	CG-CD1	6.71	1.47	1.39
1	E	143	PHE	CD2-CE2	6.70	1.52	1.39
1	E	37	VAL	CB-CG1	-6.65	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	LYS	CE-NZ	6.64	1.65	1.49
1	B	28	VAL	CB-CG1	6.64	1.66	1.52
1	L	177	TYR	CE1-CZ	6.62	1.47	1.38
1	I	215	TRP	CB-CG	-6.60	1.38	1.50
1	H	176	TYR	CG-CD1	6.60	1.47	1.39
1	E	102	PHE	CE2-CZ	6.53	1.49	1.37
1	B	170	VAL	CB-CG2	6.52	1.66	1.52
1	C	15	GLN	CG-CD	6.51	1.66	1.51
1	H	78	LYS	CE-NZ	6.51	1.65	1.49
1	G	181	ASP	CB-CG	6.51	1.65	1.51
1	D	95	PHE	CG-CD1	6.47	1.48	1.38
1	L	116	PHE	CE1-CZ	6.47	1.49	1.37
1	E	143	PHE	CD1-CE1	6.47	1.52	1.39
1	I	72	GLU	CD-OE2	6.46	1.32	1.25
1	A	54	LYS	CD-CE	6.45	1.67	1.51
1	D	177	TYR	CD1-CE1	6.40	1.49	1.39
1	F	95	PHE	CE1-CZ	6.37	1.49	1.37
1	C	33	TYR	CB-CG	-6.36	1.42	1.51
1	C	81	GLU	CD-OE2	6.36	1.32	1.25
1	G	176	TYR	CE1-CZ	6.34	1.46	1.38
1	E	196	CYS	CB-SG	-6.31	1.71	1.82
1	A	150	TRP	CE3-CZ3	6.28	1.49	1.38
1	F	69	ALA	CA-CB	6.27	1.65	1.52
1	E	56	TYR	CG-CD1	-6.27	1.31	1.39
1	A	74	ARG	CB-CG	6.26	1.69	1.52
1	H	183	VAL	CB-CG2	6.26	1.66	1.52
1	H	55	PHE	CE1-CZ	6.26	1.49	1.37
1	I	37	VAL	CB-CG2	-6.25	1.39	1.52
1	D	54	LYS	CD-CE	6.24	1.66	1.51
1	L	153	PHE	CE1-CZ	6.23	1.49	1.37
1	H	167	PHE	CB-CG	6.23	1.61	1.51
1	B	176	TYR	CG-CD1	6.22	1.47	1.39
1	I	55	PHE	CD1-CE1	6.22	1.51	1.39
1	C	176	TYR	CD1-CE1	6.22	1.48	1.39
1	G	146	SER	CB-OG	-6.19	1.34	1.42
1	B	16	TRP	CG-CD1	6.19	1.45	1.36
1	J	190	GLN	CB-CG	6.17	1.69	1.52
1	H	206	ASN	C-O	6.16	1.35	1.23
1	H	160	VAL	CA-CB	6.15	1.67	1.54
1	F	151	VAL	CB-CG2	-6.14	1.40	1.52
1	A	166	PHE	CE1-CZ	6.13	1.49	1.37
1	A	153	PHE	CD1-CE1	6.13	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	126	CYS	CB-SG	-6.12	1.71	1.82
1	B	67	MET	CB-CG	6.11	1.70	1.51
1	A	22	PHE	CE2-CZ	6.10	1.49	1.37
1	D	211	TYR	CB-CG	-6.10	1.42	1.51
1	H	157	ASP	CA-CB	-6.10	1.40	1.53
1	C	23	GLU	CG-CD	6.09	1.61	1.51
1	C	27	SER	C-O	6.09	1.34	1.23
1	D	22	PHE	CE1-CZ	6.09	1.49	1.37
1	I	92	TYR	CE2-CZ	6.08	1.46	1.38
1	D	138	PHE	CE2-CZ	6.07	1.48	1.37
1	K	177	TYR	CE2-CZ	6.07	1.46	1.38
1	L	97	GLU	CD-OE1	6.07	1.32	1.25
1	D	8	TYR	CG-CD1	6.07	1.47	1.39
1	J	140	GLU	CD-OE2	6.05	1.32	1.25
1	L	153	PHE	CD1-CE1	6.02	1.51	1.39
1	G	24	ALA	CA-CB	-6.02	1.39	1.52
1	K	159	ASN	CB-CG	6.01	1.64	1.51
1	C	153	PHE	CE1-CZ	5.99	1.48	1.37
1	A	95	PHE	CE1-CZ	5.99	1.48	1.37
1	C	127	TYR	CD1-CE1	5.98	1.48	1.39
1	I	177	TYR	CD1-CE1	5.97	1.48	1.39
1	A	26	GLN	CB-CG	-5.96	1.36	1.52
1	I	159	ASN	CB-CG	5.93	1.64	1.51
1	I	183	VAL	CB-CG2	5.93	1.65	1.52
1	H	64	ALA	CA-CB	-5.92	1.40	1.52
1	B	194	ALA	CA-CB	5.92	1.64	1.52
1	D	134	PHE	CE1-CZ	5.92	1.48	1.37
1	I	4	LYS	CB-CG	5.92	1.68	1.52
1	H	56	TYR	CD2-CE2	5.92	1.48	1.39
1	A	140	GLU	CD-OE1	5.92	1.32	1.25
1	A	169	PRO	CA-C	5.92	1.64	1.52
1	I	4	LYS	N-CA	5.90	1.58	1.46
1	G	171	PHE	CD1-CE1	5.89	1.51	1.39
1	A	134	PHE	CB-CG	5.88	1.61	1.51
1	A	176	TYR	CE2-CZ	5.88	1.46	1.38
1	A	191	VAL	CA-CB	-5.88	1.42	1.54
1	I	114	ARG	CG-CD	5.87	1.66	1.51
1	D	210	GLN	CG-CD	5.86	1.64	1.51
1	D	216	GLN	CG-CD	5.85	1.64	1.51
1	H	176	TYR	CD1-CE1	5.85	1.48	1.39
1	D	111	ASP	CB-CG	-5.85	1.39	1.51
1	B	109	TYR	CD1-CE1	5.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	28	VAL	CB-CG1	5.85	1.65	1.52
1	D	105	LEU	CG-CD1	5.84	1.73	1.51
1	H	144	PHE	C-O	5.82	1.34	1.23
1	B	190	GLN	CB-CG	-5.82	1.36	1.52
1	F	109	TYR	CD2-CE2	-5.81	1.30	1.39
1	E	170	VAL	CB-CG2	5.80	1.65	1.52
1	A	95	PHE	CG-CD2	5.80	1.47	1.38
1	F	22	PHE	CE2-CZ	5.79	1.48	1.37
1	D	177	TYR	CG-CD2	5.78	1.46	1.39
1	B	200	HIS	C-O	-5.78	1.12	1.23
1	G	167	PHE	CG-CD2	5.78	1.47	1.38
1	D	133	TYR	CG-CD1	5.75	1.46	1.39
1	K	189	ILE	CA-CB	5.75	1.68	1.54
1	H	167	PHE	CD1-CE1	5.75	1.50	1.39
1	D	211	TYR	C-O	-5.74	1.12	1.23
1	A	167	PHE	CB-CG	5.73	1.61	1.51
1	H	79	ASP	CB-CG	5.72	1.63	1.51
1	J	16	TRP	CG-CD1	5.72	1.44	1.36
1	C	102	PHE	CD1-CE1	5.71	1.50	1.39
1	C	83	VAL	CB-CG1	-5.71	1.40	1.52
1	D	145	VAL	CB-CG2	-5.70	1.40	1.52
1	I	140	GLU	CG-CD	5.70	1.60	1.51
1	A	59	PHE	CD1-CE1	5.70	1.50	1.39
1	D	114	ARG	CG-CD	5.69	1.66	1.51
1	I	194	ALA	C-O	5.68	1.34	1.23
1	A	95	PHE	CG-CD1	5.66	1.47	1.38
1	I	15	GLN	CB-CG	5.66	1.67	1.52
1	C	127	TYR	CE2-CZ	5.66	1.46	1.38
1	D	170	VAL	CA-CB	-5.62	1.43	1.54
1	H	150	TRP	CE3-CZ3	5.62	1.48	1.38
1	A	196	CYS	CB-SG	-5.62	1.72	1.81
1	I	195	VAL	CB-CG1	5.61	1.64	1.52
1	D	171	PHE	C-O	5.60	1.33	1.23
1	D	109	TYR	CD2-CE2	5.60	1.47	1.39
1	H	219	ALA	N-CA	5.59	1.57	1.46
1	K	12	ASP	CB-CG	5.59	1.63	1.51
1	C	65	ARG	CG-CD	-5.59	1.38	1.51
1	L	176	TYR	CD1-CE1	5.58	1.47	1.39
1	K	98	GLN	CB-CG	5.58	1.67	1.52
1	H	55	PHE	CD2-CE2	5.57	1.50	1.39
1	A	65	ARG	NE-CZ	5.56	1.40	1.33
1	B	127	TYR	CZ-OH	5.56	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	48	VAL	CB-CG2	-5.56	1.41	1.52
1	B	58	ALA	CA-CB	5.55	1.64	1.52
1	L	94	VAL	CA-CB	5.55	1.66	1.54
1	G	171	PHE	CE2-CZ	5.55	1.47	1.37
1	I	4	LYS	CG-CD	5.55	1.71	1.52
1	D	183	VAL	CB-CG2	5.54	1.64	1.52
1	F	8	TYR	CD1-CE1	-5.53	1.31	1.39
1	H	74	ARG	CZ-NH1	5.53	1.40	1.33
1	F	170	VAL	C-O	5.53	1.33	1.23
1	G	162	ASN	CB-CG	5.52	1.63	1.51
1	B	140	GLU	CG-CD	5.52	1.60	1.51
1	E	102	PHE	CD1-CE1	5.52	1.50	1.39
1	G	156	PHE	CE1-CZ	-5.51	1.26	1.37
1	I	104	SER	CB-OG	-5.49	1.35	1.42
1	L	55	PHE	CB-CG	-5.49	1.42	1.51
1	K	81	GLU	CG-CD	5.48	1.60	1.51
1	F	95	PHE	CE2-CZ	5.48	1.47	1.37
1	I	133	TYR	CB-CG	-5.47	1.43	1.51
1	A	156	PHE	CD1-CE1	5.46	1.50	1.39
1	G	95	PHE	C-O	-5.46	1.12	1.23
1	I	88	VAL	CB-CG2	-5.46	1.41	1.52
1	A	143	PHE	CD2-CE2	-5.45	1.28	1.39
1	H	186	PRO	C-O	5.45	1.34	1.23
1	A	23	GLU	CD-OE2	5.44	1.31	1.25
1	C	58	ALA	CA-CB	5.44	1.63	1.52
1	G	28	VAL	CB-CG1	5.44	1.64	1.52
1	E	92	TYR	CD2-CE2	5.44	1.47	1.39
1	J	28	VAL	CB-CG2	5.43	1.64	1.52
1	E	106	TRP	CE3-CZ3	5.42	1.47	1.38
1	A	211	TYR	CG-CD1	5.42	1.46	1.39
1	J	74	ARG	CB-CG	5.39	1.67	1.52
1	B	25	PHE	CE2-CZ	-5.39	1.27	1.37
1	D	88	VAL	CA-CB	-5.39	1.43	1.54
1	D	133	TYR	CE1-CZ	5.39	1.45	1.38
1	K	28	VAL	CB-CG2	5.39	1.64	1.52
1	A	134	PHE	CD1-CE1	5.37	1.50	1.39
1	C	138	PHE	CD1-CE1	5.35	1.50	1.39
1	L	156	PHE	CD2-CE2	-5.35	1.28	1.39
1	H	109	TYR	CD1-CE1	-5.35	1.31	1.39
1	A	59	PHE	CE2-CZ	5.35	1.47	1.37
1	H	68	ASN	CB-CG	5.35	1.63	1.51
1	H	95	PHE	CE2-CZ	5.35	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	84	ILE	CB-CG2	5.34	1.69	1.52
1	I	48	VAL	CB-CG1	5.34	1.64	1.52
1	L	176	TYR	CE1-CZ	5.34	1.45	1.38
1	E	176	TYR	CD1-CE1	5.33	1.47	1.39
1	C	102	PHE	CE2-CZ	5.33	1.47	1.37
1	A	160	VAL	CB-CG2	-5.32	1.41	1.52
1	C	95	PHE	CG-CD1	5.31	1.46	1.38
1	L	145	VAL	CB-CG2	-5.29	1.41	1.52
1	C	95	PHE	CG-CD2	5.29	1.46	1.38
1	I	55	PHE	CG-CD2	5.29	1.46	1.38
1	C	75	MET	C-O	5.27	1.33	1.23
1	D	100	GLU	CD-OE2	5.27	1.31	1.25
1	I	115	GLN	CG-CD	5.26	1.63	1.51
1	A	33	TYR	CE2-CZ	5.25	1.45	1.38
1	F	28	VAL	CB-CG2	5.25	1.63	1.52
1	A	54	LYS	CG-CD	5.24	1.70	1.52
1	C	177	TYR	CG-CD2	5.24	1.46	1.39
1	B	156	PHE	CD2-CE2	5.24	1.49	1.39
1	J	144	PHE	CE2-CZ	5.24	1.47	1.37
1	A	138	PHE	CD1-CE1	5.24	1.49	1.39
1	G	152	SER	CA-CB	5.23	1.60	1.52
1	H	127	TYR	CD1-CE1	5.23	1.47	1.39
1	I	90	PRO	CG-CD	5.22	1.67	1.50
1	F	154	THR	N-CA	-5.22	1.35	1.46
1	C	44	PHE	CE2-CZ	-5.22	1.27	1.37
1	K	144	PHE	CD2-CE2	5.21	1.49	1.39
1	C	133	TYR	CE2-CZ	5.20	1.45	1.38
1	H	56	TYR	CD1-CE1	5.20	1.47	1.39
1	D	143	PHE	CE2-CZ	5.20	1.47	1.37
1	A	34	ASN	CG-ND2	5.19	1.45	1.32
1	G	33	TYR	CG-CD1	5.19	1.45	1.39
1	A	29	ALA	N-CA	-5.19	1.35	1.46
1	L	133	TYR	CE2-CZ	5.19	1.45	1.38
1	A	175	LYS	CB-CG	5.18	1.66	1.52
1	E	69	ALA	CA-CB	5.18	1.63	1.52
1	A	81	GLU	CD-OE2	5.17	1.31	1.25
1	D	55	PHE	CE1-CZ	5.17	1.47	1.37
1	F	33	TYR	C-O	5.16	1.33	1.23
1	A	132	ALA	CA-CB	5.16	1.63	1.52
1	G	176	TYR	CG-CD1	5.16	1.45	1.39
1	J	8	TYR	CE2-CZ	5.15	1.45	1.38
1	D	95	PHE	CE2-CZ	5.15	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	108	GLU	CD-OE2	5.15	1.31	1.25
1	L	143	PHE	CG-CD1	5.15	1.46	1.38
1	D	124	VAL	CB-CG1	5.14	1.63	1.52
1	L	25	PHE	CE1-CZ	5.14	1.47	1.37
1	L	59	PHE	CD1-CE1	5.14	1.49	1.39
1	C	161	ALA	CA-CB	-5.14	1.41	1.52
1	K	23	GLU	CD-OE2	5.13	1.31	1.25
1	E	149	PRO	CA-C	-5.12	1.42	1.52
1	D	83	VAL	CA-CB	-5.12	1.44	1.54
1	E	180	GLY	C-O	5.12	1.31	1.23
1	C	170	VAL	C-O	5.11	1.33	1.23
1	D	211	TYR	CZ-OH	-5.11	1.29	1.37
1	C	56	TYR	CB-CG	5.10	1.59	1.51
1	F	109	TYR	CD1-CE1	-5.10	1.31	1.39
1	B	46	LYS	CB-CG	5.10	1.66	1.52
1	A	47	THR	C-O	5.09	1.33	1.23
1	J	35	GLN	C-O	5.08	1.33	1.23
1	F	167	PHE	CE1-CZ	5.08	1.47	1.37
1	D	49	LYS	CE-NZ	5.08	1.61	1.49
1	E	177	TYR	CE1-CZ	5.08	1.45	1.38
1	A	102	PHE	CD2-CE2	-5.08	1.29	1.39
1	L	35	GLN	CB-CG	-5.07	1.38	1.52
1	A	134	PHE	CE1-CZ	5.07	1.47	1.37
1	E	95	PHE	CG-CD2	5.07	1.46	1.38
1	D	88	VAL	CB-CG1	5.06	1.63	1.52
1	G	196	CYS	CB-SG	-5.06	1.73	1.81
1	D	28	VAL	CB-CG2	5.06	1.63	1.52
1	H	167	PHE	CE2-CZ	5.06	1.47	1.37
1	J	33	TYR	CE2-CZ	5.05	1.45	1.38
1	H	171	PHE	CE2-CZ	5.05	1.47	1.37
1	A	28	VAL	CB-CG2	5.04	1.63	1.52
1	F	74	ARG	CZ-NH1	5.04	1.39	1.33
1	F	159	ASN	CB-CG	5.04	1.62	1.51
1	A	52	LYS	CD-CE	5.04	1.63	1.51
1	F	16	TRP	CB-CG	5.04	1.59	1.50
1	D	151	VAL	CA-CB	5.03	1.65	1.54
1	A	23	GLU	CD-OE1	5.03	1.31	1.25
1	L	143	PHE	CG-CD2	5.01	1.46	1.38
1	H	62	ILE	CA-C	5.01	1.66	1.52
1	A	167	PHE	CD2-CE2	5.00	1.49	1.39
1	B	72	GLU	CD-OE2	5.00	1.31	1.25
