



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:34 AM GMT

PDB ID : 3DKT  
Title : Crystal structure of Thermotoga maritima encapsulin  
Authors : Sutter, M.; Boehringer, D.; Gutmann, S.; Weber-Ban, E.; Ban, N.  
Deposited on : 2008-06-26  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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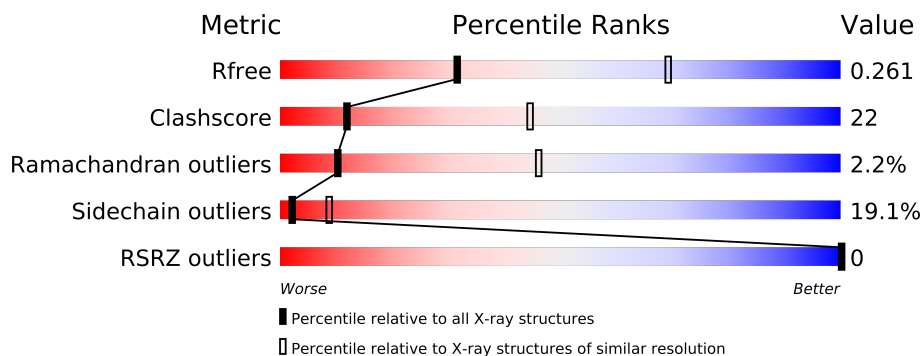
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	B	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	C	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	D	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	E	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	F	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	G	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	H	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	I	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	J	265	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	K	8	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	L	8	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	M	8	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	N	8	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
2	O	8	
2	P	8	
2	Q	8	
2	R	8	
2	S	8	
2	T	8	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22070 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Maritimacin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	B	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	C	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	D	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	E	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	F	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	G	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	H	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	I	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	J	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	L	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	M	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	N	8	Total	C	N	O	0	0	0
			56	34	12	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	P	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	Q	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	R	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	S	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	T	8	Total	C	N	O	0	0	0
			56	34	12	10			

- Molecule 3 is water.

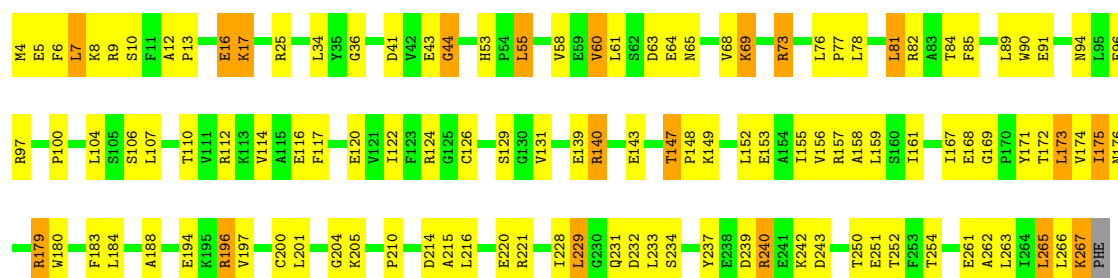
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	11	Total	O	0	0
			11	11		
3	C	9	Total	O	0	0
			9	9		
3	D	12	Total	O	0	0
			12	12		
3	E	9	Total	O	0	0
			9	9		
3	F	11	Total	O	0	0
			11	11		
3	G	9	Total	O	0	0
			9	9		
3	H	11	Total	O	0	0
			11	11		
3	I	9	Total	O	0	0
			9	9		
3	J	10	Total	O	0	0
			10	10		

### 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 errors 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.

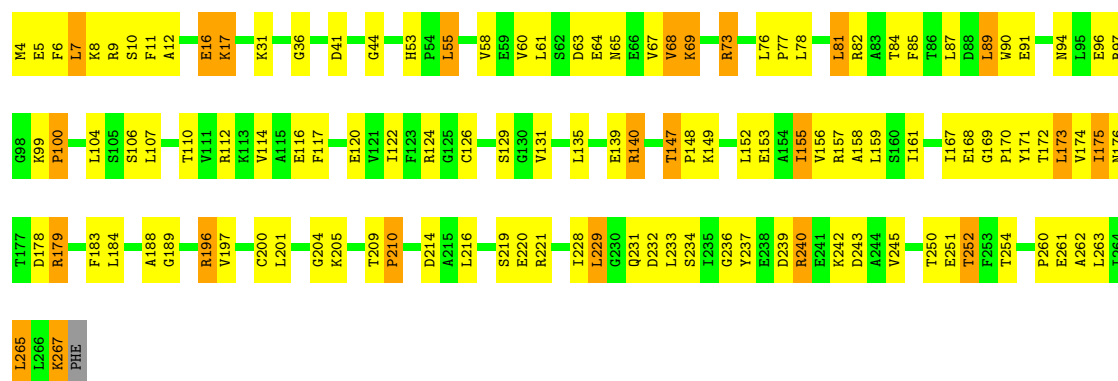
#### • Molecule 1: Maritimacin

Chain A:



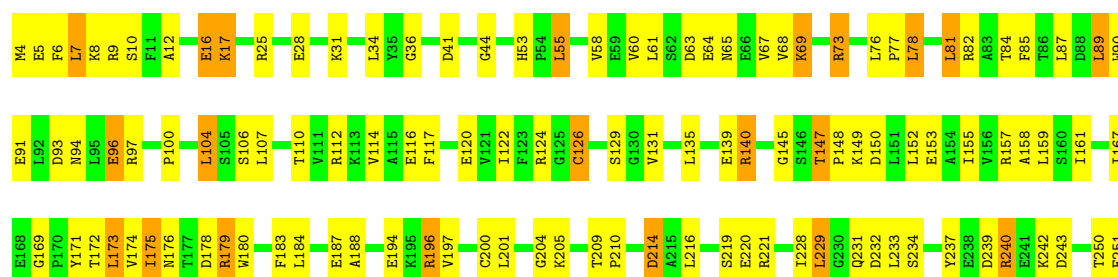
#### • Molecule 1: Maritimacin

Chain B:



#### • Molecule 1: Maritimacin

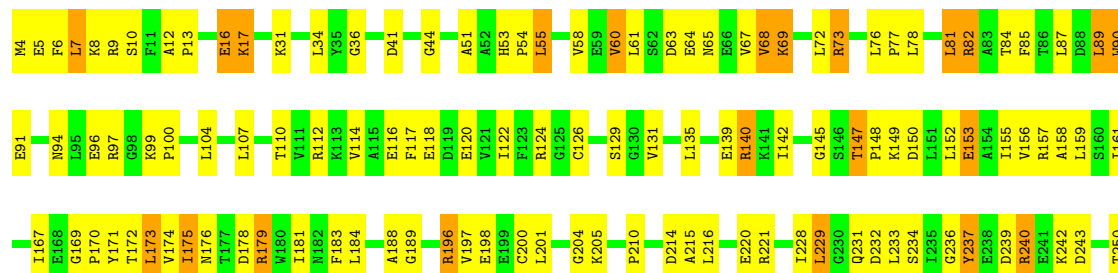
Chain C:





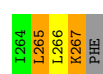
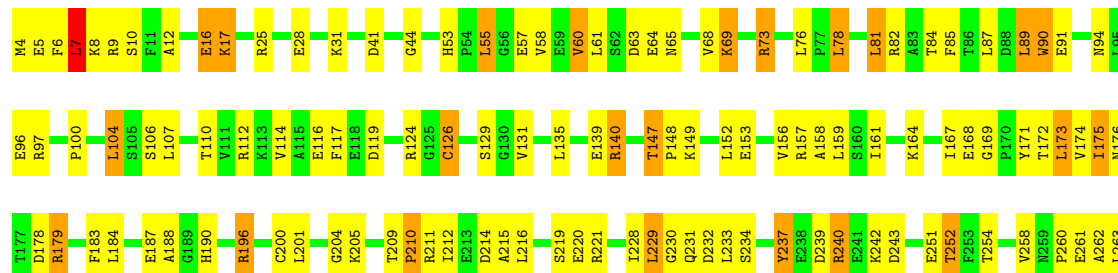
• Molecule 1: Maritimacin

Chain D:



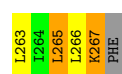
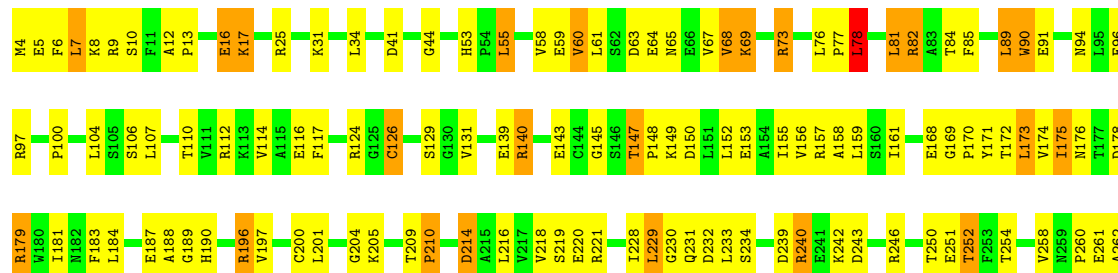
• Molecule 1: Maritimacin

Chain E:



• Molecule 1: Maritimacin

Chain F:



• Molecule 1: Maritimacin

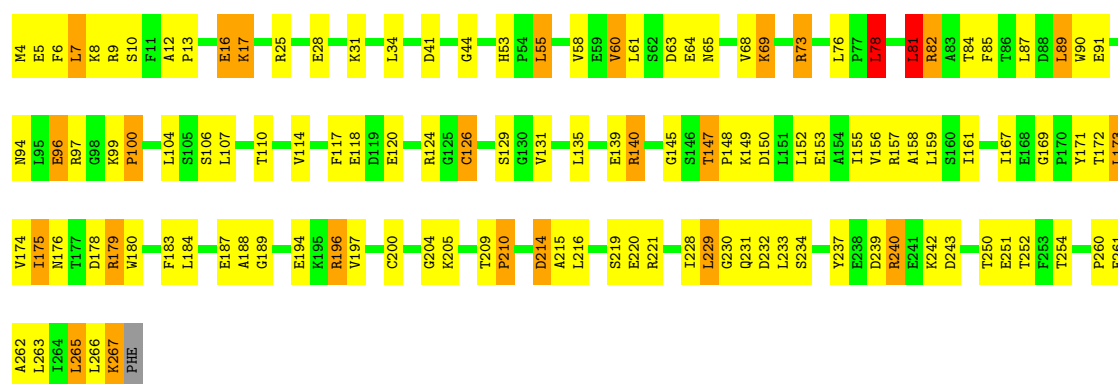
Chain G:





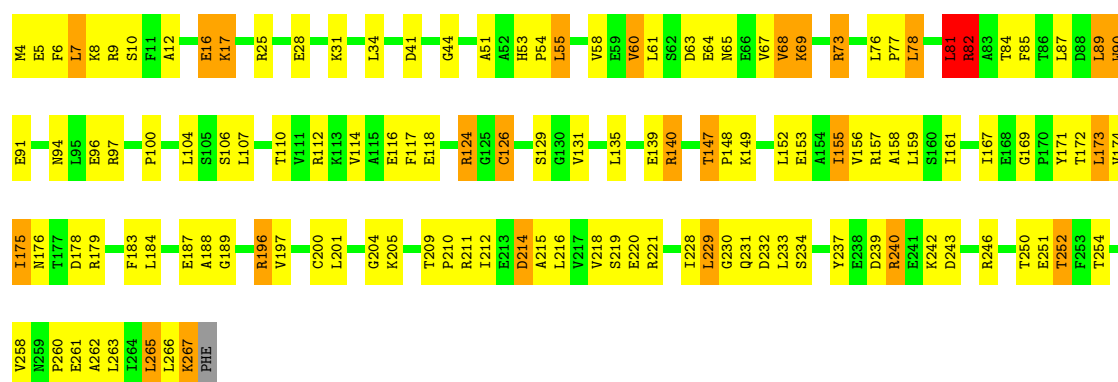
• Molecule 1: Maritimacin

Chain H:



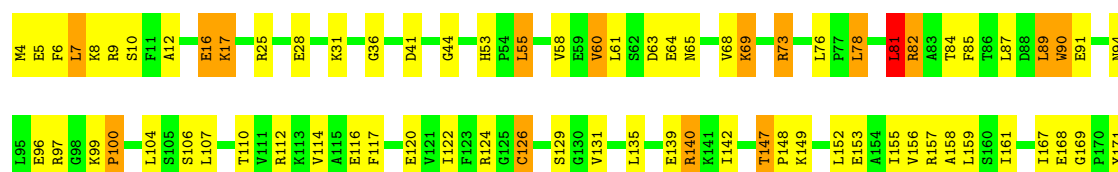
• Molecule 1: Maritimacin

Chain I:

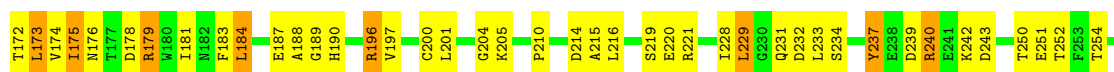


• Molecule 1: Maritimacin

Chain J:

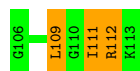






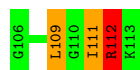
- Molecule 2: Putative uncharacterized protein

Chain K:



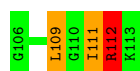
- Molecule 2: Putative uncharacterized protein

Chain L:



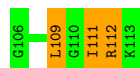
- Molecule 2: Putative uncharacterized protein

Chain M:



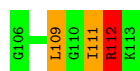
- Molecule 2: Putative uncharacterized protein

Chain N:



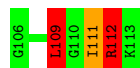
- Molecule 2: Putative uncharacterized protein

Chain O:



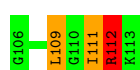
- Molecule 2: Putative uncharacterized protein

Chain P:



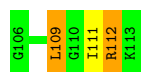
- Molecule 2: Putative uncharacterized protein

Chain Q:



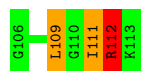
- Molecule 2: Putative uncharacterized protein

Chain R: 



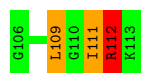
- Molecule 2: Putative uncharacterized protein

Chain S: 



- Molecule 2: Putative uncharacterized protein

Chain T: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	669.04Å 669.04Å 669.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 3.10 49.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.87-3.10) 96.5 (49.87-3.10)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.219 , 0.239 0.246 , 0.261	Depositor DCC
$R_{free}$ test set	10960 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 81.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 219258 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.44	0/2182	0.66	0/2945
1	B	0.45	0/2182	0.66	0/2945
1	C	0.45	0/2182	0.67	0/2945
1	D	0.45	0/2182	0.66	0/2945
1	E	0.44	0/2182	0.66	1/2945 (0.0%)
1	F	0.51	0/2182	0.72	2/2945 (0.1%)
1	G	0.47	0/2182	0.68	1/2945 (0.0%)
1	H	0.46	0/2182	0.67	3/2945 (0.1%)
1	I	0.47	0/2182	0.69	3/2945 (0.1%)
1	J	0.45	0/2182	0.66	3/2945 (0.1%)
2	K	0.67	0/55	0.91	0/70
2	L	0.73	0/55	1.03	0/70
2	M	0.68	0/55	0.89	0/70
2	N	0.66	0/55	0.89	0/70
2	O	0.66	0/55	1.00	0/70
2	P	0.65	0/55	0.94	0/70
2	Q	0.70	0/55	1.02	0/70
2	R	0.69	0/55	1.04	0/70
2	S	0.78	0/55	1.00	0/70
2	T	0.67	0/55	0.95	0/70
All	All	0.47	0/22370	0.68	13/30150 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	82	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	F	78	LEU	CA-CB-CG	6.32	129.83	115.30
1	I	82	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	J	82	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	E	78	LEU	CA-CB-CG	5.47	127.87	115.30
1	G	81	LEU	CA-CB-CG	5.43	127.78	115.30
1	H	82	ARG	NE-CZ-NH1	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	78	LEU	CA-CB-CG	5.42	127.75	115.30
1	I	81	LEU	CA-CB-CG	5.36	127.63	115.30
1	J	78	LEU	CA-CB-CG	5.26	127.40	115.30
1	J	81	LEU	CA-CB-CG	5.12	127.08	115.30
1	I	78	LEU	CA-CB-CG	5.07	126.95	115.30
1	H	81	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2141	0	2148	87	0
1	B	2141	0	2148	97	0
1	C	2141	0	2148	92	0
1	D	2141	0	2148	111	0
1	E	2141	0	2148	95	0
1	F	2141	0	2148	106	0
1	G	2141	0	2148	102	0
1	H	2141	0	2148	94	0
1	I	2141	0	2148	104	0
1	J	2141	0	2148	97	0
2	K	56	0	60	6	0
2	L	56	0	60	5	0
2	M	56	0	60	5	0
2	N	56	0	60	6	0
2	O	56	0	60	5	0
2	P	56	0	60	6	0
2	Q	56	0	60	8	0
2	R	56	0	60	6	0
2	S	56	0	60	7	0
2	T	56	0	60	6	0
3	A	9	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	0	4	0
3	C	9	0	0	2	0
3	D	12	0	0	4	0
3	E	9	0	0	2	0
3	F	11	0	0	4	0
3	G	9	0	0	2	0
3	H	11	0	0	2	0
3	I	9	0	0	3	0
3	J	10	0	0	2	0
All	All	22070	0	22080	953	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (953) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:196:ARG:HG3	1:H:196:ARG:HH11	1.11	1.16
1:I:196:ARG:HH11	1:I:196:ARG:HG3	1.12	1.15
1:B:196:ARG:HG3	1:B:196:ARG:HH11	1.12	1.14
1:J:196:ARG:HG3	1:J:196:ARG:HH11	1.12	1.13
2:R:109:LEU:HD12	2:R:111:ILE:HD11	1.27	1.13
2:Q:109:LEU:HD12	2:Q:111:ILE:HD11	1.28	1.11
2:S:109:LEU:HD12	2:S:111:ILE:HD11	1.31	1.11
1:D:196:ARG:HH11	1:D:196:ARG:HG3	1.14	1.11
1:G:196:ARG:HG3	1:G:196:ARG:HH11	1.11	1.10
2:T:109:LEU:HD12	2:T:111:ILE:HD11	1.32	1.09
2:M:109:LEU:HD12	2:M:111:ILE:HD11	1.30	1.09
1:E:196:ARG:HH11	1:E:196:ARG:HG3	1.09	1.09
1:F:196:ARG:HG3	1:F:196:ARG:HH11	1.09	1.09