1	J	13	ILE	CA-CB	5.00	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	98	GLN	CB-CG	5.00	1.66	1.52

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	111	ASP	CB-CG-OD2	13.02	130.02	118.30
1	A	65	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	C	157	ASP	CB-CG-OD2	11.45	128.60	118.30
1	C	18	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	I	181	ASP	CB-CG-OD2	11.01	128.21	118.30
1	A	197	ASP	CB-CG-OD1	10.86	128.07	118.30
1	B	112	ASP	CB-CG-OD1	10.58	127.82	118.30
1	J	111	ASP	CB-CG-OD1	10.52	127.77	118.30
1	J	40	ASP	CB-CG-OD2	10.32	127.59	118.30
1	B	111	ASP	CB-CG-OD2	10.26	127.53	118.30
1	J	86	ASP	CB-CG-OD2	10.22	127.50	118.30
1	F	40	ASP	CB-CG-OD2	10.10	127.39	118.30
1	B	18	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	D	157	ASP	CB-CG-OD2	9.80	127.12	118.30
1	C	86	ASP	CB-CG-OD2	9.77	127.09	118.30
1	C	18	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	H	86	ASP	CB-CG-OD2	9.56	126.90	118.30
1	J	197	ASP	CB-CG-OD2	9.41	126.77	118.30
1	J	157	ASP	CB-CG-OD1	-9.39	109.85	118.30
1	D	40	ASP	CB-CG-OD2	9.39	126.75	118.30
1	I	67	MET	CG-SD-CE	-9.27	85.37	100.20
1	H	213	ASP	CB-CG-OD2	9.22	126.60	118.30
1	I	163	MET	CG-SD-CE	9.21	114.93	100.20
1	B	111	ASP	CB-CG-OD1	-9.19	110.03	118.30
1	B	123	ASP	CB-CG-OD2	9.17	126.55	118.30
1	F	213	ASP	CB-CG-OD2	9.08	126.47	118.30
1	L	111	ASP	CB-CG-OD2	9.05	126.44	118.30
1	H	5	ILE	C-N-CA	8.99	144.17	121.70
1	G	45	LEU	CB-CG-CD2	8.98	126.27	111.00
1	K	40	ASP	CB-CG-OD2	8.98	126.38	118.30
1	E	86	ASP	CB-CG-OD2	8.96	126.36	118.30
1	A	217	GLY	C-N-CA	-8.92	103.56	122.30
1	K	86	ASP	CB-CG-OD2	8.70	126.13	118.30
1	H	111	ASP	CB-CG-OD1	8.68	126.11	118.30
1	H	39	LEU	CB-CG-CD2	8.68	125.75	111.00
1	L	181	ASP	CB-CG-OD2	8.62	126.06	118.30
1	J	157	ASP	CB-CG-OD2	8.59	126.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	79	ASP	CB-CG-OD2	8.52	125.97	118.30
1	G	111	ASP	CB-CG-OD1	-8.52	110.64	118.30
1	G	157	ASP	CB-CG-OD2	8.43	125.89	118.30
1	A	32	THR	N-CA-CB	-8.42	94.30	110.30
1	B	187	LEU	CB-CG-CD2	8.36	125.22	111.00
1	D	65	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	F	86	ASP	CB-CG-OD2	8.33	125.80	118.30
1	G	181	ASP	CB-CG-OD2	8.27	125.74	118.30
1	F	12	ASP	CB-CG-OD2	8.19	125.67	118.30
1	C	203	ARG	NE-CZ-NH1	-8.11	116.24	120.30
1	G	40	ASP	CB-CG-OD2	8.06	125.56	118.30
1	H	112	ASP	CB-CG-OD1	8.01	125.51	118.30
1	F	181	ASP	CB-CG-OD2	7.97	125.47	118.30
1	H	66	LEU	CB-CG-CD2	-7.95	97.49	111.00
1	H	52	LYS	CA-C-N	-7.94	99.73	117.20
1	F	12	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	H	39	LEU	CA-CB-CG	7.87	133.40	115.30
1	I	164	ASP	CB-CG-OD2	7.85	125.37	118.30
1	G	12	ASP	CB-CG-OD1	7.78	125.30	118.30
1	J	74	ARG	NE-CZ-NH1	-7.71	116.45	120.30
1	H	157	ASP	CB-CG-OD1	-7.67	111.40	118.30
1	H	6	THR	N-CA-C	7.66	131.67	111.00
1	B	28	VAL	N-CA-CB	7.65	128.33	111.50
1	J	157	ASP	CB-CA-C	-7.63	95.14	110.40
1	C	181	ASP	CB-CG-OD2	7.56	125.10	118.30
1	A	18	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	I	79	ASP	CB-CG-OD2	7.55	125.10	118.30
1	D	158	LEU	CB-CG-CD2	-7.51	98.22	111.00
1	J	32	THR	OG1-CB-CG2	-7.50	92.74	110.00
1	F	151	VAL	CG1-CB-CG2	-7.49	98.91	110.90
1	A	12	ASP	CB-CG-OD2	7.46	125.02	118.30
1	I	28	VAL	CG1-CB-CG2	7.46	122.84	110.90
1	J	12	ASP	CB-CG-OD2	7.33	124.90	118.30
1	G	111	ASP	CB-CG-OD2	7.33	124.89	118.30
1	J	128	GLY	N-CA-C	-7.31	94.82	113.10
1	G	32	THR	N-CA-CB	-7.30	96.43	110.30
1	I	28	VAL	CB-CA-C	7.25	125.17	111.40
1	C	157	ASP	CB-CG-OD1	-7.24	111.79	118.30
1	E	154	THR	N-CA-CB	-7.18	96.66	110.30
1	D	181	ASP	CB-CG-OD2	7.17	124.76	118.30
1	H	87	SER	CB-CA-C	-7.17	96.49	110.10
1	J	6	THR	C-N-CA	-7.14	107.30	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	97	GLU	CB-CA-C	-7.08	96.25	110.40
1	H	12	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	111	ASP	CB-CG-OD2	7.05	124.64	118.30
1	D	12	ASP	CB-CG-OD2	7.05	124.64	118.30
1	F	123	ASP	CB-CG-OD2	7.04	124.64	118.30
1	L	164	ASP	CB-CG-OD2	7.03	124.62	118.30
1	C	86	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	A	39	LEU	CB-CG-CD2	6.90	122.73	111.00
1	H	8	TYR	CB-CG-CD2	6.84	125.11	121.00
1	C	87	SER	CB-CA-C	-6.81	97.17	110.10
1	H	6	THR	N-CA-CB	-6.78	97.41	110.30
1	J	67	MET	CG-SD-CE	6.77	111.03	100.20
1	H	83	VAL	N-CA-CB	-6.77	96.61	111.50
1	L	187	LEU	CA-CB-CG	-6.76	99.76	115.30
1	J	65	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	B	40	ASP	CB-CG-OD2	6.75	124.37	118.30
1	A	197	ASP	OD1-CG-OD2	-6.74	110.49	123.30
1	A	49	LYS	CD-CE-NZ	-6.74	96.20	111.70
1	C	213	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	97	GLU	CA-CB-CG	6.73	128.20	113.40
1	G	112	ASP	CB-CG-OD2	6.70	124.33	118.30
1	E	187	LEU	CB-CG-CD2	6.70	122.39	111.00
1	E	40	ASP	CB-CG-OD2	6.69	124.33	118.30
1	I	12	ASP	CB-CG-OD2	6.67	124.30	118.30
1	H	219	ALA	N-CA-CB	6.64	119.39	110.10
1	E	187	LEU	CA-CB-CG	-6.62	100.08	115.30
1	A	181	ASP	CB-CG-OD2	6.61	124.25	118.30
1	J	18	ARG	CG-CD-NE	6.60	125.65	111.80
1	H	5	ILE	CA-C-N	-6.59	102.71	117.20
1	I	40	ASP	CB-CG-OD2	6.57	124.22	118.30
1	A	203	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	39	LEU	CB-CG-CD2	6.56	122.15	111.00
1	F	121	SER	N-CA-CB	6.55	120.33	110.50
1	B	51	ASN	C-N-CA	-6.53	105.38	121.70
1	D	213	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	176	TYR	CB-CG-CD2	-6.51	117.10	121.00
1	B	74	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	E	32	THR	N-CA-CB	-6.49	97.97	110.30
1	G	51	ASN	N-CA-C	-6.46	93.56	111.00
1	L	39	LEU	CA-CB-CG	6.45	130.12	115.30
1	B	181	ASP	CB-CG-OD2	6.44	124.10	118.30
1	D	54	LYS	CD-CE-NZ	6.43	126.48	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	123	ASP	CB-CG-OD2	6.42	124.08	118.30
1	C	32	THR	N-CA-CB	-6.38	98.17	110.30
1	B	105	LEU	CB-CG-CD2	-6.38	100.15	111.00
1	A	213	ASP	CB-CG-OD2	6.37	124.03	118.30
1	G	197	ASP	CB-CG-OD1	6.37	124.03	118.30
1	D	32	THR	N-CA-CB	-6.36	98.21	110.30
1	H	52	LYS	C-N-CA	6.36	137.60	121.70
1	D	51	ASN	C-N-CA	-6.36	105.81	121.70
1	A	217	GLY	O-C-N	-6.34	112.42	123.20
1	F	18	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	86	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	87	SER	CB-CA-C	-6.29	98.15	110.10
1	B	77	MET	CG-SD-CE	-6.29	90.14	100.20
1	G	63	LEU	CB-CG-CD1	6.28	121.68	111.00
1	I	123	ASP	CB-CG-OD2	6.27	123.94	118.30
1	C	12	ASP	CB-CG-OD2	6.26	123.94	118.30
1	K	187	LEU	CA-CB-CG	-6.25	100.92	115.30
1	D	52	LYS	CB-CA-C	6.24	122.89	110.40
1	B	86	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	12	ASP	CB-CG-OD2	6.24	123.91	118.30
1	G	45	LEU	CA-CB-CG	6.23	129.63	115.30
1	D	111	ASP	N-CA-CB	-6.23	99.39	110.60
1	A	205	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	A	79	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	39	LEU	CB-CA-C	-6.22	98.38	110.20
1	G	145	VAL	CB-CA-C	-6.21	99.61	111.40
1	G	146	SER	CB-CA-C	-6.19	98.34	110.10
1	L	187	LEU	CB-CG-CD1	6.19	121.52	111.00
1	I	105	LEU	CB-CG-CD1	-6.17	100.52	111.00
1	F	94	VAL	N-CA-C	-6.16	94.36	111.00
1	F	117	LEU	CB-CG-CD2	6.16	121.47	111.00
1	F	163	MET	CG-SD-CE	-6.16	90.34	100.20
1	D	74	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	75	MET	CG-SD-CE	6.16	110.06	100.20
1	C	154	THR	N-CA-CB	-6.16	98.60	110.30
1	H	114	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	G	19	LYS	CB-CA-C	-6.14	98.11	110.40
1	A	27	SER	CB-CA-C	-6.09	98.52	110.10
1	B	154	THR	CA-CB-CG2	6.09	120.92	112.40
1	C	162	ASN	CB-CA-C	-6.09	98.23	110.40
1	B	19	LYS	CD-CE-NZ	-6.08	97.72	111.70
1	G	196	CYS	CA-CB-SG	-6.07	103.07	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	136	LYS	CB-CA-C	-6.06	98.28	110.40
1	L	169	PRO	N-CD-CG	-6.06	94.11	103.20
1	J	213	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	18	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	F	39	LEU	CB-CG-CD2	6.05	121.29	111.00
1	C	40	ASP	CB-CG-OD2	6.04	123.73	118.30
1	D	77	MET	CG-SD-CE	-6.04	90.54	100.20
1	J	152	SER	N-CA-CB	-6.03	101.45	110.50
1	G	50	LYS	CD-CE-NZ	-6.03	97.83	111.70
1	A	62	ILE	CG1-CB-CG2	-6.03	98.14	111.40
1	A	105	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	I	135	PRO	N-CD-CG	-6.02	94.16	103.20
1	J	131	LEU	CA-CB-CG	6.02	129.15	115.30
1	D	86	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	40	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	74	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	J	79	ASP	CB-CG-OD2	6.01	123.71	118.30
1	J	123	ASP	CB-CG-OD1	6.00	123.70	118.30
1	E	114	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	K	37	VAL	N-CA-C	-5.99	94.84	111.00
1	A	154	THR	N-CA-CB	-5.96	98.98	110.30
1	C	78	LYS	CD-CE-NZ	-5.95	98.01	111.70
1	F	65	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	G	217	GLY	N-CA-C	-5.92	98.30	113.10
1	B	123	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	B	28	VAL	CA-CB-CG2	5.89	119.74	110.90
1	F	158	LEU	CB-CG-CD1	-5.89	100.99	111.00
1	L	123	ASP	CB-CG-OD2	5.88	123.59	118.30
1	J	181	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	187	LEU	CB-CG-CD2	5.85	120.94	111.00
1	F	186	PRO	N-CD-CG	-5.84	94.43	103.20
1	C	83	VAL	CG1-CB-CG2	5.82	120.22	110.90
1	C	158	LEU	CB-CG-CD2	5.82	120.89	111.00