1:C:196:ARG:HH11	1:C:196:ARG:HG3	1.10	1.08
2:N:109:LEU:HD12	2:N:111:ILE:HD11	1.36	1.08
2:O:109:LEU:HD12	2:O:111:ILE:HD11	1.35	1.08
2:K:109:LEU:HD12	2:K:111:ILE:HD11	1.35	1.06
2:L:109:LEU:HD12	2:L:111:ILE:HD11	1.37	1.06
1:A:196:ARG:HH11	1:A:196:ARG:HG3	1.13	1.04
1:A:176:ASN:HD22	1:A:179:ARG:H	1.09	0.98
1:F:176:ASN:HD22	1:F:179:ARG:H	1.09	0.98
2:P:109:LEU:HD12	2:P:111:ILE:HD11	1.43	0.98
1:E:176:ASN:HD22	1:E:179:ARG:H	1.13	0.96
1:I:188:ALA:HB1	1:J:149:LYS:HG2	1.44	0.96
1:G:252:THR:HG21	3:G:1043:HOH:O	1.65	0.95
1:H:176:ASN:HD22	1:H:179:ARG:H	1.13	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:176:ASN:HD22	1:G:179:ARG:H	1.09	0.94
1:I:176:ASN:HD22	1:I:179:ARG:H	1.13	0.94
1:E:252:THR:HG21	3:E:1043:HOH:O	1.66	0.94
1:F:252:THR:HG21	3:F:1004:HOH:O	1.69	0.93
1:C:176:ASN:HD22	1:C:179:ARG:H	1.11	0.92
1:J:176:ASN:HD22	1:J:179:ARG:H	1.10	0.92
1:D:176:ASN:HD22	1:D:179:ARG:H	1.08	0.92
1:I:252:THR:HG21	3:I:1043:HOH:O	1.70	0.91
1:D:252:THR:HG21	3:D:1010:HOH:O	1.70	0.90
1:I:16:GLU:OE1	1:I:16:GLU:HA	1.73	0.89
1:B:176:ASN:HD22	1:B:179:ARG:H	1.14	0.89
1:J:252:THR:HG21	3:J:1006:HOH:O	1.73	0.88
1:E:196:ARG:NH1	1:E:196:ARG:HG3	1.89	0.86
1:F:196:ARG:HG3	1:F:196:ARG:NH1	1.89	0.86
1:C:252:THR:HG21	3:C:1043:HOH:O	1.77	0.84
1:F:16:GLU:OE1	1:F:16:GLU:HA	1.77	0.83
1:C:196:ARG:CG	1:C:196:ARG:HH11	1.93	0.82
1:A:147:THR:HG21	1:A:149:LYS:HE3	1.61	0.82
1:C:147:THR:HG21	1:C:149:LYS:HE3	1.62	0.82
1:B:252:THR:HG21	3:B:1009:HOH:O	1.80	0.81
1:I:196:ARG:NH1	1:I:196:ARG:HG3	1.92	0.81
1:H:252:THR:HG21	3:H:1009:HOH:O	1.80	0.81
1:G:196:ARG:HG3	1:G:196:ARG:NH1	1.90	0.81
1:A:252:THR:HG21	3:A:1043:HOH:O	1.80	0.81
1:B:16:GLU:HA	1:B:16:GLU:OE1	1.79	0.81
1:E:16:GLU:HA	1:E:16:GLU:OE1	1.78	0.81
1:A:16:GLU:HA	1:A:16:GLU:OE1	1.81	0.81
1:J:16:GLU:OE1	1:J:16:GLU:HA	1.81	0.81
1:I:188:ALA:CB	1:J:149:LYS:HG2	2.10	0.80
1:H:157:ARG:O	1:H:161:ILE:HD12	1.81	0.80
1:D:157:ARG:O	1:D:161:ILE:HD12	1.80	0.80
1:A:157:ARG:O	1:A:161:ILE:HD12	1.81	0.80
1:D:188:ALA:HB1	1:E:149:LYS:HG2	1.64	0.79
1:H:216:LEU:HD11	1:H:263:LEU:HD11	1.64	0.79
1:G:147:THR:HG21	1:G:149:LYS:HE3	1.62	0.79
1:H:188:ALA:HB1	1:I:149:LYS:HG2	1.64	0.79
1:E:147:THR:HG21	1:E:149:LYS:HE3	1.66	0.78
1:D:16:GLU:OE1	1:D:16:GLU:HA	1.81	0.78
1:G:16:GLU:OE1	1:G:16:GLU:HA	1.84	0.78
1:J:157:ARG:O	1:J:161:ILE:HD12	1.83	0.77
1:I:157:ARG:O	1:I:161:ILE:HD12	1.85	0.77
1:B:188:ALA:HB1	1:C:149:LYS:HG2	1.67	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:157:ARG:O	1:E:161:ILE:HD12	1.85	0.77
1:A:196:ARG:NH1	1:A:196:ARG:HG3	1.93	0.76
1:C:16:GLU:HA	1:C:16:GLU:OE1	1.83	0.76
1:F:157:ARG:O	1:F:161:ILE:HD12	1.86	0.76
1:C:157:ARG:O	1:C:161:ILE:HD12	1.86	0.75
1:I:147:THR:HG21	1:I:149:LYS:HE3	1.68	0.74
1:D:196:ARG:NH1	1:D:196:ARG:HG3	1.93	0.74
1:E:196:ARG:HH11	1:E:196:ARG:CG	1.95	0.74
1:G:157:ARG:O	1:G:161:ILE:HD12	1.87	0.74
1:H:16:GLU:OE1	1:H:16:GLU:HA	1.87	0.74
1:J:196:ARG:CG	1:J:196:ARG:HH11	1.97	0.74
1:I:196:ARG:HH11	1:I:196:ARG:CG	1.97	0.74
1:J:147:THR:HG21	1:J:149:LYS:HE3	1.68	0.74
1:H:196:ARG:HH11	1:H:196:ARG:CG	1.96	0.74
1:J:196:ARG:HG3	1:J:196:ARG:NH1	1.92	0.74
1:H:147:THR:HG21	1:H:149:LYS:HE3	1.70	0.73
1:B:147:THR:HG22	1:B:148:PRO:HD2	1.70	0.73
1:A:216:LEU:HD11	1:A:263:LEU:HD11	1.69	0.73
1:A:91:GLU:O	1:A:94:ASN:HB2	1.88	0.73
1:B:157:ARG:O	1:B:161:ILE:HD12	1.88	0.72
1:F:196:ARG:CG	1:F:196:ARG:HH11	1.94	0.72
1:F:188:ALA:HB1	1:G:149:LYS:HG2	1.72	0.72
1:I:216:LEU:HD11	1:I:263:LEU:HD11	1.72	0.72
1:G:216:LEU:HD11	1:G:263:LEU:HD11	1.71	0.71
1:H:196:ARG:HG3	1:H:196:ARG:NH1	1.91	0.71
1:B:196:ARG:HH11	1:B:196:ARG:CG	1.97	0.71
1:B:216:LEU:HD11	1:B:263:LEU:HD11	1.71	0.71
1:D:6:PHE:HB3	1:H:96:GLU:HG2	1.72	0.71
1:F:73:ARG:HH21	1:J:97:ARG:HD3	1.55	0.71
1:G:176:ASN:ND2	1:G:179:ARG:H	1.86	0.70
1:A:174:VAL:HB	1:A:216:LEU:HB3	1.73	0.70
1:G:91:GLU:O	1:G:94:ASN:HB2	1.91	0.70
1:D:216:LEU:HD11	1:D:263:LEU:HD11	1.72	0.70
1:J:216:LEU:HD11	1:J:263:LEU:HD11	1.72	0.70
1:F:147:THR:HG22	1:F:148:PRO:HD2	1.72	0.70
1:C:196:ARG:NH1	1:C:196:ARG:HG3	1.91	0.69
1:G:188:ALA:HB1	1:H:149:LYS:HG2	1.74	0.69
1:C:91:GLU:O	1:C:94:ASN:HB2	1.91	0.69
1:E:17:LYS:HA	1:E:17:LYS:HE3	1.74	0.69
1:E:147:THR:HG22	1:E:148:PRO:HD2	1.74	0.69
1:E:216:LEU:HD11	1:E:263:LEU:HD11	1.73	0.69
1:I:97:ARG:HD3	1:J:73:ARG:HH21	1.57	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:147:THR:HG21	1:B:149:LYS:HE3	1.74	0.69
1:F:174:VAL:HB	1:F:216:LEU:HB3	1.73	0.69
1:H:174:VAL:HB	1:H:216:LEU:HB3	1.75	0.69
1:A:188:ALA:HB1	1:B:149:LYS:HG2	1.74	0.69
1:D:147:THR:HG21	1:D:149:LYS:HE3	1.74	0.69
1:I:147:THR:HG22	1:I:148:PRO:HD2	1.75	0.68
1:H:91:GLU:O	1:H:94:ASN:HB2	1.92	0.68
1:D:174:VAL:HB	1:D:216:LEU:HB3	1.75	0.68
1:F:149:LYS:HG2	1:J:188:ALA:HB1	1.74	0.68
1:G:196:ARG:HH11	1:G:196:ARG:CG	1.97	0.68
1:I:179:ARG:O	1:I:183:PHE:HD1	1.77	0.67
1:B:229:LEU:HD12	1:B:232:ASP:HA	1.76	0.67
1:D:91:GLU:O	1:D:94:ASN:HB2	1.94	0.67
1:H:179:ARG:O	1:H:183:PHE:HD1	1.78	0.67
1:F:97:ARG:HD3	1:G:73:ARG:HH21	1.59	0.67
1:F:179:ARG:O	1:F:183:PHE:HD1	1.77	0.67
1:C:176:ASN:ND2	1:C:179:ARG:H	1.91	0.67
1:J:174:VAL:HB	1:J:216:LEU:HB3	1.75	0.67
1:J:91:GLU:O	1:J:94:ASN:HB2	1.95	0.67
1:D:196:ARG:CG	1:D:196:ARG:HH11	1.99	0.67
1:C:179:ARG:O	1:C:183:PHE:HD1	1.77	0.67
1:F:147:THR:HG21	1:F:149:LYS:HE3	1.75	0.67
1:F:55:LEU:HD12	1:F:76:LEU:HB2	1.77	0.67
1:B:196:ARG:HG3	1:B:196:ARG:NH1	1.92	0.67
1:D:176:ASN:ND2	1:D:179:ARG:H	1.88	0.67
1:C:174:VAL:HB	1:C:216:LEU:HB3	1.76	0.67
1:C:229:LEU:HD12	1:C:232:ASP:HA	1.77	0.67
1:H:129:SER:HB2	3:H:1013:HOH:O	1.94	0.66
1:G:85:PHE:CZ	1:G:107:LEU:HD13	2.30	0.66
1:D:179:ARG:O	1:D:183:PHE:HD1	1.78	0.66
1:E:64:GLU:HA	1:E:69:LYS:NZ	2.10	0.66
1:C:216:LEU:HD11	1:C:263:LEU:HD11	1.77	0.66
1:G:174:VAL:HB	1:G:216:LEU:HB3	1.77	0.66
1:H:78:LEU:HD12	1:H:252:THR:CG2	2.26	0.66
1:I:91:GLU:O	1:I:94:ASN:HB2	1.95	0.66
1:F:176:ASN:ND2	1:F:179:ARG:H	1.90	0.65
1:E:91:GLU:O	1:E:94:ASN:HB2	1.97	0.65
1:F:188:ALA:CB	1:G:149:LYS:HG2	2.26	0.65
1:F:216:LEU:HD11	1:F:263:LEU:HD11	1.77	0.65
1:A:229:LEU:HD12	1:A:232:ASP:HA	1.76	0.65
1:F:189:GLY:HA3	1:G:187:GLU:OE2	1.96	0.65
1:J:176:ASN:ND2	1:J:179:ARG:H	1.89	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:60:VAL:O	1:F:61:LEU:HD12	1.96	0.65
1:I:176:ASN:ND2	1:I:179:ARG:H	1.91	0.65
1:B:174:VAL:HB	1:B:216:LEU:HB3	1.79	0.65
1:G:64:GLU:HA	1:G:69:LYS:NZ	2.12	0.65
1:J:147:THR:HG22	1:J:148:PRO:HD2	1.79	0.65
1:F:91:GLU:O	1:F:94:ASN:HB2	1.96	0.65
1:B:91:GLU:O	1:B:94:ASN:HB2	1.97	0.65
1:F:17:LYS:HA	1:F:17:LYS:HE3	1.79	0.65
1:B:179:ARG:HH11	1:B:179:ARG:HG2	1.61	0.65
1:B:60:VAL:O	1:B:61:LEU:HD12	1.97	0.64
1:J:179:ARG:O	1:J:183:PHE:HD1	1.80	0.64
1:B:85:PHE:CZ	1:B:107:LEU:HD13	2.33	0.64
1:A:196:ARG:CG	1:A:196:ARG:HH11	2.00	0.64
1:C:78:LEU:HD12	1:C:252:THR:CG2	2.28	0.64
1:E:174:VAL:HB	1:E:216:LEU:HB3	1.77	0.64
1:H:60:VAL:O	1:H:61:LEU:HD12	1.98	0.64
1:A:179:ARG:O	1:A:183:PHE:HD1	1.80	0.64
1:D:147:THR:HG22	1:D:148:PRO:HD2	1.79	0.64
1:D:179:ARG:HG2	1:D:179:ARG:HH11	1.63	0.64
1:E:229:LEU:HD12	1:E:232:ASP:HA	1.80	0.64
1:G:229:LEU:HD12	1:G:232:ASP:HA	1.80	0.64
1:G:97:ARG:HD3	1:H:73:ARG:HH21	1.63	0.63
1:A:176:ASN:ND2	1:A:179:ARG:H	1.89	0.63
1:F:78:LEU:HD12	1:F:252:THR:CG2	2.28	0.63
1:I:174:VAL:HB	1:I:216:LEU:HB3	1.80	0.63
1:J:229:LEU:HD12	1:J:232:ASP:HA	1.80	0.63
1:B:78:LEU:HD12	1:B:252:THR:CG2	2.29	0.63
1:B:64:GLU:HA	1:B:69:LYS:NZ	2.13	0.63
1:E:179:ARG:O	1:E:183:PHE:HD1	1.82	0.62