1	K	187	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	175	LYS	CD-CE-NZ	-5.80	98.35	111.70
1	L	203	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	L	74	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	32	THR	N-CA-CB	-5.75	99.37	110.30
1	K	12	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	117	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	74	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	152	SER	N-CA-C	-5.72	95.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	158	LEU	CB-CG-CD2	5.72	120.73	111.00
1	K	208	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	C	178	THR	CA-CB-CG2	-5.72	104.39	112.40
1	D	111	ASP	CB-CA-C	-5.72	98.97	110.40
1	E	123	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	47	THR	OG1-CB-CG2	-5.68	96.93	110.00
1	A	187	LEU	CB-CG-CD1	-5.63	101.44	111.00
1	A	54	LYS	CD-CE-NZ	5.62	124.63	111.70
1	D	51	ASN	O-C-N	-5.62	113.70	122.70
1	G	51	ASN	C-N-CA	-5.61	107.68	121.70
1	B	90	PRO	N-CD-CG	-5.60	94.81	103.20
1	I	143	PHE	N-CA-C	-5.58	95.92	111.00
1	L	176	TYR	CB-CG-CD1	5.58	124.35	121.00
1	C	77	MET	CG-SD-CE	-5.58	91.28	100.20
1	A	37	VAL	CG1-CB-CG2	5.58	119.82	110.90
1	J	178	THR	OG1-CB-CG2	-5.56	97.21	110.00
1	A	65	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
1	C	203	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	L	173	MET	CB-CG-SD	-5.54	95.78	112.40
1	F	94	VAL	CG1-CB-CG2	-5.54	102.04	110.90
1	I	5	ILE	N-CA-C	5.53	125.92	111.00
1	B	136	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	D	49	LYS	CD-CE-NZ	5.50	124.36	111.70
1	G	79	ASP	CB-CG-OD1	5.50	123.25	118.30
1	I	9	THR	OG1-CB-CG2	-5.49	97.37	110.00
1	E	189	ILE	CG1-CB-CG2	-5.49	99.32	111.40
1	B	117	LEU	CA-CB-CG	5.48	127.90	115.30
1	C	127	TYR	CD1-CE1-CZ	-5.48	114.87	119.80
1	A	13	ILE	CG1-CB-CG2	-5.47	99.36	111.40
1	K	32	THR	N-CA-CB	-5.44	99.96	110.30
1	B	28	VAL	CG1-CB-CG2	5.44	119.60	110.90
1	D	79	ASP	CB-CG-OD1	5.43	123.19	118.30
1	H	52	LYS	O-C-N	5.43	131.38	122.70
1	E	211	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	E	183	VAL	CB-CA-C	-5.41	101.12	111.40
1	D	208	LEU	CB-CG-CD2	5.40	120.18	111.00
1	H	65	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	H	143	PHE	N-CA-C	-5.36	96.52	111.00
1	B	117	LEU	CB-CG-CD2	5.35	120.10	111.00
1	I	178	THR	OG1-CB-CG2	-5.35	97.70	110.00
1	G	98	GLN	CA-CB-CG	5.34	125.15	113.40
1	D	160	VAL	CB-CA-C	5.33	121.54	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	89	HIS	CB-CA-C	5.33	121.06	110.40
1	C	27	SER	CB-CA-C	-5.32	99.99	110.10
1	I	74	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	G	178	THR	OG1-CB-CG2	-5.31	97.78	110.00
1	L	211	TYR	CB-CG-CD1	5.31	124.19	121.00
1	D	89	HIS	CB-CA-C	5.31	121.01	110.40
1	F	117	LEU	CA-CB-CG	5.30	127.50	115.30
1	G	158	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	87	SER	CA-CB-OG	-5.29	96.90	111.20
1	J	39	LEU	CA-CB-CG	5.29	127.47	115.30
1	C	111	ASP	N-CA-CB	-5.28	101.10	110.60
1	F	187	LEU	CA-CB-CG	-5.28	103.16	115.30
1	C	118	HIS	N-CA-CB	5.27	120.09	110.60
1	H	77	MET	N-CA-C	-5.27	96.76	111.00
1	I	111	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	111	ASP	OD1-CG-OD2	-5.26	113.30	123.30
1	G	160	VAL	CG1-CB-CG2	5.25	119.30	110.90
1	H	5	ILE	O-C-N	5.25	131.10	122.70
1	B	150	TRP	C-N-CA	-5.25	108.58	121.70
1	D	36	THR	OG1-CB-CG2	-5.25	97.93	110.00
1	I	32	THR	N-CA-CB	-5.23	100.36	110.30
1	G	37	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	L	57	PRO	N-CD-CG	-5.23	95.35	103.20
1	B	154	THR	N-CA-CB	-5.22	100.38	110.30
1	H	218	GLY	C-N-CA	-5.21	108.66	121.70
1	I	16	TRP	CA-CB-CG	5.20	123.58	113.70
1	B	77	MET	CA-CB-CG	-5.20	104.46	113.30
1	G	35	GLN	CA-CB-CG	5.20	124.84	113.40
1	K	208	LEU	CB-CG-CD1	5.20	119.83	111.00
1	D	90	PRO	N-CD-CG	-5.20	95.41	103.20
1	H	181	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	142	MET	CG-SD-CE	5.19	108.50	100.20
1	J	204	MET	CG-SD-CE	-5.19	91.90	100.20
1	F	46	LYS	CD-CE-NZ	-5.18	99.78	111.70
1	A	18	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	E	164	ASP	CB-CG-OD2	5.18	122.96	118.30
1	I	4	LYS	N-CA-C	5.17	124.97	111.00
1	I	154	THR	N-CA-CB	-5.17	100.48	110.30
1	L	211	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	E	63	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	F	91	CYS	CB-CA-C	5.16	120.72	110.40
1	J	86	ASP	CB-CG-OD1	-5.15	113.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	157	ASP	CB-CG-OD1	5.14	122.93	118.30
1	L	40	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	170	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	C	29	ALA	N-CA-C	5.13	124.86	111.00
1	E	65	ARG	N-CA-CB	5.11	119.79	110.60
1	H	86	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	A	190	GLN	C-N-CA	-5.10	108.95	121.70
1	F	83	VAL	N-CA-CB	-5.08	100.31	111.50
1	L	112	ASP	CB-CG-OD1	5.08	122.87	118.30
1	L	118	HIS	N-CA-C	-5.07	97.31	111.00
1	B	45	LEU	CB-CG-CD1	5.07	119.61	111.00
1	C	9	THR	CA-CB-CG2	5.06	119.48	112.40
1	F	123	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	F	18	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	C	66	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	A	123	ASP	CB-CG-OD1	5.04	122.83	118.30
1	J	142	MET	CB-CA-C	-5.03	100.34	110.40
1	D	114	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	187	LEU	CB-CG-CD2	5.02	119.53	111.00
1	C	95	PHE	CB-CA-C	5.02	120.43	110.40
1	B	184	LEU	CA-CB-CG	5.01	126.83	115.30
1	G	105	LEU	CA-CB-CG	5.01	126.83	115.30
1	F	169	PRO	N-CD-CG	-5.01	95.68	103.20
1	H	18	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	65	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	F	62	ILE	CG1-CB-CG2	5.01	122.41	111.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	ALA	Mainchain
1	C	28	VAL	Peptide
1	C	52	LYS	Peptide
1	G	217	GLY	Peptide
1	I	4	LYS	Peptide
1	J	127	TYR	Peptide
1	J	13	ILE	Peptide
1	J	153	PHE	Peptide
1	K	50	LYS	Peptide
1	L	128	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1647	72	0
1	B	1789	0	1684	58	0
1	C	1763	0	1647	83	0
1	D	1763	0	1647	79	0
1	E	1785	0	1681	61	0
1	F	1759	0	1644	56	0
1	G	1763	0	1647	83	0
1	H	1785	0	1675	72	0
1	I	1776	0	1668	104	0
1	J	1755	0	1641	115	0
1	K	1763	0	1657	92	0
1	L	1746	0	1633	94	0
2	A	19	0	0	1	0
2	B	22	0	0	1	0
2	C	19	0	0	1	0
2	D	21	0	0	2	0
2	E	15	0	0	1	0
2	F	16	0	0	1	0
2	G	20	0	0	3	0
2	H	36	0	0	3	0
2	I	17	0	0	0	0
2	J	11	0	0	5	0
2	K	4	0	0	1	0
2	L	8	0	0	0	0
All	All	21418	0	19871	881	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 21.

All (881) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ILE:CG1	1:C:13:ILE:CD1	1.83	1.56
1:I:6:THR:CG2	1:I:6:THR:CB	1.74	1.55
1:I:139:ILE:N	1:I:142:MET:HE3	1.19	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:ILE:H	1:I:142:MET:CE	1.36	1.37
1:I:171:PHE:CZ	1:I:204:MET:HE3	1.61	1.35
1:I:171:PHE:HZ	1:I:204:MET:CE	1.41	1.34
1:I:171:PHE:CZ	1:I:204:MET:CE	2.12	1.31
1:A:67:MET:CE	1:A:171:PHE:HE1	1.46	1.26
1:C:145:VAL:CG1	1:C:173:MET:CE	2.18	1.21
1:E:59:PHE:HD2	1:E:173:MET:CE	1.57	1.17
1:G:32:THR:HG22	1:I:159:ASN:HB3	1.26	1.17
1:H:67:MET:HE3	1:H:73:PHE:HB3	1.18	1.15
1:I:6:THR:HG21	1:I:141:ASN:HD21	1.11	1.15
1:B:158:LEU:CD1	1:B:160:VAL:HG23	1.77	1.13
1:C:145:VAL:HG12	1:C:173:MET:HE3	1.32	1.12
1:C:145:VAL:CG1	1:C:173:MET:HE2	1.80	1.11
1:J:154:THR:HG22	1:K:154:THR:O	1.47	1.11
1:K:154:THR:HG23	1:L:154:THR:O	1.50	1.11
1:A:67:MET:CE	1:A:171:PHE:CE1	2.34	1.11
1:A:67:MET:HE2	1:A:171:PHE:CE1	1.87	1.08
1:J:159:ASN:HB3	1:K:32:THR:HG22	1.34	1.06
1:C:67:MET:CE	1:C:73:PHE:CG	2.39	1.06
1:A:67:MET:HE2	1:A:171:PHE:HE1	0.96	1.05
1:K:8:TYR:CZ	1:K:78:LYS:HD3	1.91	1.05
1:L:129:GLU:OE2	1:L:129:GLU:HA	1.36	1.05
1:E:59:PHE:HD2	1:E:173:MET:HE1	1.20	1.04
1:I:138:PHE:HA	1:I:142:MET:HE1	1.41	1.03
1:I:67:MET:HE1	1:I:169:PRO:HG2	1.07	1.03
1:C:67:MET:HE1	1:C:73:PHE:CG	1.95	1.02
1:I:171:PHE:HZ	1:I:204:MET:HE3	0.92	1.02
1:C:67:MET:HE3	1:C:73:PHE:CB	1.90	1.02
1:E:59:PHE:CD2	1:E:173:MET:CE	2.44	1.01
1:H:67:MET:CE	1:H:73:PHE:HB3	1.90	1.01
1:I:67:MET:CE	1:I:169:PRO:HG2	1.89	1.01
1:J:159:ASN:HD22	1:L:159:ASN:HD21	1.02	1.00
1:A:159:ASN:HB3	1:B:32:THR:HG22	1.39	0.98
1:A:154:THR:HG23	1:B:154:THR:O	1.61	0.98
1:J:67:MET:HA	1:J:67:MET:HE2	1.41	0.97
1:A:154:THR:O	1:C:154:THR:HG23	1.65	0.96
1:D:67:MET:CE	1:D:169:PRO:HG2	1.95	0.96
1:L:67:MET:HE3	1:L:73:PHE:HB3	1.43	0.96
1:C:67:MET:CE	1:C:73:PHE:HB3	1.95	0.95
1:H:32:THR:HG21	2:H:224:HOH:O	1.65	0.95
1:B:158:LEU:HD11	1:B:160:VAL:HG23	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:ASN:ND2	1:L:159:ASN:HD21	1.65	0.95
1:L:106:TRP:CD1	1:L:142:MET:HE3	2.02	0.94
1:I:171:PHE:CZ	1:I:204:MET:HE1	2.02	0.94
1:A:123:ASP:OD1	1:A:136:LYS:NZ	2.01	0.93
1:C:67:MET:CE	1:C:73:PHE:CB	2.45	0.93
1:I:112:ASP:OD2	1:I:115:GLN:HG2	1.68	0.93
1:B:149:PRO:O	1:B:175:LYS:HG3	1.67	0.93
1:C:145:VAL:HG11	1:C:173:MET:CE	1.98	0.93
1:A:56:TYR:HE1	1:A:173:MET:HE3	1.31	0.92
1:B:67:MET:CE	1:B:169:PRO:HG2	1.99	0.92
1:H:67:MET:HE3	1:H:73:PHE:CB	1.99	0.92
1:J:67:MET:CE	1:J:67:MET:HA	1.98	0.92
1:K:148:ASN:HD22	1:K:150:TRP:HE3	1.17	0.92
1:A:56:TYR:CD1	1:A:173:MET:HE1	2.03	0.92
1:C:56:TYR:HB3	1:C:57:PRO:HD3	1.51	0.92
1:G:59:PHE:HD2	1:G:173:MET:CE	1.82	0.92