1:C:97:ARG:HD3	1:D:73:ARG:HH21	1.65	0.62
1:I:64:GLU:HA	1:I:69:LYS:NZ	2.15	0.62
1:B:179:ARG:O	1:B:183:PHE:HD1	1.82	0.62
1:D:82:ARG:NH2	1:H:90:TRP:CZ3	2.68	0.62
1:C:64:GLU:HA	1:C:69:LYS:NZ	2.14	0.62
1:F:229:LEU:HD12	1:F:232:ASP:HA	1.82	0.62
1:D:229:LEU:HD12	1:D:232:ASP:HA	1.82	0.62
1:H:147:THR:HG22	1:H:148:PRO:HD2	1.82	0.62
1:G:129:SER:HB2	3:G:1053:HOH:O	1.99	0.62
1:C:96:GLU:HG2	1:I:6:PHE:HB3	1.81	0.62
1:H:179:ARG:HH11	1:H:179:ARG:HG2	1.65	0.62
1:G:179:ARG:O	1:G:183:PHE:HD1	1.83	0.62
1:A:78:LEU:HD12	1:A:252:THR:CG2	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:78:LEU:HD12	1:G:252:THR:CG2	2.30	0.61
1:D:85:PHE:CZ	1:D:107:LEU:HD13	2.35	0.61
1:D:6:PHE:O	1:D:8:LYS:HG2	2.00	0.61
1:D:17:LYS:HE3	1:D:17:LYS:HA	1.82	0.61
1:I:229:LEU:HD12	1:I:232:ASP:HA	1.81	0.61
1:A:149:LYS:HG2	1:E:188:ALA:HB1	1.81	0.61
1:J:179:ARG:HG2	1:J:179:ARG:HH11	1.66	0.60
1:C:147:THR:HG22	1:C:148:PRO:HD2	1.83	0.60
1:H:229:LEU:HD12	1:H:232:ASP:HA	1.83	0.60
1:E:176:ASN:ND2	1:E:179:ARG:H	1.91	0.60
1:J:78:LEU:HD12	1:J:252:THR:CG2	2.31	0.60
1:H:6:PHE:O	1:H:8:LYS:HG2	2.01	0.60
1:D:189:GLY:HA3	1:E:187:GLU:OE2	2.02	0.60
1:J:64:GLU:HA	1:J:69:LYS:NZ	2.16	0.60
1:B:17:LYS:HE3	1:B:17:LYS:HA	1.83	0.60
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.65	0.60
1:G:12:ALA:HB2	1:G:237:TYR:CD1	2.36	0.60
1:C:76:LEU:HD22	1:C:254:THR:OG1	2.02	0.60
1:H:173:LEU:HD13	1:H:175:ILE:HB	1.83	0.60
1:I:189:GLY:HA3	1:J:187:GLU:OE2	2.02	0.60
1:D:64:GLU:HA	1:D:69:LYS:NZ	2.16	0.59
1:C:110:THR:O	1:C:114:VAL:HG23	2.02	0.59
1:E:6:PHE:O	1:E:8:LYS:HG2	2.01	0.59
1:A:147:THR:HG22	1:A:148:PRO:HD2	1.84	0.59
1:A:6:PHE:O	1:A:8:LYS:HG2	2.03	0.59
1:F:73:ARG:NH2	1:J:97:ARG:HD3	2.18	0.59
1:H:85:PHE:CZ	1:H:107:LEU:HD13	2.37	0.59
1:I:60:VAL:O	1:I:61:LEU:HD12	2.02	0.59
1:F:6:PHE:O	1:F:8:LYS:HG2	2.03	0.59
1:I:6:PHE:O	1:I:8:LYS:HG2	2.02	0.59
1:B:176:ASN:ND2	1:B:179:ARG:H	1.93	0.58
1:G:60:VAL:O	1:G:61:LEU:HD12	2.03	0.58
1:E:90:TRP:CD1	1:E:90:TRP:O	2.56	0.58
1:J:60:VAL:O	1:J:61:LEU:HD12	2.04	0.58
1:D:60:VAL:O	1:D:61:LEU:HD12	2.02	0.58
1:G:205:LYS:HE2	1:G:220:GLU:OE1	2.04	0.58
1:I:12:ALA:HB2	1:I:237:TYR:CD1	2.38	0.58
1:I:17:LYS:HE3	1:I:17:LYS:HA	1.86	0.58
1:A:53:HIS:CG	1:A:228:ILE:HD13	2.39	0.58
1:F:179:ARG:HG2	1:F:179:ARG:HH11	1.69	0.58
1:E:76:LEU:HD22	1:E:254:THR:OG1	2.04	0.58
1:J:17:LYS:HE3	1:J:17:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:179:ARG:HH11	1:C:179:ARG:HG2	1.68	0.57
1:A:231:GLN:H	1:A:252:THR:HB	1.69	0.57
1:B:196:ARG:NH1	1:B:196:ARG:CG	2.64	0.57
1:G:17:LYS:HE3	1:G:17:LYS:HA	1.85	0.57
1:G:231:GLN:H	1:G:252:THR:HB	1.69	0.57
1:G:147:THR:HG22	1:G:148:PRO:HD2	1.86	0.57
1:A:64:GLU:HA	1:A:69:LYS:NZ	2.18	0.57
1:G:76:LEU:HD22	1:G:254:THR:OG1	2.04	0.57
1:I:78:LEU:HD12	1:I:252:THR:CG2	2.34	0.57
1:B:188:ALA:CB	1:C:149:LYS:HG2	2.35	0.57
1:H:97:ARG:HD3	1:I:73:ARG:HH21	1.70	0.57
1:D:76:LEU:HD22	1:D:254:THR:OG1	2.04	0.57
1:C:6:PHE:O	1:C:8:LYS:HG2	2.04	0.57
1:I:205:LYS:HE2	1:I:220:GLU:OE1	2.04	0.57
1:F:189:GLY:O	1:G:190:HIS:HB2	2.05	0.57
2:P:111:ILE:N	2:P:111:ILE:HD12	2.20	0.57
1:C:17:LYS:HA	1:C:17:LYS:HE3	1.87	0.57
1:I:85:PHE:CZ	1:I:107:LEU:HD13	2.40	0.57
1:D:205:LYS:HE2	1:D:220:GLU:OE1	2.05	0.57
1:D:129:SER:HB2	3:D:1014:HOH:O	2.05	0.57
1:A:97:ARG:HD3	1:B:73:ARG:HH21	1.70	0.57
1:E:205:LYS:HE2	1:E:220:GLU:OE1	2.04	0.57
1:A:129:SER:HB2	3:A:1053:HOH:O	2.05	0.56
1:B:173:LEU:HD13	1:B:175:ILE:HB	1.86	0.56
1:H:188:ALA:CB	1:I:149:LYS:HG2	2.33	0.56
1:G:90:TRP:CD1	1:G:90:TRP:O	2.59	0.56
1:I:155:ILE:HG22	1:I:156:VAL:N	2.20	0.56
1:F:64:GLU:HA	1:F:69:LYS:NZ	2.20	0.56
1:J:6:PHE:O	1:J:8:LYS:HG2	2.04	0.56
1:D:78:LEU:HD12	1:D:252:THR:CG2	2.36	0.56
1:C:231:GLN:H	1:C:252:THR:HB	1.69	0.56