1:F:110:HIS:HD2	1:F:119:ILE:HD11	1.34	0.91
1:D:154:THR:O	1:F:154:THR:HG23	1.71	0.91
1:G:32:THR:CG2	1:I:159:ASN:HB3	1.99	0.91
1:E:59:PHE:CD2	1:E:173:MET:SD	2.65	0.90
1:I:6:THR:HG21	1:I:141:ASN:ND2	1.84	0.90
1:J:154:THR:CG2	1:K:154:THR:O	2.19	0.90
1:D:163:MET:O	1:D:164:ASP:HB2	1.71	0.90
1:A:67:MET:HE1	1:A:171:PHE:CE1	2.04	0.90
1:H:192:HIS:HD1	1:H:194:ALA:H	1.14	0.89
1:E:139:ILE:H	1:E:142:MET:HE3	1.35	0.89
1:I:67:MET:HE1	1:I:169:PRO:CG	1.99	0.89
1:L:7:GLY:HA3	1:L:86:ASP:OD1	1.70	0.88
1:H:54:LYS:HD3	2:H:249:HOH:O	1.73	0.88
1:L:67:MET:CE	1:L:169:PRO:HG2	2.04	0.88
1:A:56:TYR:CE1	1:A:173:MET:HE3	2.09	0.88
1:C:114:ARG:HH11	1:C:114:ARG:CG	1.86	0.88
1:H:91:CYS:HB2	1:H:142:MET:HE2	1.55	0.88
1:C:114:ARG:HH11	1:C:114:ARG:HG2	1.40	0.86
1:C:216:GLN:HA	1:C:216:GLN:HE21	1.40	0.86
1:G:59:PHE:CD2	1:G:173:MET:CE	2.59	0.85
1:D:67:MET:HE3	1:D:73:PHE:HB3	1.59	0.85
1:J:106:TRP:CD1	1:J:142:MET:HE3	2.12	0.84
1:J:154:THR:O	1:L:154:THR:HG23	1.78	0.84
1:K:47:THR:O	1:K:49:LYS:N	2.11	0.84
1:G:59:PHE:HD2	1:G:173:MET:HE1	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:171:PHE:CE2	1:I:204:MET:CE	2.60	0.83
1:J:30:GLN:NE2	1:J:163:MET:O	2.11	0.83
1:K:171:PHE:CZ	1:K:204:MET:CE	2.63	0.82
1:E:59:PHE:CD2	1:E:173:MET:HE1	2.07	0.82
2:A:220:HOH:O	1:C:159:ASN:HB2	1.79	0.82
1:D:67:MET:HE1	1:D:169:PRO:HG2	1.60	0.82
1:A:56:TYR:HD1	1:A:173:MET:HE1	1.43	0.82
1:D:8:TYR:N	1:D:8:TYR:CD2	2.44	0.82
1:F:106:TRP:CD1	1:F:142:MET:CE	2.62	0.81
1:A:56:TYR:CE1	1:A:173:MET:CE	2.64	0.81
1:C:49:LYS:O	1:C:51:ASN:N	2.13	0.81
1:C:145:VAL:CG1	1:C:173:MET:HE3	1.95	0.81
1:G:154:THR:HG23	1:H:154:THR:O	1.82	0.80
1:J:159:ASN:HD21	1:K:159:ASN:ND2	1.80	0.80
1:D:67:MET:CE	1:D:73:PHE:HB3	2.11	0.80
1:F:110:HIS:CD2	1:F:119:ILE:HD11	2.17	0.80
1:L:91:CYS:HB2	1:L:142:MET:HE2	1.63	0.79
1:K:154:THR:CG2	1:L:154:THR:O	2.28	0.79
1:L:192:HIS:HD1	1:L:194:ALA:H	1.30	0.79
1:C:145:VAL:HG11	1:C:173:MET:HE2	1.56	0.79
1:A:192:HIS:HD1	1:A:194:ALA:H	1.29	0.79
1:G:171:PHE:HZ	1:G:204:MET:HE3	1.47	0.79
1:I:139:ILE:N	1:I:142:MET:CE	2.13	0.79
1:J:138:PHE:CD2	1:J:138:PHE:O	2.36	0.79
1:J:89:HIS:CE1	1:J:108:GLU:HG3	2.18	0.79
1:G:171:PHE:CZ	1:G:204:MET:HE3	2.18	0.78
1:K:171:PHE:CZ	1:K:204:MET:HE3	2.19	0.78
1:K:25:PHE:O	1:K:30:GLN:HG3	1.84	0.78
1:G:50:LYS:C	1:G:51:ASN:O	2.12	0.78
1:E:106:TRP:CE2	1:E:136:LYS:HD2	2.18	0.78
1:D:154:THR:HG23	1:E:154:THR:O	1.84	0.77
1:J:192:HIS:HD1	1:J:194:ALA:H	1.33	0.77
1:F:100:GLU:OE1	1:J:6:THR:HG22	1.85	0.77
1:B:67:MET:HE1	1:B:169:PRO:HG2	1.63	0.77
1:F:192:HIS:HD1	1:F:194:ALA:H	1.29	0.77
1:C:145:VAL:HG13	1:C:173:MET:HE2	1.65	0.77
1:L:106:TRP:CD1	1:L:142:MET:CE	2.68	0.77
1:E:34:ASN:ND2	1:E:190:GLN:HB3	2.00	0.77
1:E:67:MET:HE3	1:E:171:PHE:CE1	2.20	0.77
1:K:8:TYR:CE2	1:K:78:LYS:HD3	2.19	0.77
1:G:91:CYS:SG	1:G:142:MET:HE2	2.25	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:HIS:HD1	1:G:194:ALA:H	1.33	0.76
1:I:171:PHE:CE2	1:I:204:MET:HE3	2.17	0.76
1:C:112:ASP:HB3	1:C:115:GLN:HG3	1.68	0.75
1:A:154:THR:CG2	1:B:154:THR:O	2.35	0.75
1:E:67:MET:CE	1:E:171:PHE:CE1	2.70	0.75
1:D:159:ASN:HB3	1:E:32:THR:HG22	1.68	0.75
1:L:67:MET:HE1	1:L:169:PRO:HG2	1.67	0.75
1:J:10:THR:HG23	1:J:10:THR:O	1.86	0.75
1:G:15:GLN:HA	1:G:15:GLN:HE21	1.51	0.74
1:G:171:PHE:CZ	1:G:204:MET:CE	2.70	0.74
1:J:6:THR:O	1:J:6:THR:HG23	1.84	0.74
1:K:59:PHE:CD2	1:K:173:MET:SD	2.80	0.74
1:J:40:ASP:HA	1:J:184:LEU:HD23	1.67	0.74
1:G:13:ILE:O	1:G:19:LYS:HG3	1.86	0.74
1:K:10:THR:OG1	1:K:83:VAL:HG23	1.87	0.74
1:B:154:THR:HG23	1:C:154:THR:O	1.88	0.74
1:L:106:TRP:HB3	1:L:142:MET:HE2	1.70	0.74
1:A:56:TYR:CD1	1:A:173:MET:CE	2.71	0.73
1:E:139:ILE:O	1:E:142:MET:SD	2.46	0.73
1:F:106:TRP:O	1:F:136:LYS:NZ	2.22	0.73
1:J:190:GLN:C	1:J:190:GLN:HE21	1.91	0.73
1:C:67:MET:HE3	1:C:73:PHE:CG	2.19	0.73
1:E:59:PHE:HD2	1:E:173:MET:SD	2.06	0.72
1:J:106:TRP:CD1	1:J:142:MET:CE	2.72	0.72
1:D:163:MET:O	1:D:164:ASP:CB	2.36	0.72
1:J:123:ASP:OD1	1:J:136:LYS:HE2	1.88	0.72
1:J:159:ASN:CB	1:K:32:THR:HG22	2.18	0.72
1:D:75:MET:HE3	2:D:235:HOH:O	1.88	0.72
1:J:35:GLN:HG3	1:L:156:PHE:HD1	1.54	0.72
1:C:67:MET:HE2	1:C:73:PHE:HB3	1.70	0.72
1:L:129:GLU:OE2	1:L:129:GLU:CA	2.26	0.72
1:B:155:SER:HB2	1:C:155:SER:HB2	1.71	0.71
1:J:35:GLN:HG3	1:L:156:PHE:CD1	2.24	0.71
1:K:45:LEU:HD22	1:K:49:LYS:HD2	1.71	0.71
1:K:106:TRP:CD1	1:K:142:MET:CE	2.74	0.71
1:L:59:PHE:CD2	1:L:173:MET:HE1	2.26	0.71
1:H:47:THR:O	1:H:51:ASN:ND2	2.24	0.71
1:I:171:PHE:CE2	1:I:204:MET:HE1	2.22	0.71
1:G:159:ASN:ND2	1:I:159:ASN:ND2	2.39	0.70
1:D:65:ARG:CD	1:J:111:ASP:OD2	2.39	0.70
1:E:3:LYS:O	1:E:4:LYS:HG2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:O	1:C:154:THR:CG2	2.39	0.70
1:K:72:GLU:HA	1:K:75:MET:HE2	1.72	0.70
1:C:145:VAL:HG12	1:C:173:MET:CE	1.94	0.70
1:G:171:PHE:HZ	1:G:204:MET:CE	2.03	0.70
1:I:59:PHE:CD2	1:I:173:MET:SD	2.84	0.70
1:L:59:PHE:HD2	1:L:173:MET:HE1	1.57	0.70
1:B:34:ASN:CG	1:B:157:ASP:HB2	2.12	0.70
1:B:204:MET:HE1	1:B:205:LEU:HD23	1.73	0.69
1:H:149:PRO:O	1:H:175:LYS:HD3	1.91	0.69
1:A:34:ASN:HB2	1:A:157:ASP:OD2	1.93	0.69
1:H:159:ASN:HB3	1:I:32:THR:HG22	1.74	0.69
1:D:65:ARG:HD3	1:J:111:ASP:OD2	1.92	0.69
1:F:190:GLN:C	1:F:190:GLN:HE21	1.96	0.69
1:G:59:PHE:CD2	1:G:173:MET:HE1	2.24	0.69
1:G:154:THR:O	1:I:154:THR:HG23	1.93	0.69
1:C:67:MET:HE1	1:C:73:PHE:CD2	2.28	0.69
1:A:204:MET:HE2	1:A:205:LEU:HG	1.73	0.69
1:E:132:ALA:O	1:E:135:PRO:HD3	1.92	0.68
1:E:67:MET:CE	1:E:171:PHE:HE1	2.06	0.68
1:I:59:PHE:HD2	1:I:173:MET:HE1	1.58	0.68
1:J:159:ASN:ND2	1:K:159:ASN:ND2	2.40	0.68
1:I:138:PHE:CA	1:I:142:MET:HE1	2.21	0.68
1:L:8:TYR:HB2	1:L:83:VAL:HG13	1.74	0.68
1:C:13:ILE:H	1:C:13:ILE:HD12	1.58	0.68
1:D:34:ASN:ND2	1:D:158:LEU:H	1.92	0.68
1:E:159:ASN:HB3	1:F:32:THR:HG22	1.76	0.68
1:C:57:PRO:HG3	1:C:120:TYR:CE2	2.29	0.68
1:J:35:GLN:HA	1:L:155:SER:O	1.94	0.68
1:H:67:MET:CE	1:H:169:PRO:HG2	2.24	0.68
1:I:145:VAL:HG11	1:I:173:MET:CE	2.24	0.67
1:J:44:PHE:HB2	1:J:212:CYS:O	1.95	0.67
1:C:67:MET:HE3	1:C:73:PHE:HB3	1.59	0.67
1:C:192:HIS:HD1	1:C:194:ALA:H	1.40	0.67
1:F:34:ASN:ND2	1:F:190:GLN:HB2	2.08	0.67
1:H:91:CYS:HB2	1:H:142:MET:CE	2.24	0.67
1:J:171:PHE:CZ	1:J:204:MET:HE3	2.29	0.67
1:F:110:HIS:HD2	1:F:119:ILE:CD1	2.06	0.67
1:A:32:THR:HG22	1:C:159:ASN:HB3	1.77	0.67
1:F:92:TYR:HA	1:F:145:VAL:O	1.94	0.67
1:L:214:GLU:O	1:L:215:TRP:C	2.33	0.67
1:F:214:GLU:O	1:F:215:TRP:C	2.32	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:PHE:HZ	1:J:204:MET:HE3	1.60	0.66
1:B:34:ASN:ND2	1:B:190:GLN:HB3	2.11	0.66
1:H:113:PHE:H	1:H:219:ALA:HB3	1.59	0.66
1:H:67:MET:HE1	1:H:73:PHE:CD2	2.30	0.66
1:B:156:PHE:O	1:B:157:ASP:HB3	1.95	0.66
1:E:3:LYS:O	1:E:4:LYS:CG	2.42	0.66
1:J:65:ARG:HD3	2:J:229:HOH:O	1.95	0.66
1:F:30:GLN:HE22	1:F:164:ASP:HA	1.60	0.66
1:I:6:THR:CG2	1:I:6:THR:CA	2.69	0.66
1:F:120:TYR:O	1:F:124:VAL:HG23	1.95	0.66
1:I:145:VAL:HG11	1:I:173:MET:HE3	1.77	0.66
1:J:16:TRP:CE2	1:J:18:ARG:HB2	2.30	0.66
1:H:56:TYR:HD1	1:H:173:MET:HE1	1.61	0.65
1:G:30:GLN:HB3	1:I:161:ALA:HB3	1.78	0.65
1:J:10:THR:CG2	1:J:10:THR:O	2.44	0.65
1:I:7:GLY:CA	1:I:86:ASP:OD1	2.44	0.65
1:J:176:TYR:HB3	1:J:185:MET:HB2	1.77	0.65
1:H:67:MET:HE1	1:H:169:PRO:HG2	1.78	0.65
1:F:106:TRP:CD1	1:F:142:MET:HE3	2.31	0.65
1:I:7:GLY:C	1:I:86:ASP:OD1	2.36	0.65
1:D:32:THR:HG21	2:D:220:HOH:O	1.96	0.64
1:C:110:HIS:CD2	1:C:119:ILE:HD13	2.32	0.64
1:K:67:MET:HE2	1:K:67:MET:HA	1.79	0.64
1:H:56:TYR:CD1	1:H:173:MET:HE1	2.32	0.64
1:J:13:ILE:HG22	1:J:19:LYS:HD2	1.80	0.64
1:A:56:TYR:O	1:A:60:ILE:HG13	1.99	0.63
1:L:123:ASP:OD1	1:L:136:LYS:HE3	1.97	0.63
1:L:59:PHE:HD2	1:L:173:MET:CE	2.10	0.63
1:A:204:MET:HE1	1:A:205:LEU:CD2	2.29	0.63
1:A:56:TYR:N	1:A:57:PRO:HD2	2.13	0.63
1:G:159:ASN:HD22	1:I:159:ASN:CG	2.01	0.63
1:I:139:ILE:HG13	1:I:142:MET:CE	2.28	0.63
1:G:154:THR:O	1:I:154:THR:CG2	2.47	0.63
1:J:106:TRP:HB3	1:J:142:MET:HE2	1.81	0.63
1:E:106:TRP:CZ2	1:E:136:LYS:HD2	2.33	0.63
1:F:40:ASP:HA	1:F:184:LEU:HD23	1.81	0.63
1:H:22:PHE:CE2	1:H:82:LEU:HD22	2.34	0.63
1:H:91:CYS:SG	1:H:142:MET:HE1	2.38	0.63
1:K:57:PRO:HG3	1:K:120:TYR:CE2	2.34	0.63
1:K:159:ASN:HB3	1:L:32:THR:HG23	1.80	0.62
1:K:56:TYR:HB3	1:K:57:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:148:ASN:ND2	1:K:150:TRP:HE3	1.92	0.62
1:D:34:ASN:HD21	1:D:158:LEU:H	1.46	0.62
1:E:139:ILE:H	1:E:142:MET:CE	2.10	0.62
1:I:190:GLN:HE21	1:I:190:GLN:C	2.01	0.62
1:C:114:ARG:CG	1:C:114:ARG:NH1	2.51	0.62
1:J:10:THR:HB	2:J:225:HOH:O	2.00	0.62
1:L:115:GLN:O	1:L:118:HIS:O	2.17	0.62
1:F:179:GLN:O	1:F:180:GLY:C	2.38	0.62
1:H:57:PRO:HG3	1:H:120:TYR:CE2	2.35	0.62
1:I:7:GLY:HA3	1:I:86:ASP:OD1	1.99	0.61
1:A:34:ASN:OD1	1:A:157:ASP:OD2	2.18	0.61
1:E:67:MET:HE3	1:E:171:PHE:HE1	1.62	0.61
1:A:39:LEU:O	1:A:184:LEU:HA	2.00	0.61
1:J:49:LYS:O	1:J:51:ASN:O	2.18	0.61
1:L:66:LEU:CD2	1:L:211:TYR:CE2	2.83	0.61
1:K:117:LEU:HD22	1:K:117:LEU:O	2.00	0.61
1:L:66:LEU:HD23	1:L:211:TYR:CE2	2.36	0.61
1:A:34:ASN:CB	1:A:157:ASP:OD2	2.49	0.61
1:D:59:PHE:CD2	1:D:173:MET:SD	2.94	0.61
1:H:58:ALA:HA	1:H:113:PHE:CE1	2.36	0.61
1:K:34:ASN:ND2	1:K:190:GLN:HB2	2.15	0.61
1:A:34:ASN:CG	1:A:157:ASP:OD2	2.39	0.61
1:J:158:LEU:HD13	1:J:160:VAL:HG23	1.81	0.61
1:I:138:PHE:HA	1:I:142:MET:CE	2.23	0.61
1:K:171:PHE:HZ	1:K:204:MET:SD	2.23	0.60
1:A:83:VAL:CG1	1:A:84:ILE:N	2.64	0.60
1:L:26:GLN:HA	1:L:26:GLN:NE2	2.16	0.60
1:H:65:ARG:HH22	1:H:219:ALA:HB1	1.66	0.60
1:K:171:PHE:CE2	1:K:204:MET:HE1	2.36	0.60
1:I:148:ASN:O	1:I:174:GLY:HA2	2.01	0.60
1:I:112:ASP:OD2	1:I:115:GLN:CG	2.48	0.60
1:B:67:MET:HE3	1:B:169:PRO:HG2	1.84	0.60
1:G:154:THR:CG2	1:H:154:THR:O	2.47	0.60
1:A:83:VAL:HG13	1:A:84:ILE:N	2.17	0.60
1:L:59:PHE:CD2	1:L:173:MET:CE	2.84	0.60
1:I:67:MET:CE	1:I:169:PRO:CG	2.71	0.59
1:C:13:ILE:H	1:C:13:ILE:CD1	2.15	0.59
1:L:127:TYR:O	1:L:129:GLU:N	2.34	0.59
1:F:139:ILE:HG13	1:F:142:MET:HG3	1.84	0.59
1:C:110:HIS:CD2	1:C:119:ILE:CD1	2.86	0.59
1:G:59:PHE:CE2	1:G:63:LEU:HD11	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:TYR:C	1:H:8:TYR:CD1	2.75	0.59
1:D:57:PRO:HG3	1:D:120:TYR:CE2	2.38	0.58
1:E:154:THR:CG2	1:F:154:THR:O	2.51	0.58
1:A:67:MET:HE3	1:A:169:PRO:HB2	1.84	0.58
1:D:35:GLN:OE1	1:F:151:VAL:HG11	2.03	0.58
1:H:22:PHE:CZ	1:H:82:LEU:HD22	2.38	0.58
1:L:106:TRP:HB3	1:L:142:MET:CE	2.33	0.58
1:E:8:TYR:CE2	1:E:78:LYS:HE2	2.38	0.58
1:H:139:ILE:HD12	1:H:141:ASN:OD1	2.03	0.58
1:I:138:PHE:C	1:I:142:MET:HE3	2.14	0.58
1:D:8:TYR:HD1	1:D:83:VAL:HG22	1.69	0.58
1:F:110:HIS:CD2	1:F:119:ILE:CD1	2.84	0.58
1:H:25:PHE:HB2	1:H:194:ALA:HA	1.85	0.58
1:A:187:LEU:CD2	1:A:208:LEU:HD21	2.34	0.58
1:F:57:PRO:HG3	1:F:120:TYR:CE2	2.39	0.58
1:L:106:TRP:HD1	1:L:142:MET:CE	2.14	0.58
1:C:9:THR:HG22	2:C:228:HOH:O	2.03	0.58
1:B:67:MET:CE	1:B:169:PRO:CG	2.79	0.58
1:C:49:LYS:C	1:C:51:ASN:N	2.56	0.58
1:H:127:TYR:CE2	1:H:136:LYS:HG2	2.38	0.58
1:A:204:MET:CE	1:A:205:LEU:HD23	2.33	0.57
1:E:192:HIS:HD1	1:E:194:ALA:H	1.52	0.57
1:G:113:PHE:HD2	1:G:218:GLY:HA3	1.67	0.57
1:K:47:THR:O	1:K:48:VAL:C	2.42	0.57
1:B:158:LEU:HD12	1:B:160:VAL:HG23	1.82	0.57
1:I:38:GLN:NE2	1:I:177:TYR:OH	2.37	0.57
1:A:204:MET:CE	1:A:205:LEU:HG	2.35	0.57
1:G:159:ASN:ND2	1:H:159:ASN:ND2	2.53	0.57
1:J:149:PRO:O	1:J:175:LYS:HB2	2.04	0.57
1:C:56:TYR:HB3	1:C:57:PRO:CD	2.30	0.57
1:K:106:TRP:CD1	1:K:142:MET:HE1	2.39	0.57
1:A:204:MET:HE1	1:A:205:LEU:HD23	1.87	0.57
1:G:72:GLU:N	1:G:72:GLU:OE2	2.30	0.57
1:K:171:PHE:HZ	1:K:204:MET:CE	2.15	0.57
1:K:192:HIS:HD1	1:K:194:ALA:H	1.53	0.57
1:J:138:PHE:CG	1:J:138:PHE:O	2.57	0.57
1:H:4:LYS:HB2	1:H:89:HIS:HE2	1.70	0.56
1:I:149:PRO:HD2	1:I:150:TRP:CZ3	2.39	0.56
1:G:53:HIS:HE1	1:G:114:ARG:NH1	2.02	0.56
1:G:14:SER:HA	1:G:19:LYS:HE2	1.87	0.56
1:C:49:LYS:O	1:C:50:LYS:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:TYR:HA	1:E:145:VAL:O	2.05	0.56
1:G:155:SER:O	1:H:35:GLN:HA	2.05	0.56
1:F:157:ASP:OD2	1:F:157:ASP:N	2.37	0.56
1:I:59:PHE:HD2	1:I:173:MET:SD	2.27	0.56
1:I:59:PHE:HD2	1:I:173:MET:CE	2.18	0.56
1:D:67:MET:CE	1:D:169:PRO:CG	2.79	0.56
1:H:48:VAL:HG13	1:H:53:HIS:O	2.06	0.56
1:C:114:ARG:HG3	1:C:114:ARG:NH1	2.19	0.56
1:D:56:TYR:HB3	1:D:57:PRO:HD3	1.86	0.56
1:K:171:PHE:CE2	1:K:204:MET:CE	2.89	0.56
1:L:179:GLN:HE21	1:L:184:LEU:HD12	1.70	0.56
1:L:30:GLN:HE22	1:L:164:ASP:HA	1.71	0.56
1:B:67:MET:HE1	1:B:169:PRO:CG	2.35	0.56
1:G:59:PHE:HD2	1:G:173:MET:HE2	1.69	0.56
1:L:45:LEU:HD23	1:L:45:LEU:C	2.25	0.56
1:A:89:HIS:O	1:A:142:MET:HA	2.06	0.56
1:D:8:TYR:CD1	1:D:83:VAL:HG22	2.40	0.56
1:G:159:ASN:ND2	1:I:159:ASN:HD21	2.04	0.56
1:L:118:HIS:O	1:L:119:ILE:HB	2.06	0.56
1:L:37:VAL:HG13	1:L:38:GLN:N	2.21	0.56
1:I:118:HIS:CE1	1:I:122:GLN:NE2	2.73	0.55
1:I:77:MET:HE1	1:I:82:LEU:HB2	1.87	0.55
1:J:67:MET:HE1	1:J:73:PHE:CG	2.41	0.55
1:I:118:HIS:ND1	1:I:122:GLN:NE2	2.53	0.55
1:J:106:TRP:HD1	1:J:142:MET:CE	2.19	0.55
1:D:65:ARG:HD2	1:J:111:ASP:OD2	2.06	0.55
1:J:25:PHE:O	1:J:30:GLN:HG3	2.06	0.55
1:K:74:ARG:HD2	1:K:88:VAL:HG13	1.89	0.55
1:E:25:PHE:O	1:E:30:GLN:HG3	2.07	0.55
1:L:26:GLN:HA	1:L:26:GLN:HE21	1.70	0.55
1:L:77:MET:HG3	1:L:165:ASN:OD1	2.07	0.55
1:H:45:LEU:HD13	1:H:49:LYS:NZ	2.22	0.55
1:J:57:PRO:HA	1:J:60:ILE:HB	1.88	0.55
1:K:34:ASN:OD1	1:K:157:ASP:HB3	2.07	0.55
1:C:49:LYS:C	1:C:51:ASN:H	2.10	0.55
1:A:115:GLN:O	1:A:119:ILE:HD12	2.07	0.55
1:B:156:PHE:C	1:B:156:PHE:CD2	2.80	0.55
1:I:34:ASN:ND2	1:I:158:LEU:H	2.04	0.55
1:D:203:ARG:O	1:D:207:GLU:HG3	2.07	0.55
1:H:65:ARG:HH22	1:H:219:ALA:CB	2.20	0.55
1:H:38:GLN:NE2	1:H:177:TYR:OH	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:PHE:CA	1:I:142:MET:CE	2.84	0.54
1:K:90:PRO:HD2	1:K:107:SER:O	2.07	0.54
1:B:204:MET:CE	1:B:205:LEU:HD23	2.37	0.54
1:D:110:HIS:HD2	1:D:112:ASP:H	1.54	0.54
1:J:29:ALA:O	1:J:30:GLN:C	2.45	0.54
1:K:106:TRP:CD1	1:K:142:MET:HE3	2.43	0.54
1:G:72:GLU:HG3	1:G:200:HIS:HB3	1.89	0.54
1:I:34:ASN:HD21	1:I:158:LEU:H	1.55	0.54
1:I:75:MET:HA	1:I:83:VAL:O	2.08	0.54
1:J:67:MET:HE1	1:J:73:PHE:CD1	2.42	0.54
1:G:159:ASN:HB3	1:H:32:THR:HG22	1.90	0.54
1:C:148:ASN:O	1:C:174:GLY:HA2	2.08	0.54
1:D:25:PHE:O	1:D:30:GLN:HG3	2.08	0.54
1:I:118:HIS:CE1	1:I:122:GLN:HE21	2.25	0.54
1:K:159:ASN:HB3	1:L:32:THR:CG2	2.38	0.54
1:G:93:THR:HG23	1:G:146:SER:HB3	1.90	0.54
1:G:159:ASN:HD22	1:I:159:ASN:ND2	2.06	0.54
1:G:91:CYS:HB2	1:G:142:MET:HE2	1.90	0.54
1:J:27:SER:OG	1:J:28:VAL:HG22	2.08	0.54
1:F:11:VAL:HG21	1:F:82:LEU:HD23	1.89	0.54
1:K:106:TRP:CG	1:K:142:MET:CE	2.91	0.54
1:C:67:MET:HE3	1:C:67:MET:HA	1.90	0.54
1:K:56:TYR:HB3	1:K:57:PRO:CD	2.37	0.54
1:L:66:LEU:HD21	1:L:211:TYR:CD2	2.43	0.54
1:G:59:PHE:HE2	1:G:63:LEU:HD11	1.72	0.53
1:H:4:LYS:HB2	1:H:89:HIS:NE2	2.23	0.53
1:I:6:THR:CG2	1:I:141:ASN:HD21	2.01	0.53
1:J:159:ASN:HB3	1:K:32:THR:CG2	2.24	0.53
1:J:62:ILE:HD11	1:J:215:TRP:CD1	2.43	0.53
1:B:78:LYS:O	1:B:81:GLU:N	2.39	0.53
1:J:171:PHE:CZ	1:J:204:MET:CE	2.91	0.53
1:D:190:GLN:O	1:D:190:GLN:HG3	2.06	0.53
1:E:148:ASN:N	1:E:149:PRO:HD3	2.22	0.53
1:G:59:PHE:CD2	1:G:173:MET:SD	3.02	0.53
1:J:40:ASP:HA	1:J:184:LEU:CD2	2.38	0.53
1:A:187:LEU:CD2	1:A:208:LEU:CD2	2.85	0.53
1:F:177:TYR:OH	2:F:233:HOH:O	2.19	0.53
1:E:44:PHE:O	1:E:48:VAL:HG23	2.09	0.53
1:E:154:THR:HG23	1:F:154:THR:O	2.08	0.53
1:K:171:PHE:CZ	1:K:204:MET:SD	3.01	0.53
1:C:190:GLN:C	1:C:190:GLN:HE21	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:THR:CG2	1:G:146:SER:HB3	2.39	0.53
1:G:98:GLN:HB2	1:G:99:THR:HG23	1.90	0.53
1:J:123:ASP:OD1	1:J:136:LYS:CE	2.56	0.53
1:H:26:GLN:HE21	1:H:26:GLN:HA	1.74	0.53
1:H:5:ILE:HA	1:H:6:THR:HG23	1.90	0.53
1:J:27:SER:OG	1:J:28:VAL:N	2.40	0.53
1:J:30:GLN:NE2	2:J:226:HOH:O	2.41	0.53
1:D:110:HIS:HD2	1:D:111:ASP:N	2.06	0.53
1:G:139:ILE:HG13	1:G:142:MET:CG	2.38	0.53
1:J:99:THR:HB	1:K:17:HIS:HD2	1.73	0.53
1:K:154:THR:HG22	1:L:36:THR:HB	1.90	0.53
1:C:216:GLN:HA	1:C:216:GLN:NE2	2.17	0.52
1:A:56:TYR:N	1:A:57:PRO:CD	2.71	0.52
1:G:12:ASP:OD2	1:G:15:GLN:HG2	2.10	0.52
1:H:56:TYR:HB3	1:H:57:PRO:HD3	1.91	0.52
1:I:143:PHE:HB2	1:I:169:PRO:HD2	1.92	0.52
1:E:156:PHE:C	1:E:156:PHE:CD2	2.82	0.52
1:L:57:PRO:HG2	1:L:58:ALA:N	2.23	0.52
1:L:67:MET:HE1	1:L:73:PHE:CD2	2.44	0.52
1:E:187:LEU:HG	1:E:188:ALA:N	2.21	0.52
1:H:30:GLN:NE2	1:H:163:MET:HG3	2.25	0.52
1:G:187:LEU:CD2	1:G:208:LEU:HD21	2.40	0.52
1:G:75:MET:HA	1:G:83:VAL:O	2.08	0.52
1:J:130:ASN:HB3	1:J:135:PRO:HG3	1.92	0.52
1:K:106:TRP:HB3	1:K:142:MET:HE1	1.92	0.52
1:L:35:GLN:O	1:L:188:ALA:HA	2.09	0.52
1:B:154:THR:HG21	1:C:38:GLN:OE1	2.10	0.52
1:C:67:MET:HE3	1:C:73:PHE:HB2	1.88	0.52
1:D:214:GLU:OE2	1:J:115:GLN:HG3	2.10	0.52
1:B:187:LEU:HG	1:B:188:ALA:N	2.18	0.52
1:C:47:THR:O	1:C:48:VAL:C	2.48	0.52
1:J:59:PHE:HD2	1:J:173:MET:HE1	1.74	0.52
1:K:34:ASN:HD21	1:K:190:GLN:HB2	1.75	0.52
1:C:67:MET:HE1	1:C:73:PHE:CD1	2.44	0.52
1:D:16:TRP:CE2	1:D:18:ARG:HB2	2.45	0.52
1:G:133:TYR:O	1:G:135:PRO:HD3	2.10	0.52
1:L:171:PHE:HA	1:L:188:ALA:O	2.10	0.51
1:A:129:GLU:HA	1:A:129:GLU:OE1	2.10	0.51
1:A:56:TYR:HB3	1:A:57:PRO:HD3	1.92	0.51
1:C:29:ALA:O	1:C:30:GLN:C	2.45	0.51
1:D:110:HIS:CD2	1:D:112:ASP:H	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:O	1:D:189:ILE:HG23	2.10	0.51
1:C:113:PHE:CD2	1:C:215:TRP:HZ2	2.29	0.51
1:D:73:PHE:HB3	1:D:169:PRO:HG2	1.91	0.51
1:E:90:PRO:HD2	1:E:107:SER:O	2.10	0.51
1:I:30:GLN:NE2	1:I:192:HIS:NE2	2.47	0.51
1:J:145:VAL:CG1	1:J:173:MET:HE3	2.41	0.51
1:L:106:TRP:CG	1:L:142:MET:HE3	2.43	0.51
1:D:27:SER:O	1:D:28:VAL:C	2.45	0.51
1:A:204:MET:CE	1:A:205:LEU:CD2	2.88	0.51
1:B:78:LYS:O	1:B:80:GLY:N	2.43	0.51
1:G:45:LEU:HD12	1:G:183:VAL:HG11	1.92	0.51
1:F:89:HIS:ND1	1:F:109:TYR:HB3	2.25	0.51
1:I:30:GLN:NE2	1:I:163:MET:HG3	2.26	0.51
1:I:49:LYS:O	1:I:51:ASN:O	2.29	0.51
1:K:59:PHE:HD2	1:K:173:MET:CE	2.24	0.51
1:D:148:ASN:ND2	1:D:150:TRP:HE3	2.09	0.51
1:I:25:PHE:O	1:I:30:GLN:HG3	2.10	0.51
1:K:171:PHE:CZ	1:K:189:ILE:HD13	2.46	0.51
1:B:5:ILE:N	1:B:5:ILE:CD1	2.74	0.51
1:D:8:TYR:CD1	1:D:83:VAL:CG2	2.94	0.51
1:G:34:ASN:ND2	2:G:232:HOH:O	2.44	0.51
1:H:59:PHE:CD2	1:H:173:MET:SD	3.04	0.51
1:A:77:MET:HG3	1:A:165:ASN:OD1	2.11	0.50
1:F:106:TRP:CD1	1:F:142:MET:HE2	2.45	0.50
1:F:151:VAL:CG1	1:F:153:PHE:HB3	2.40	0.50
1:G:127:TYR:CE2	1:G:136:LYS:HG2	2.46	0.50
1:I:110:HIS:HB3	1:I:115:GLN:OE1	2.11	0.50
1:K:172:THR:HB	1:K:188:ALA:HB3	1.93	0.50
1:C:62:ILE:HG21	1:C:208:LEU:HD12	1.94	0.50
1:E:67:MET:CE	1:E:171:PHE:CZ	2.93	0.50