1:H:176:ASN:ND2	1:H:179:ARG:H	1.94	0.56
1:G:196:ARG:NH1	1:G:196:ARG:CG	2.63	0.56
1:E:64:GLU:HA	1:E:69:LYS:HZ2	1.69	0.56
1:A:152:LEU:O	1:A:156:VAL:HG13	2.05	0.56
1:H:12:ALA:HB2	1:H:237:TYR:CD1	2.40	0.56
1:H:231:GLN:H	1:H:252:THR:HB	1.70	0.56
1:G:53:HIS:CG	1:G:228:ILE:HD13	2.40	0.56
1:E:179:ARG:HG2	1:E:179:ARG:HH11	1.71	0.56
1:I:64:GLU:HA	1:I:69:LYS:HZ1	1.69	0.56
1:D:53:HIS:CG	1:D:228:ILE:HD13	2.41	0.56
1:D:188:ALA:CB	1:E:149:LYS:HG2	2.34	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:231:GLN:H	1:E:252:THR:HB	1.70	0.56
1:G:64:GLU:HA	1:G:69:LYS:HZ1	1.70	0.55
1:A:85:PHE:CZ	1:A:107:LEU:HD13	2.41	0.55
1:J:76:LEU:HD22	1:J:254:THR:OG1	2.06	0.55
1:C:188:ALA:HB1	1:D:149:LYS:HG2	1.87	0.55
1:E:173:LEU:HD13	1:E:175:ILE:HB	1.88	0.55
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.66	0.55
1:I:76:LEU:HD22	1:I:254:THR:OG1	2.06	0.55
1:G:152:LEU:HD12	1:G:200:CYS:SG	2.47	0.55
1:E:78:LEU:HD12	1:E:252:THR:CG2	2.36	0.55
1:D:63:ASP:HB2	1:D:65:ASN:HB2	1.89	0.55
1:C:90:TRP:CD1	1:C:90:TRP:O	2.60	0.55
1:H:17:LYS:HA	1:H:17:LYS:HE3	1.88	0.55
1:F:155:ILE:HG22	1:F:156:VAL:N	2.22	0.55
1:A:76:LEU:HD22	1:A:254:THR:OG1	2.06	0.55
1:I:173:LEU:HD13	1:I:175:ILE:HB	1.87	0.55
1:G:233:LEU:O	2:Q:109:LEU:CB	2.55	0.55
1:J:85:PHE:CZ	1:J:107:LEU:HD13	2.40	0.55
1:B:6:PHE:O	1:B:8:LYS:HG2	2.06	0.55
1:J:173:LEU:HD13	1:J:175:ILE:HB	1.89	0.54
1:I:90:TRP:CD1	1:I:90:TRP:O	2.60	0.54
1:C:233:LEU:O	2:M:109:LEU:CB	2.56	0.54
1:D:158:ALA:HA	1:D:161:ILE:HD13	1.88	0.54
1:F:76:LEU:HD22	1:F:254:THR:OG1	2.07	0.54
1:C:90:TRP:CZ3	1:I:82:ARG:NH2	2.75	0.54
1:J:205:LYS:HE2	1:J:220:GLU:OE1	2.08	0.54
1:J:129:SER:HB2	3:J:1009:HOH:O	2.06	0.54
1:J:231:GLN:H	1:J:252:THR:HB	1.73	0.54
1:F:110:THR:O	1:F:114:VAL:HG23	2.08	0.54
1:J:196:ARG:NH1	1:J:196:ARG:CG	2.64	0.54
1:E:81:LEU:C	1:E:81:LEU:HD23	2.28	0.54
1:I:110:THR:O	1:I:114:VAL:HG23	2.07	0.54
1:B:231:GLN:H	1:B:252:THR:HB	1.72	0.54
1:A:173:LEU:HD13	1:A:175:ILE:HB	1.90	0.54
1:G:173:LEU:HD13	1:G:175:ILE:HB	1.90	0.54
1:H:126:CYS:HB2	1:H:129:SER:OG	2.08	0.54
1:D:110:THR:O	1:D:114:VAL:HG23	2.08	0.54
1:C:60:VAL:O	1:C:61:LEU:HD12	2.07	0.54
1:J:53:HIS:CG	1:J:228:ILE:HD13	2.43	0.54
1:D:97:ARG:HD3	1:E:73:ARG:HH21	1.73	0.54
1:F:173:LEU:HD13	1:F:175:ILE:HB	1.90	0.54
1:A:55:LEU:HD12	1:A:76:LEU:HB2	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:12:ALA:HB2	1:E:237:TYR:CD1	2.42	0.54
1:F:90:TRP:CD1	1:F:90:TRP:O	2.61	0.53
1:G:233:LEU:O	2:Q:109:LEU:HB3	2.08	0.53
1:J:90:TRP:CD1	1:J:90:TRP:O	2.62	0.53
1:A:205:LYS:HE2	1:A:220:GLU:OE1	2.08	0.53
1:D:173:LEU:HD13	1:D:175:ILE:HB	1.90	0.53
1:B:112:ARG:O	1:B:116:GLU:HG3	2.09	0.53
1:D:126:CYS:HB2	1:D:129:SER:OG	2.08	0.53
1:B:205:LYS:HE2	1:B:220:GLU:OE1	2.07	0.53
1:B:76:LEU:HD22	1:B:254:THR:OG1	2.08	0.53
1:I:229:LEU:CD1	1:I:232:ASP:HA	2.39	0.53
1:F:181:ILE:HG12	1:G:156:VAL:HG21	1.90	0.53
1:F:85:PHE:CZ	1:F:107:LEU:HD13	2.44	0.53
1:G:229:LEU:CD1	1:G:232:ASP:HA	2.39	0.53
1:I:129:SER:HB2	3:I:1053:HOH:O	2.08	0.53
1:F:53:HIS:CG	1:F:228:ILE:HD13	2.43	0.53
1:A:229:LEU:CD1	1:A:232:ASP:HA	2.39	0.53
1:I:53:HIS:CG	1:I:228:ILE:HD13	2.44	0.53
1:G:6:PHE:O	1:G:8:LYS:HG2	2.07	0.53
1:F:129:SER:HB2	3:F:1008:HOH:O	2.09	0.53
1:H:55:LEU:HD12	1:H:76:LEU:HB2	1.91	0.53
1:G:55:LEU:HD12	1:G:76:LEU:HB2	1.91	0.53
1:C:112:ARG:O	1:C:116:GLU:HG3	2.09	0.53
1:H:53:HIS:CG	1:H:228:ILE:HD13	2.44	0.53
1:B:97:ARG:HD3	1:C:73:ARG:HH21	1.74	0.53
1:I:215:ALA:HB3	1:I:266:LEU:HD12	1.90	0.53
1:E:233:LEU:O	2:O:109:LEU:CB	2.57	0.52
1:C:239:ASP:CG	1:C:240:ARG:H	2.13	0.52
1:H:233:LEU:O	2:R:109:LEU:CB	2.58	0.52
2:S:111:ILE:C	2:S:112:ARG:HG2	2.29	0.52
1:I:179:ARG:HG2	1:I:179:ARG:HH11	1.73	0.52
1:F:149:LYS:HG2	1:J:188:ALA:CB	2.38	0.52