1:E:26:GLN:HA	1:E:26:GLN:HE21	1.76	0.50
1:I:40:ASP:HB3	1:I:209:GLN:OE1	2.12	0.50
1:J:163:MET:SD	1:L:161:ALA:HB2	2.51	0.50
1:K:139:ILE:HG13	1:K:142:MET:HG2	1.93	0.50
1:G:159:ASN:ND2	1:H:159:ASN:HD21	2.10	0.50
1:G:59:PHE:CD2	1:G:173:MET:HE2	2.42	0.50
1:D:114:ARG:CG	1:D:114:ARG:HH11	2.25	0.50
1:J:56:TYR:CZ	1:J:147:ALA:HB2	2.46	0.50
1:L:179:GLN:HE21	1:L:184:LEU:CD1	2.24	0.50
1:D:113:PHE:O	1:D:117:LEU:HB2	2.12	0.50
1:D:159:ASN:OD1	1:E:159:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:CYS:CB	1:G:142:MET:HE2	2.42	0.50
1:C:204:MET:CE	1:C:205:LEU:HD23	2.41	0.50
1:D:56:TYR:HB3	1:D:57:PRO:CD	2.41	0.50
1:F:68:ASN:OD1	1:F:87:SER:HA	2.10	0.50
1:J:159:ASN:ND2	1:K:159:ASN:HD22	2.10	0.50
1:B:34:ASN:CB	1:B:157:ASP:HB2	2.41	0.50
1:I:67:MET:HE1	1:I:73:PHE:HB3	1.93	0.50
1:J:34:ASN:ND2	1:J:190:GLN:HB2	2.27	0.50
1:L:84:ILE:HG22	1:L:85:TRP:O	2.12	0.50
1:C:110:HIS:HD2	1:C:119:ILE:HD13	1.76	0.50
1:D:30:GLN:HE22	1:D:164:ASP:HA	1.77	0.50
1:G:18:ARG:O	1:G:19:LYS:C	2.50	0.50
1:D:148:ASN:ND2	1:D:150:TRP:CE3	2.81	0.49
1:K:10:THR:O	1:K:10:THR:CG2	2.60	0.49
1:L:153:PHE:O	1:L:186:PRO:HB3	2.11	0.49
1:F:39:LEU:HD13	1:F:41:ILE:CG2	2.42	0.49
1:G:91:CYS:SG	1:G:142:MET:CE	2.96	0.49
1:J:106:TRP:HB3	1:J:142:MET:CE	2.42	0.49
1:L:123:ASP:OD1	1:L:136:LYS:CE	2.60	0.49
1:K:8:TYR:OH	1:K:78:LYS:HD3	2.12	0.49
1:D:110:HIS:CD2	1:D:111:ASP:N	2.81	0.49
1:D:38:GLN:NE2	1:D:177:TYR:OH	2.44	0.49
1:A:13:ILE:HG22	1:A:19:LYS:HG3	1.95	0.49
1:J:106:TRP:O	1:J:136:LYS:HE3	2.12	0.49
1:J:34:ASN:O	1:L:157:ASP:N	2.45	0.49
1:E:56:TYR:HB3	1:E:57:PRO:CD	2.42	0.49
1:G:26:GLN:NE2	2:G:225:HOH:O	2.37	0.49
1:H:5:ILE:O	1:H:5:ILE:HG22	2.12	0.49
1:K:22:PHE:CE1	1:K:26:GLN:HG3	2.47	0.49
1:B:99:THR:O	1:B:100:GLU:HB2	2.12	0.49
2:B:240:HOH:O	1:C:17:HIS:HD2	1.94	0.49
1:D:25:PHE:HB2	1:D:194:ALA:HA	1.95	0.49
1:D:67:MET:HE1	1:D:169:PRO:CG	2.40	0.49
1:I:14:SER:HA	1:I:19:LYS:HD2	1.95	0.49
1:J:179:GLN:O	1:J:179:GLN:CG	2.60	0.49
1:L:103:SER:HB3	1:L:132:ALA:O	2.12	0.49
1:L:8:TYR:HB2	1:L:83:VAL:CG1	2.41	0.49
1:B:67:MET:HE2	1:B:169:PRO:HB2	1.94	0.49
1:D:38:GLN:NE2	1:D:177:TYR:HE2	2.09	0.49
1:E:67:MET:HE2	1:E:171:PHE:CE1	2.48	0.49
1:G:127:TYR:CE2	1:G:136:LYS:CG	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:MET:CE	1:J:73:PHE:CG	2.96	0.49
1:K:171:PHE:CE2	1:K:189:ILE:HD13	2.47	0.49
1:B:191:VAL:HG21	1:B:201:VAL:HG21	1.95	0.49
1:A:90:PRO:HD2	1:A:107:SER:O	2.12	0.49
1:D:38:GLN:NE2	1:D:177:TYR:CE2	2.81	0.49
1:G:92:TYR:HA	1:G:145:VAL:O	2.13	0.48
1:I:145:VAL:CG1	1:I:173:MET:CE	2.91	0.48
1:K:44:PHE:HB2	1:K:212:CYS:HB3	1.94	0.48
1:D:36:THR:HB	1:F:155:SER:HB3	1.94	0.48
1:L:178:THR:O	1:L:179:GLN:HB3	2.14	0.48
1:I:150:TRP:HB2	1:I:151:VAL:HG23	1.95	0.48
1:J:10:THR:CB	2:J:225:HOH:O	2.59	0.48
1:J:44:PHE:O	1:J:48:VAL:HG23	2.13	0.48
1:B:215:TRP:CZ2	1:B:217:GLY:HA2	2.49	0.48
1:D:87:SER:O	1:D:141:ASN:ND2	2.43	0.48
1:E:134:PHE:O	1:E:135:PRO:C	2.50	0.48
1:H:25:PHE:O	1:H:30:GLN:HG3	2.13	0.48
1:I:110:HIS:CD2	1:I:119:ILE:HD12	2.48	0.48
1:I:139:ILE:HG13	1:I:142:MET:HE2	1.95	0.48
1:J:159:ASN:ND2	1:L:159:ASN:ND2	2.48	0.48
1:I:148:ASN:HD22	1:I:150:TRP:HE3	1.60	0.48
1:K:138:PHE:CD2	1:K:138:PHE:N	2.81	0.48
1:F:151:VAL:HG12	1:F:153:PHE:HD2	1.79	0.48
1:K:11:VAL:HG23	1:K:82:LEU:O	2.14	0.48
1:E:30:GLN:HE22	1:E:164:ASP:HA	1.79	0.48
1:F:123:ASP:OD1	1:F:136:LYS:CE	2.62	0.48
1:A:187:LEU:HD22	1:A:208:LEU:HD21	1.95	0.48
1:A:157:ASP:HB2	1:C:157:ASP:OD2	2.14	0.48
1:G:35:GLN:O	1:G:188:ALA:HA	2.14	0.48
1:I:67:MET:CE	1:I:73:PHE:HB3	2.44	0.48
1:K:10:THR:HG22	1:K:10:THR:O	2.13	0.48
1:J:63:LEU:HD13	1:J:171:PHE:CD1	2.49	0.47
1:K:67:MET:HG3	1:K:143:PHE:CG	2.48	0.47
1:L:89:HIS:ND1	1:L:109:TYR:N	2.49	0.47
1:D:136:LYS:O	1:D:137:GLY:C	2.51	0.47
1:G:22:PHE:O	1:G:23:GLU:C	2.50	0.47
1:K:72:GLU:HA	1:K:75:MET:CE	2.41	0.47
1:L:66:LEU:HD23	1:L:211:TYR:HE2	1.79	0.47
1:G:154:THR:HG22	1:H:36:THR:HB	1.97	0.47
1:G:161:ALA:HB2	1:H:163:MET:SD	2.54	0.47
1:J:57:PRO:O	1:J:58:ALA:C	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:MET:HE3	1:E:165:ASN:OD1	2.15	0.47
1:J:159:ASN:CG	1:K:159:ASN:HD22	2.17	0.47
1:K:92:TYR:HA	1:K:145:VAL:O	2.13	0.47
1:A:123:ASP:OD1	1:A:136:LYS:CE	2.62	0.47
1:B:109:TYR:O	1:B:110:HIS:CG	2.68	0.47
1:B:151:VAL:CG1	1:B:152:SER:N	2.78	0.47
1:F:204:MET:HE2	1:F:205:LEU:HA	1.96	0.47
1:J:57:PRO:HB3	1:J:120:TYR:CE2	2.49	0.47
1:A:192:HIS:HD1	1:A:194:ALA:N	2.05	0.47
1:A:29:ALA:O	1:A:30:GLN:C	2.52	0.47
1:C:120:TYR:CZ	1:C:124:VAL:HG21	2.49	0.47
1:I:109:TYR:O	1:I:110:HIS:CD2	2.68	0.47
1:I:92:TYR:HA	1:I:145:VAL:O	2.14	0.47
1:I:59:PHE:CD2	1:I:173:MET:HE1	2.45	0.47
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.63	0.47
1:B:5:ILE:N	1:B:5:ILE:HD13	2.29	0.47
1:D:67:MET:HE3	1:D:169:PRO:HG2	1.92	0.47
1:I:139:ILE:HG13	1:I:142:MET:HE3	1.92	0.47
1:G:30:GLN:HB3	1:I:161:ALA:CB	2.43	0.47
1:J:67:MET:CE	1:J:67:MET:CA	2.84	0.47
1:J:85:TRP:CD2	1:J:141:ASN:HB3	2.50	0.47
1:L:67:MET:CE	1:L:169:PRO:CG	2.85	0.47
1:K:190:GLN:C	1:K:190:GLN:HE21	2.17	0.47
1:K:77:MET:HE2	1:K:82:LEU:HD13	1.97	0.47
1:D:59:PHE:HD2	1:D:173:MET:CE	2.28	0.47
1:B:67:MET:HG3	1:B:143:PHE:CG	2.50	0.46
1:D:59:PHE:CE2	1:D:63:LEU:HD11	2.50	0.46
1:K:157:ASP:OD2	1:L:157:ASP:OD2	2.33	0.46
1:A:26:GLN:O	1:A:26:GLN:HG3	2.15	0.46
1:B:151:VAL:HG12	1:B:152:SER:N	2.29	0.46
1:J:189:ILE:HG23	1:J:189:ILE:O	2.14	0.46
1:J:18:ARG:HE	1:J:197:ASP:CG	2.19	0.46
1:K:8:TYR:CD1	1:K:8:TYR:O	2.68	0.46
1:B:171:PHE:HA	1:B:188:ALA:O	2.15	0.46
1:E:153:PHE:O	1:E:186:PRO:HB3	2.16	0.46
1:J:45:LEU:HD23	1:J:45:LEU:HA	1.77	0.46
1:K:165:ASN:HA	1:K:167:PHE:CZ	2.50	0.46
1:B:39:LEU:O	1:B:185:MET:N	2.44	0.46
1:E:56:TYR:HB3	1:E:57:PRO:HD3	1.97	0.46
1:F:202:GLY:O	1:F:203:ARG:C	2.54	0.46
1:J:64:ALA:O	1:J:68:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:MET:CE	1:B:205:LEU:HA	2.45	0.46
1:E:105:LEU:HD21	1:E:127:TYR:HB2	1.97	0.46
1:E:59:PHE:CE2	1:E:173:MET:SD	3.08	0.46
1:J:122:GLN:O	1:J:126:CYS:HB3	2.16	0.46
1:J:145:VAL:HG11	1:J:173:MET:HE3	1.97	0.46
1:L:67:MET:HB3	1:L:88:VAL:HG21	1.97	0.46
1:A:204:MET:HE2	1:A:205:LEU:N	2.31	0.46
1:B:155:SER:O	1:C:35:GLN:HA	2.16	0.46
1:D:51:ASN:H	1:D:51:ASN:ND2	2.12	0.46
1:E:67:MET:HE2	1:E:171:PHE:HE1	1.79	0.46
1:J:106:TRP:CG	1:J:142:MET:HE3	2.49	0.46
1:A:139:ILE:HG12	1:A:142:MET:HE3	1.98	0.46
1:I:145:VAL:CG1	1:I:173:MET:HE2	2.46	0.46
1:K:154:THR:HG21	1:L:38:GLN:OE1	2.16	0.46
1:K:34:ASN:HB3	1:K:157:ASP:OD1	2.16	0.46
1:E:26:GLN:HA	1:E:26:GLN:NE2	2.30	0.46
1:G:113:PHE:CG	1:G:113:PHE:O	2.68	0.46
1:B:105:LEU:HA	1:B:105:LEU:HD23	1.61	0.45
1:E:59:PHE:CD2	1:E:173:MET:HE2	2.45	0.45
1:I:67:MET:HG3	1:I:143:PHE:CG	2.51	0.45
1:J:124:VAL:O	1:J:128:GLY:CA	2.65	0.45
1:J:90:PRO:HD2	1:J:107:SER:O	2.16	0.45
1:C:51:ASN:HB3	1:C:52:LYS:H	1.57	0.45
1:H:26:GLN:NE2	1:H:26:GLN:HA	2.30	0.45
1:F:26:GLN:HA	1:F:26:GLN:NE2	2.31	0.45
1:J:159:ASN:HD22	1:L:159:ASN:ND2	1.87	0.45
1:A:175:LYS:HZ3	1:A:175:LYS:HG3	1.40	0.45
1:A:35:GLN:O	1:A:188:ALA:HA	2.17	0.45
1:A:40:ASP:HA	1:A:184:LEU:HD23	1.98	0.45
1:B:158:LEU:HD13	1:B:160:VAL:HG23	1.87	0.45
1:B:19:LYS:HE3	1:B:23:GLU:OE2	2.17	0.45
1:H:192:HIS:HD1	1:H:194:ALA:N	1.97	0.45
1:I:6:THR:CG2	1:I:6:THR:OG1	2.52	0.45
1:J:63:LEU:HD13	1:J:171:PHE:CG	2.51	0.45
1:K:59:PHE:CE2	1:K:173:MET:SD	3.09	0.45
1:L:74:ARG:HB2	1:L:84:ILE:HG23	1.97	0.45
1:I:171:PHE:HA	1:I:188:ALA:O	2.16	0.45
1:L:182:LYS:HZ2	1:L:182:LYS:HG2	1.62	0.45
1:A:145:VAL:CG1	1:A:173:MET:HE2	2.46	0.45
1:H:205:LEU:O	1:H:208:LEU:HB3	2.17	0.45
1:J:89:HIS:CE1	1:J:108:GLU:CG	2.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:TRP:HD1	1:L:142:MET:HE1	1.82	0.45
1:C:56:TYR:CE1	1:C:173:MET:HE1	2.52	0.45
1:D:36:THR:HG22	1:F:154:THR:HG22	1.99	0.45
1:G:36:THR:HB	1:I:155:SER:HB3	1.98	0.45
1:L:149:PRO:HD2	1:L:150:TRP:CZ3	2.52	0.45
1:L:144:PHE:HB2	1:L:170:VAL:HG22	1.99	0.45
1:C:96:HIS:CE1	1:C:128:GLY:O	2.70	0.45
1:C:56:TYR:HE1	1:C:173:MET:CE	2.29	0.45
1:F:26:GLN:HA	1:F:26:GLN:HE21	1.81	0.45
1:H:101:THR:HB	2:H:231:HOH:O	2.16	0.45
1:K:49:LYS:C	1:K:51:ASN:O	2.55	0.45
1:A:13:ILE:H	1:A:13:ILE:HD12	1.82	0.45
1:B:204:MET:HE2	1:B:205:LEU:HG	1.99	0.45
1:C:67:MET:CE	1:C:73:PHE:CD1	2.99	0.45
1:D:77:MET:HB2	1:D:165:ASN:HB3	1.99	0.45
1:F:204:MET:HE2	1:F:205:LEU:CA	2.47	0.45
1:J:93:THR:HA	1:J:103:SER:O	2.16	0.45
1:K:205:LEU:HD23	1:K:205:LEU:HA	1.85	0.45
1:J:159:ASN:HD21	1:K:159:ASN:HD21	1.60	0.45
1:J:6:THR:O	1:J:6:THR:CG2	2.53	0.45
1:A:149:PRO:O	1:A:175:LYS:HB2	2.18	0.44
1:B:78:LYS:O	1:B:79:ASP:C	2.55	0.44
1:G:30:GLN:NE2	2:G:225:HOH:O	2.50	0.44
1:H:113:PHE:N	1:H:219:ALA:HB3	2.30	0.44
1:J:25:PHE:HB2	1:J:194:ALA:HA	1.99	0.44
1:J:98:GLN:N	1:J:98:GLN:HE21	2.16	0.44
1:I:57:PRO:HB3	1:I:120:TYR:CD2	2.52	0.44
1:J:203:ARG:HG2	1:J:207:GLU:OE2	2.17	0.44
1:J:75:MET:HA	1:J:83:VAL:O	2.17	0.44
1:C:30:GLN:HE22	1:C:164:ASP:HA	1.83	0.44
1:D:67:MET:HE1	1:D:73:PHE:HB3	1.92	0.44
1:E:6:THR:HG21	1:E:89:HIS:HE2	1.82	0.44
1:H:132:ALA:O	1:H:135:PRO:HD3	2.16	0.44
1:H:35:GLN:NE2	1:H:201:VAL:HG11	2.32	0.44
1:K:187:LEU:HG	1:K:188:ALA:N	2.30	0.44
1:D:159:ASN:ND2	1:F:159:ASN:CG	2.70	0.44
1:G:171:PHE:HA	1:G:188:ALA:O	2.17	0.44
1:H:155:SER:HB3	1:I:36:THR:HB	1.98	0.44
1:G:106:TRP:HB3	1:G:142:MET:HE3	2.00	0.44
1:I:94:VAL:N	1:I:103:SER:O	2.38	0.44
1:J:124:VAL:O	1:J:128:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:PHE:O	1:J:60:ILE:C	2.55	0.44
1:E:139:ILE:N	1:E:142:MET:HE3	2.18	0.44
1:F:59:PHE:O	1:F:60:ILE:C	2.55	0.44
1:H:57:PRO:HG3	1:H:120:TYR:CZ	2.53	0.44
1:H:67:MET:CE	1:H:73:PHE:CB	2.73	0.44
1:L:130:ASN:HB2	1:L:135:PRO:HB3	2.00	0.44
1:L:25:PHE:HB2	1:L:194:ALA:HA	2.00	0.44
1:A:159:ASN:OD1	1:B:159:ASN:ND2	2.47	0.44
1:A:30:GLN:HE22	1:A:164:ASP:HA	1.82	0.44
1:C:63:LEU:HD23	1:C:208:LEU:HD13	1.99	0.44
1:G:38:GLN:NE2	1:G:177:TYR:OH	2.50	0.44
1:H:34:ASN:ND2	1:H:158:LEU:H	2.15	0.44
1:D:163:MET:HG2	1:D:163:MET:H	1.61	0.44
1:D:185:MET:HA	1:D:186:PRO:HD3	1.75	0.44
1:D:20:GLU:OE1	1:F:133:TYR:N	2.42	0.44
1:I:149:PRO:HD2	1:I:150:TRP:CE3	2.52	0.44
1:I:77:MET:CE	1:I:82:LEU:HB2	2.47	0.44
1:K:66:LEU:HD23	1:K:66:LEU:HA	1.71	0.44
1:K:72:GLU:HG2	1:K:73:PHE:H	1.83	0.44
1:E:4:LYS:HB3	1:E:4:LYS:HE3	1.30	0.44
1:K:59:PHE:O	1:K:60:ILE:C	2.56	0.44
1:G:85:TRP:CH2	1:G:140:GLU:HG3	2.53	0.43
1:G:159:ASN:CG	1:H:159:ASN:ND2	2.72	0.43
1:I:192:HIS:HD1	1:I:194:ALA:H	1.64	0.43
1:G:29:ALA:O	1:G:30:GLN:C	2.56	0.43
1:L:92:TYR:HA	1:L:145:VAL:O	2.18	0.43
1:B:66:LEU:O	1:B:67:MET:C	2.50	0.43
1:D:85:TRP:CZ2	1:D:140:GLU:HB3	2.53	0.43
1:D:85:TRP:CG	1:D:141:ASN:HB3	2.53	0.43
1:H:156:PHE:CD2	1:H:157:ASP:N	2.85	0.43
1:J:32:THR:HG22	1:J:163:MET:SD	2.59	0.43
1:C:203:ARG:O	1:C:207:GLU:HG3	2.18	0.43
1:E:77:MET:HE3	1:E:77:MET:HB2	1.52	0.43
1:G:15:GLN:HA	1:G:15:GLN:NE2	2.25	0.43
1:H:210:GLN:O	1:H:211:TYR:C	2.57	0.43
1:I:91:CYS:HA	1:I:105:LEU:O	2.19	0.43
1:D:168:ALA:HA	1:D:169:PRO:HD3	1.79	0.43
1:G:30:GLN:HG2	1:G:163:MET:SD	2.58	0.43
1:H:168:ALA:HA	1:H:169:PRO:HD3	1.88	0.43
1:I:4:LYS:HB3	1:I:5:ILE:HD13	2.01	0.43
1:I:6:THR:CG2	1:I:6:THR:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:PHE:CD2	1:J:173:MET:HE1	2.53	0.43
1:L:92:TYR:CD1	1:L:92:TYR:O	2.72	0.43
1:G:50:LYS:HA	1:G:50:LYS:HD2	1.68	0.43
1:B:47:THR:HG21	1:B:215:TRP:O	2.19	0.43
1:C:38:GLN:HE22	1:C:186:PRO:HG3	1.83	0.43
1:H:45:LEU:HD23	1:H:45:LEU:HA	1.91	0.43
1:H:67:MET:CE	1:H:73:PHE:CG	3.02	0.43
1:J:18:ARG:NH2	1:J:193:HIS:O	2.52	0.43
1:J:22:PHE:O	1:J:26:GLN:N	2.47	0.43
1:L:57:PRO:HG2	1:L:58:ALA:H	1.81	0.43
1:C:27:SER:OG	1:C:28:VAL:N	2.45	0.43
1:C:56:TYR:N	1:C:57:PRO:CD	2.81	0.43
1:C:70:HIS:HB3	1:C:72:GLU:OE1	2.19	0.43
1:D:159:ASN:ND2	1:F:159:ASN:ND2	2.67	0.43
1:H:25:PHE:CZ	1:H:193:HIS:CE1	3.06	0.43
1:D:187:LEU:HD22	1:D:208:LEU:CD2	2.48	0.43
1:F:38:GLN:NE2	1:F:177:TYR:OH	2.51	0.43
1:H:63:LEU:O	1:H:67:MET:HG2	2.18	0.43
1:J:171:PHE:CE2	1:J:204:MET:CE	3.01	0.43
1:K:67:MET:HG3	1:K:143:PHE:CD2	2.54	0.43
1:L:56:TYR:HB3	1:L:57:PRO:CD	2.49	0.43
1:B:112:ASP:HB3	1:B:115:GLN:HB2	1.99	0.43
1:G:40:ASP:HA	1:G:184:LEU:HD23	2.01	0.43
1:L:206:ASN:O	1:L:210:GLN:HB2	2.19	0.43
1:L:66:LEU:HD21	1:L:211:TYR:CE2	2.51	0.43
1:C:105:LEU:HA	1:C:105:LEU:HD23	1.89	0.42
1:H:25:PHE:HB2	1:H:194:ALA:CA	2.48	0.42
1:J:57:PRO:HB3	1:J:120:TYR:CD2	2.54	0.42
1:L:67:MET:HE1	1:L:169:PRO:CG	2.42	0.42
1:C:19:LYS:HE2	1:C:23:GLU:OE2	2.19	0.42
1:C:25:PHE:O	1:C:30:GLN:HG3	2.18	0.42
1:D:93:THR:HA	1:D:103:SER:O	2.19	0.42
1:L:47:THR:HA	1:L:50:LYS:HD3	2.01	0.42
1:C:66:LEU:HD11	1:C:208:LEU:HA	2.01	0.42
1:C:89:HIS:O	1:C:142:MET:HA	2.19	0.42
1:D:59:PHE:CD2	1:D:173:MET:CE	3.02	0.42
1:D:42:THR:OG1	1:D:182:LYS:HA	2.20	0.42
1:E:147:ALA:C	1:E:149:PRO:HD3	2.39	0.42
1:I:57:PRO:HB3	1:I:120:TYR:CE2	2.55	0.42
1:J:59:PHE:HD2	1:J:173:MET:CE	2.32	0.42
1:A:28:VAL:HG23	1:A:29:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:TYR:CE2	1:D:134:PHE:HE1	2.37	0.42
1:D:50:LYS:C	1:D:51:ASN:O	2.56	0.42
1:G:25:PHE:HB2	1:G:194:ALA:HA	2.01	0.42
1:H:34:ASN:HD21	1:H:158:LEU:H	1.67	0.42
1:A:190:GLN:CG	1:A:190:GLN:O	2.66	0.42
1:C:56:TYR:CE1	1:C:173:MET:CE	3.02	0.42
1:D:29:ALA:O	1:D:30:GLN:C	2.57	0.42
1:I:132:ALA:O	1:I:135:PRO:HD3	2.20	0.42
1:I:6:THR:CG2	1:I:141:ASN:ND2	2.67	0.42
1:K:176:TYR:HA	1:K:184:LEU:O	2.19	0.42
1:K:73:PHE:CZ	1:K:204:MET:HB2	2.54	0.42
1:L:158:LEU:HB3	1:L:190:GLN:HG3	2.02	0.42
1:A:56:TYR:H	1:A:57:PRO:HD2	1.84	0.42
1:F:56:TYR:HB3	1:F:57:PRO:HD3	2.01	0.42
1:G:56:TYR:HB3	1:G:57:PRO:CD	2.49	0.42
1:J:154:THR:O	1:L:154:THR:CG2	2.58	0.42
1:J:34:ASN:HB2	1:L:157:ASP:HB2	2.01	0.42
1:E:34:ASN:ND2	1:E:190:GLN:CB	2.77	0.42
1:H:35:GLN:O	1:H:188:ALA:HA	2.19	0.42
1:B:100:GLU:HG2	1:C:199:PHE:CE1	2.55	0.42
1:L:197:ASP:O	1:L:201:VAL:HG23	2.19	0.42
1:A:106:TRP:HB3	1:A:142:MET:HE2	2.01	0.42
1:E:120:TYR:CD2	1:E:120:TYR:C	2.93	0.42
1:F:204:MET:HE2	1:F:205:LEU:N	2.35	0.42
1:G:184:LEU:HD23	1:G:184:LEU:HA	1.71	0.42
1:G:32:THR:HG22	1:I:159:ASN:CB	2.20	0.42
1:K:122:GLN:HG3	1:K:122:GLN:O	2.19	0.42
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.96	0.41
1:F:25:PHE:O	1:F:30:GLN:HA	2.19	0.41
1:J:132:ALA:O	1:J:135:PRO:HD3	2.19	0.41
1:L:22:PHE:O	1:L:26:GLN:HG2	2.19	0.41
1:G:156:PHE:C	1:G:156:PHE:CD2	2.93	0.41
1:I:145:VAL:HG11	1:I:173:MET:HE2	2.01	0.41
1:L:105:LEU:HD21	1:L:127:TYR:HB2	2.02	0.41
1:L:70:HIS:NE2	1:L:207:GLU:OE1	2.47	0.41
1:K:57:PRO:HB3	1:K:120:TYR:CD2	2.56	0.41
1:D:182:LYS:HZ3	1:D:182:LYS:HG3	1.46	0.41
1:K:59:PHE:CD2	1:K:173:MET:CE	3.03	0.41
1:L:205:LEU:HD23	1:L:205:LEU:HA	1.96	0.41
1:D:114:ARG:CG	1:D:114:ARG:NH1	2.83	0.41
1:D:85:TRP:CD2	1:D:141:ASN:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ASN:HA	1:E:167:PHE:CE1	2.55	0.41
1:F:153:PHE:O	1:F:186:PRO:HB3	2.21	0.41
1:G:139:ILE:HG13	1:G:142:MET:HG3	2.02	0.41
1:K:89:HIS:O	1:K:142:MET:HA	2.20	0.41
1:A:90:PRO:O	1:A:106:TRP:HA	2.21	0.41
1:B:91:CYS:HA	1:B:105:LEU:O	2.21	0.41
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.81	0.41
1:E:41:ILE:HG13	1:E:183:VAL:O	2.19	0.41
1:E:66:LEU:HD23	1:E:66:LEU:HA	1.89	0.41
1:G:118:HIS:O	1:G:122:GLN:HG3	2.21	0.41
1:I:120:TYR:O	1:I:123:ASP:HB2	2.21	0.41
1:J:162:ASN:HB3	2:K:221:HOH:O	2.20	0.41
1:K:92:TYR:N	1:K:92:TYR:CD2	2.88	0.41
1:A:38:GLN:HE22	1:A:186:PRO:HG3	1.86	0.41
1:C:25:PHE:HB2	1:C:194:ALA:HA	2.03	0.41
1:F:151:VAL:HG12	1:F:151:VAL:O	2.21	0.41
1:L:171:PHE:CZ	1:L:189:ILE:HD13	2.55	0.41
1:B:154:THR:CG2	1:C:154:THR:O	2.65	0.41
1:F:72:GLU:HG3	1:F:200:HIS:HB3	2.03	0.41
1:H:154:THR:HG22	1:I:154:THR:O	2.21	0.41
1:J:8:TYR:CD1	1:J:83:VAL:HG21	2.55	0.41
1:L:118:HIS:O	1:L:119:ILE:CB	2.69	0.41
1:I:59:PHE:CD2	1:I:173:MET:CE	3.03	0.41
1:I:89:HIS:ND1	1:I:108:GLU:HA	2.36	0.41
1:L:67:MET:HE3	1:L:73:PHE:CB	2.31	0.41
1:C:67:MET:CE	1:C:73:PHE:CD2	2.94	0.41
1:E:65:ARG:NH2	2:E:230:HOH:O	2.53	0.41
1:K:57:PRO:HA	1:K:60:ILE:HD12	2.02	0.41
1:B:204:MET:HE3	1:B:204:MET:O	2.21	0.41
1:C:204:MET:HE2	1:C:205:LEU:HD23	2.02	0.41
1:E:64:ALA:HB1	1:E:109:TYR:CD1	2.56	0.41
1:F:204:MET:CE	1:F:205:LEU:HA	2.50	0.41
1:I:26:GLN:HA	1:I:26:GLN:HE21	1.86	0.41
1:A:27:SER:OG	1:A:28:VAL:HG22	2.20	0.40
1:B:119:ILE:O	1:B:120:TYR:C	2.59	0.40
1:B:18:ARG:NE	1:B:197:ASP:OD1	2.46	0.40
1:E:38:GLN:NE2	1:E:177:TYR:OH	2.54	0.40
1:G:56:TYR:HB3	1:G:57:PRO:HD3	2.03	0.40
1:H:91:CYS:SG	1:H:142:MET:CE	3.07	0.40
1:I:138:PHE:C	1:I:142:MET:CE	2.82	0.40
1:G:159:ASN:HD21	1:I:159:ASN:HD21	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:TYR:O	1:B:110:HIS:CD2	2.74	0.40
1:F:106:TRP:HB3	1:F:142:MET:HE2	2.03	0.40
1:F:168:ALA:HA	1:F:169:PRO:HD3	1.93	0.40
1:J:136:LYS:NZ	2:J:223:HOH:O	2.54	0.40
1:K:168:ALA:HA	1:K:169:PRO:HD3	1.96	0.40
1:L:134:PHE:O	1:L:136:LYS:N	2.55	0.40
1:A:187:LEU:HD23	1:A:208:LEU:CD2	2.51	0.40
1:B:25:PHE:HB2	1:B:194:ALA:HA	2.02	0.40
1:J:67:MET:CE	1:J:73:PHE:CD1	3.04	0.40
1:K:154:THR:HG22	1:L:36:THR:CB	2.52	0.40
1:K:75:MET:HB2	1:K:195:VAL:HG11	2.03	0.40
1:A:63:LEU:O	1:A:67:MET:HG2	2.21	0.40
1:A:8:TYR:HB2	1:A:83:VAL:HG13	2.04	0.40
1:B:204:MET:HE3	1:B:205:LEU:HA	2.02	0.40
1:D:114:ARG:NH1	1:D:114:ARG:HG3	2.36	0.40
1:F:123:ASP:OD1	1:F:136:LYS:HE3	2.21	0.40
1:K:185:MET:HA	1:K:186:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/219 (96%)	203 (96%)	7 (3%)	1 (0%)	32	53
1	B	214/219 (98%)	204 (95%)	8 (4%)	2 (1%)	20	36
1	C	211/219 (96%)	200 (95%)	8 (4%)	3 (1%)	13	23
1	D	211/219 (96%)	196 (93%)	12 (6%)	3 (1%)	13	23
1	E	213/219 (97%)	199 (93%)	12 (6%)	2 (1%)	20	36
1	F	210/219 (96%)	195 (93%)	14 (7%)	1 (0%)	32	53
1	G	211/219 (96%)	196 (93%)	14 (7%)	1 (0%)	32	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	214/219 (98%)	204 (95%)	8 (4%)	2 (1%)	20	36
1	I	212/219 (97%)	199 (94%)	11 (5%)	2 (1%)	20	36
1	J	209/219 (95%)	191 (91%)	16 (8%)	2 (1%)	18	32
1	K	210/219 (96%)	195 (93%)	10 (5%)	5 (2%)	7	11
1	L	208/219 (95%)	188 (90%)	16 (8%)	4 (2%)	9	15
All	All	2534/2628 (96%)	2370 (94%)	136 (5%)	28 (1%)	17	29

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	B	79	ASP
1	D	164	ASP
1	K	48	VAL
1	L	119	ILE
1	B	28	VAL
1	C	29	ALA
1	E	4	LYS
1	E	29	ALA
1	K	166	PHE
1	L	128	GLY
1	C	50	LYS
1	D	50	LYS
1	H	6	THR
1	H	52	LYS
1	K	29	ALA
1	I	29	ALA
1	K	47	THR
1	K	165	ASN
1	D	180	GLY
1	G	19	LYS
1	J	72	GLU
1	F	198	GLY
1	L	129	GLU
1	I	135	PRO
1	J	13	ILE
1	L	80	GLY
1	C	28	VAL

### 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	189/194 (97%)	160 (85%)	29 (15%)	3	6
1	B	192/194 (99%)	163 (85%)	29 (15%)	3	6
1	C	189/194 (97%)	163 (86%)	26 (14%)	4	8
1	D	189/194 (97%)	162 (86%)	27 (14%)	4	7
1	E	192/194 (99%)	161 (84%)	31 (16%)	3	5
1	F	189/194 (97%)	161 (85%)	28 (15%)	3	6
1	G	189/194 (97%)	164 (87%)	25 (13%)	5	8
1	H	191/194 (98%)	171 (90%)	20 (10%)	8	15
1	I	191/194 (98%)	163 (85%)	28 (15%)	3	6
1	J	189/194 (97%)	158 (84%)	31 (16%)	2	5
1	K	190/194 (98%)	150 (79%)	40 (21%)	1	2
1	L	188/194 (97%)	154 (82%)	34 (18%)	2	3
All	All	2278/2328 (98%)	1930 (85%)	348 (15%)	3	6

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	28	VAL
1	A	32	THR
1	A	37	VAL
1	A	39	LEU
1	A	45	LEU
1	A	52	LYS
1	A	54	LYS
1	A	81	GLU
1	A	83	VAL
1	A	94	VAL
1	A	97	GLU
1	A	114	ARG
1	A	135	PRO

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Mol	Chain	Res	Type
1	A	136	LYS
1	A	140	GLU
1	A	142	MET
1	A	146	SER
1	A	148	ASN
1	A	154	THR
1	A	160	VAL
1	A	173	MET
1	A	175	LYS
1	A	182	LYS
1	A	189	ILE
1	A	190	GLN
1	A	196	CYS
1	A	204	MET
1	A	211	TYR
1	B	5	ILE
1	B	9	THR
1	B	10	THR
1	B	19	LYS
1	B	28	VAL
1	B	32	THR
1	B	37	VAL
1	B	39	LEU
1	B	45	LEU
1	B	49	LYS
1	B	50	LYS
1	B	83	VAL
1	B	87	SER
1	B	94	VAL
1	B	104	SER
1	B	111	ASP
1	B	114	ARG
1	B	117	LEU
1	B	129	GLU
1	B	140	GLU
1	B	154	THR
1	B	158	LEU
1	B	159	ASN
1	B	160	VAL
1	B	175	LYS
1	B	187	LEU
1	B	189	ILE

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Mol	Chain	Res	Type
1	B	190	GLN
1	B	204	MET
1	C	6	THR
1	C	9	THR
1	C	13	ILE
1	C	23	GLU
1	C	27	SER
1	C	32	THR
1	C	39	LEU
1	C	45	LEU
1	C	50	LYS
1	C	54	LYS
1	C	62	ILE
1	C	111	ASP
1	C	114	ARG
1	C	115	GLN
1	C	117	LEU
1	C	126	CYS
1	C	139	ILE
1	C	154	THR
1	C	155	SER
1	C	158	LEU
1	C	162	ASN
1	C	179	GLN
1	C	182	LYS
1	C	190	GLN
1	C	204	MET
1	C	216	GLN
1	D	8	TYR
1	D	9	THR
1	D	13	ILE
1	D	15	GLN
1	D	19	LYS
1	D	28	VAL
1	D	32	THR
1	D	39	LEU
1	D	45	LEU
1	D	54	LYS
1	D	71	PRO
1	D	77	MET
1	D	81	GLU
1	D	83	VAL

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Mol	Chain	Res	Type
1	D	111	ASP
1	D	114	ARG
1	D	117	LEU
1	D	148	ASN
1	D	152	SER
1	D	154	THR
1	D	155	SER
1	D	160	VAL
1	D	163	MET
1	D	164	ASP
1	D	189	ILE
1	D	190	GLN
1	D	193	HIS
1	E	3	LYS
1	E	4	LYS
1	E	5	ILE
1	E	6	THR
1	E	9	THR
1	E	10	THR
1	E	15	GLN
1	E	19	LYS
1	E	20	GLU
1	E	32	THR
1	E	37	VAL
1	E	39	LEU
1	E	45	LEU
1	E	54	LYS
1	E	81	GLU
1	E	83	VAL
1	E	98	GLN
1	E	108	GLU
1	E	114	ARG
1	E	115	GLN
1	E	117	LEU
1	E	120	TYR
1	E	129	GLU
1	E	136	LYS
1	E	138	PHE
1	E	142	MET
1	E	154	THR
1	E	158	LEU
1	E	187	LEU

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Mol	Chain	Res	Type
1	E	189	ILE
1	E	190	GLN
1	F	9	THR
1	F	12	ASP
1	F	15	GLN
1	F	19	LYS
1	F	32	THR
1	F	37	VAL
1	F	39	LEU
1	F	45	LEU
1	F	50	LYS
1	F	52	LYS
1	F	54	LYS
1	F	62	ILE
1	F	77	MET
1	F	83	VAL
1	F	114	ARG
1	F	115	GLN
1	F	117	LEU
1	F	119	ILE
1	F	121	SER
1	F	136	LYS
1	F	148	ASN
1	F	151	VAL
1	F	157	ASP
1	F	189	ILE
1	F	190	GLN
1	F	204	MET
1	F	212	CYS
1	F	215	TRP
1	G	9	THR
1	G	12	ASP
1	G	15	GLN
1	G	32	THR
1	G	35	GLN
1	G	39	LEU
1	G	45	LEU
1	G	48	VAL
1	G	50	LYS
1	G	52	LYS
1	G	54	LYS
1	G	67	MET

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Mol	Chain	Res	Type
1	G	78	LYS
1	G	111	ASP
1	G	115	GLN
1	G	119	ILE
1	G	146	SER
1	G	148	ASN
1	G	151	VAL
1	G	154	THR
1	G	158	LEU
1	G	160	VAL
1	G	181	ASP
1	G	190	GLN
1	G	204	MET
1	H	4	LYS
1	H	23	GLU
1	H	32	THR
1	H	37	VAL
1	H	39	LEU
1	H	45	LEU
1	H	50	LYS
1	H	52	LYS
1	H	54	LYS
1	H	62	ILE
1	H	83	VAL
1	H	87	SER
1	H	122	GLN
1	H	129	GLU
1	H	157	ASP
1	H	158	LEU
1	H	160	VAL
1	H	181	ASP
1	H	190	GLN
1	H	212	CYS
1	I	4	LYS
1	I	10	THR
1	I	14	SER
1	I	28	VAL
1	I	32	THR
1	I	39	LEU
1	I	45	LEU
1	I	46	LYS
1	I	52	LYS

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Mol	Chain	Res	Type
1	I	54	LYS
1	I	62	ILE
1	I	81	GLU
1	I	83	VAL
1	I	97	GLU
1	I	105	LEU
1	I	112	ASP
1	I	114	ARG
1	I	115	GLN
1	I	117	LEU
1	I	126	CYS
1	I	136	LYS
1	I	139	ILE
1	I	146	SER
1	I	154	THR
1	I	157	ASP
1	I	158	LEU
1	I	160	VAL
1	I	190	GLN
1	J	9	THR
1	J	18	ARG
1	J	28	VAL
1	J	32	THR
1	J	35	GLN
1	J	39	LEU
1	J	45	LEU
1	J	50	LYS
1	J	56	TYR
1	J	67	MET
1	J	78	LYS
1	J	83	VAL
1	J	87	SER
1	J	94	VAL
1	J	98	GLN
1	J	107	SER
1	J	111	ASP
1	J	117	LEU
1	J	122	GLN
1	J	129	GLU
1	J	131	LEU
1	J	138	PHE
1	J	152	SER

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Mol	Chain	Res	Type
1	J	157	ASP
1	J	158	LEU
1	J	175	LYS
1	J	178	THR
1	J	181	ASP
1	J	182	LYS
1	J	190	GLN
1	J	215	TRP
1	K	4	LYS
1	K	9	THR
1	K	10	THR
1	K	12	ASP
1	K	14	SER
1	K	15	GLN
1	K	17	HIS
1	K	28	VAL
1	K	32	THR
1	K	37	VAL
1	K	39	LEU
1	K	45	LEU
1	K	46	LYS
1	K	52	LYS
1	K	54	LYS
1	K	77	MET
1	K	78	LYS
1	K	83	VAL
1	K	103	SER
1	K	105	LEU
1	K	108	GLU
1	K	114	ARG
1	K	117	LEU
1	K	122	GLN
1	K	126	CYS
1	K	136	LYS
1	K	140	GLU
1	K	142	MET
1	K	146	SER
1	K	151	VAL
1	K	154	THR
1	K	158	LEU
1	K	160	VAL
1	K	179	GLN

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Mol	Chain	Res	Type
1	K	181	ASP
1	K	187	LEU
1	K	190	GLN
1	K	203	ARG
1	K	204	MET
1	K	210	GLN
1	L	6	THR
1	L	10	THR
1	L	15	GLN
1	L	19	LYS
1	L	27	SER
1	L	39	LEU
1	L	50	LYS
1	L	52	LYS
1	L	54	LYS
1	L	56	TYR
1	L	77	MET
1	L	78	LYS
1	L	79	ASP
1	L	83	VAL
1	L	94	VAL
1	L	97	GLU
1	L	100	GLU
1	L	104	SER
1	L	105	LEU
1	L	111	ASP
1	L	114	ARG
1	L	117	LEU
1	L	122	GLN
1	L	129	GLU
1	L	136	LYS
1	L	146	SER
1	L	151	VAL
1	L	154	THR
1	L	158	LEU
1	L	182	LYS
1	L	190	GLN
1	L	204	MET
1	L	210	GLN
1	L	214	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	30	GLN
1	A	38	GLN
1	A	148	ASN
1	A	159	ASN
1	B	26	GLN
1	B	34	ASN
1	B	38	GLN
1	B	159	ASN
1	C	26	GLN
1	C	30	GLN
1	C	51	ASN
1	C	110	HIS
1	C	159	ASN
1	C	190	GLN
1	C	216	GLN
1	D	26	GLN
1	D	30	GLN
1	D	34	ASN
1	D	38	GLN
1	D	110	HIS
1	D	148	ASN
1	D	159	ASN
1	D	190	GLN
1	E	26	GLN
1	E	30	GLN
1	E	34	ASN
1	E	159	ASN
1	E	190	GLN
1	F	26	GLN
1	F	30	GLN
1	F	34	ASN
1	F	38	GLN
1	F	110	HIS
1	F	148	ASN
1	F	159	ASN
1	F	190	GLN
1	G	15	GLN
1	G	26	GLN
1	G	30	GLN
1	G	38	GLN
1	G	53	HIS
1	G	148	ASN

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Mol	Chain	Res	Type
1	G	159	ASN
1	G	190	GLN
1	H	26	GLN
1	H	30	GLN
1	H	34	ASN
1	H	38	GLN
1	H	159	ASN
1	I	26	GLN
1	I	30	GLN
1	I	34	ASN
1	I	38	GLN
1	I	51	ASN
1	I	122	GLN
1	I	141	ASN
1	I	148	ASN
1	I	159	ASN
1	I	190	GLN
1	J	30	GLN
1	J	34	ASN
1	J	98	GLN
1	J	148	ASN
1	J	159	ASN
1	J	190	GLN
1	K	17	HIS
1	K	30	GLN
1	K	38	GLN
1	K	122	GLN
1	K	159	ASN
1	K	179	GLN
1	K	190	GLN
1	L	26	GLN
1	L	30	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/219 (97%)	-0.07	1 (0%) 90 91	21, 34, 50, 57	0
1	B	216/219 (98%)	-0.10	1 (0%) 90 91	23, 39, 59, 71	0
1	C	213/219 (97%)	0.04	3 (1%) 75 76	24, 38, 62, 76	0
1	D	213/219 (97%)	0.06	3 (1%) 75 76	27, 42, 60, 80	0
1	E	215/219 (98%)	0.07	3 (1%) 75 76	30, 45, 64, 84	0
1	F	212/219 (96%)	0.11	5 (2%) 59 61	29, 45, 62, 74	0
1	G	213/219 (97%)	0.13	4 (1%) 67 69	31, 41, 59, 69	0
1	H	216/219 (98%)	0.09	7 (3%) 48 51	19, 37, 52, 72	0
1	I	214/219 (97%)	0.19	2 (0%) 84 85	32, 44, 62, 72	0
1	J	211/219 (96%)	0.65	27 (12%) 4 3	38, 55, 77, 81	0
1	K	212/219 (96%)	0.63	23 (10%) 6 6	43, 59, 76, 88	0
1	L	210/219 (95%)	0.74	28 (13%) 4 3	40, 55, 74, 84	0
All	All	2558/2628 (97%)	0.21	107 (4%) 37 39	19, 44, 69, 88	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	124	VAL	6.0
1	J	125	ALA	5.5
1	H	5	ILE	4.8
1	J	6	THR	4.6
1	L	6	THR	4.5
1	J	46	LYS	4.0
1	K	158	LEU	3.9
1	G	15	GLN	3.9
1	L	15	GLN	3.8
1	K	215	TRP	3.8
1	L	115	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	122	GLN	3.7
1	H	218	GLY	3.6
1	K	114	ARG	3.5
1	K	98	GLN	3.5
1	F	173	MET	3.5
1	L	113	PHE	3.5
1	L	125	ALA	3.4
1	L	181	ASP	3.4
1	L	131	LEU	3.3
1	L	118	HIS	3.3
1	D	46	LYS	3.2
1	K	50	LYS	3.2
1	J	43	ALA	3.2
1	L	114	ARG	3.2
1	J	181	ASP	3.2
1	F	77	MET	3.1
1	L	112	ASP	3.0
1	L	122	GLN	3.0
1	I	124	VAL	3.0
1	G	6	THR	3.0
1	H	219	ALA	3.0
1	G	98	GLN	2.8
1	F	211	TYR	2.8
1	C	118	HIS	2.8
1	L	23	GLU	2.7
1	J	50	LYS	2.7
1	L	71	PRO	2.7
1	J	14	SER	2.7
1	K	46	LYS	2.7
1	J	156	PHE	2.6
1	K	22	PHE	2.6
1	L	14	SER	2.6
1	L	188	ALA	2.6
1	L	89	HIS	2.6
1	H	6	THR	2.6
1	J	15	GLN	2.5
1	K	173	MET	2.5
1	J	34	ASN	2.5
1	J	97	GLU	2.5
1	J	180	GLY	2.5
1	L	179	GLN	2.5
1	L	45	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	157	ASP	2.4
1	L	77	MET	2.4
1	F	181	ASP	2.4
1	E	155	SER	2.4
1	K	15	GLN	2.4
1	J	51	ASN	2.4
1	H	154	THR	2.4
1	J	138	PHE	2.4
1	E	12	ASP	2.3
1	J	118	HIS	2.3
1	A	181	ASP	2.3
1	J	95	PHE	2.3
1	J	99	THR	2.3
1	J	98	GLN	2.3
1	L	189	ILE	2.3
1	J	188	ALA	2.3
1	L	130	ASN	2.3
1	K	42	THR	2.3
1	L	50	LYS	2.3
1	K	180	GLY	2.3
1	K	17	HIS	2.3
1	K	211	TYR	2.3
1	B	216	GLN	2.2
1	L	180	GLY	2.2
1	H	155	SER	2.2
1	K	36	THR	2.2
1	C	115	GLN	2.2
1	J	130	ASN	2.2
1	K	44	PHE	2.2
1	D	217	GLY	2.2
1	K	110	HIS	2.2
1	J	121	SER	2.2
1	D	98	GLN	2.2
1	J	13	ILE	2.2
1	K	34	ASN	2.2
1	K	12	ASP	2.1
1	E	173	MET	2.1
1	J	126	CYS	2.1
1	K	127	TYR	2.1
1	L	8	TYR	2.1
1	H	15	GLN	2.1
1	J	127	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	81	GLU	2.1
1	L	172	THR	2.1
1	C	52	LYS	2.1
1	L	83	VAL	2.1
1	F	156	PHE	2.1
1	L	127	TYR	2.0
1	K	130	ASN	2.0
1	G	157	ASP	2.0
1	J	201	VAL	2.0
1	K	48	VAL	2.0
1	K	159	ASN	2.0
1	L	7	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.