1:A:233:LEU:O	2:K:109:LEU:CB	2.57	0.52
1:C:229:LEU:CD1	1:C:232:ASP:HA	2.38	0.52
1:E:129:SER:HB2	3:E:1053:HOH:O	2.09	0.52
1:D:258:VAL:O	1:D:260:PRO:HD3	2.10	0.52
1:J:64:GLU:HA	1:J:69:LYS:HZ2	1.73	0.52
1:E:60:VAL:O	1:E:61:LEU:HD12	2.10	0.52
1:B:64:GLU:HA	1:B:69:LYS:HZ1	1.75	0.52
1:F:229:LEU:CD1	1:F:232:ASP:HA	2.40	0.52
1:A:250:THR:HG22	1:A:251:GLU:N	2.24	0.52
1:H:64:GLU:HA	1:H:69:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:205:LYS:HE2	1:F:220:GLU:OE1	2.10	0.52
1:B:53:HIS:CG	1:B:228:ILE:HD13	2.43	0.52
1:E:196:ARG:NH1	1:E:196:ARG:CG	2.61	0.52
1:D:233:LEU:O	2:N:109:LEU:CB	2.57	0.52
1:H:229:LEU:CD1	1:H:232:ASP:HA	2.40	0.52
1:H:81:LEU:HD23	1:H:81:LEU:C	2.31	0.52
2:O:111:ILE:C	2:O:112:ARG:HG2	2.30	0.51
1:J:126:CYS:HB2	1:J:129:SER:OG	2.10	0.51
1:H:81:LEU:HD23	1:H:81:LEU:O	2.09	0.51
1:B:81:LEU:C	1:B:81:LEU:HD23	2.30	0.51
1:A:17:LYS:HA	1:A:17:LYS:HE3	1.92	0.51
1:B:189:GLY:HA3	1:C:187:GLU:OE2	2.10	0.51
1:E:233:LEU:O	2:O:109:LEU:HB2	2.10	0.51
1:I:231:GLN:H	1:I:252:THR:HB	1.75	0.51
1:J:158:ALA:HA	1:J:161:ILE:HD13	1.92	0.51
1:A:90:TRP:O	1:A:90:TRP:CD1	2.63	0.51
1:B:90:TRP:CD1	1:B:90:TRP:O	2.63	0.51
1:A:73:ARG:HH21	1:E:97:ARG:HD3	1.75	0.51
1:E:265:LEU:O	1:E:266:LEU:HD23	2.11	0.51
1:F:126:CYS:HB2	1:F:129:SER:OG	2.10	0.51
1:J:110:THR:O	1:J:114:VAL:HG23	2.10	0.51
1:E:110:THR:O	1:E:114:VAL:HG23	2.11	0.51
1:E:214:ASP:OD2	1:E:267:LYS:HG2	2.10	0.51
1:I:230:GLY:HA3	1:I:252:THR:HG22	1.93	0.51
1:A:81:LEU:C	1:A:81:LEU:HD23	2.31	0.51
1:J:233:LEU:O	2:T:109:LEU:CB	2.58	0.51
1:H:214:ASP:OD2	1:H:267:LYS:HG2	2.10	0.51
1:F:258:VAL:O	1:F:260:PRO:HD3	2.10	0.51
1:E:229:LEU:CD1	1:E:232:ASP:HA	2.41	0.51
1:C:152:LEU:HD12	1:C:200:CYS:SG	2.51	0.51
1:H:110:THR:O	1:H:114:VAL:HG23	2.11	0.51
1:I:233:LEU:O	2:S:109:LEU:CB	2.59	0.51
1:E:140:ARG:HH22	1:E:161:ILE:CG2	2.24	0.51
1:H:205:LYS:HE2	1:H:220:GLU:OE1	2.11	0.51
1:C:129:SER:HB2	3:C:1053:HOH:O	2.11	0.51
1:E:53:HIS:CG	1:E:228:ILE:HD13	2.46	0.51
1:C:214:ASP:OD2	1:C:267:LYS:HG2	2.11	0.51
1:E:55:LEU:HD12	1:E:76:LEU:HB2	1.92	0.51
1:C:173:LEU:HD13	1:C:175:ILE:HB	1.92	0.51
1:I:176:ASN:HD21	1:I:178:ASP:HB2	1.76	0.50
1:H:155:ILE:HG22	1:H:156:VAL:N	2.25	0.50
1:H:196:ARG:NH1	1:H:196:ARG:CG	2.64	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:189:GLY:O	1:E:190:HIS:HB2	2.10	0.50
1:C:167:ILE:HG21	1:C:262:ALA:HA	1.94	0.50
1:C:12:ALA:HB2	1:C:237:TYR:CD1	2.45	0.50
1:E:179:ARG:NE	1:E:267:LYS:HE3	2.26	0.50
1:B:214:ASP:OD2	1:B:267:LYS:HG2	2.10	0.50
1:J:12:ALA:HB2	1:J:237:TYR:CD1	2.46	0.50
1:I:81:LEU:C	1:I:81:LEU:HD23	2.32	0.50
1:B:110:THR:O	1:B:114:VAL:HG23	2.12	0.50
1:F:140:ARG:HD3	1:F:263:LEU:O	2.11	0.50
1:G:81:LEU:O	1:G:250:THR:HG23	2.11	0.50
1:H:76:LEU:HD22	1:H:254:THR:OG1	2.11	0.50
1:H:158:ALA:HA	1:H:161:ILE:HD13	1.93	0.50
1:G:188:ALA:CB	1:H:149:LYS:HG2	2.42	0.50
1:J:229:LEU:CD1	1:J:232:ASP:HA	2.41	0.50
1:B:31:LYS:NZ	3:B:1015:HOH:O	2.43	0.50
1:D:31:LYS:NZ	3:D:1016:HOH:O	2.42	0.50
1:C:53:HIS:CG	1:C:228:ILE:HD13	2.47	0.50
1:F:112:ARG:O	1:F:116:GLU:HG3	2.12	0.50
2:Q:111:ILE:C	2:Q:112:ARG:HG2	2.31	0.50
1:C:158:ALA:HA	1:C:161:ILE:HD13	1.92	0.50
2:R:111:ILE:C	2:R:112:ARG:HG2	2.32	0.49
1:C:233:LEU:O	2:M:109:LEU:HB2	2.12	0.49
1:A:140:ARG:HH22	1:A:161:ILE:CG2	2.25	0.49
1:E:258:VAL:O	1:E:260:PRO:HD3	2.11	0.49
1:D:54:PRO:HB3	1:I:51:ALA:HB2	1.94	0.49
1:B:126:CYS:HB2	1:B:129:SER:OG	2.12	0.49
1:I:112:ARG:O	1:I:116:GLU:HG3	2.13	0.49
1:H:90:TRP:CD1	1:H:90:TRP:O	2.65	0.49
1:C:7:LEU:O	1:C:9:ARG:N	2.41	0.49
1:C:85:PHE:CZ	1:C:107:LEU:HD13	2.46	0.49
1:B:233:LEU:O	2:L:109:LEU:CB	2.60	0.49
1:B:140:ARG:HD3	1:B:263:LEU:O	2.11	0.49
1:A:126:CYS:HB2	1:A:129:SER:OG	2.13	0.49
1:E:7:LEU:O	1:E:9:ARG:N	2.44	0.49
1:B:229:LEU:CD1	1:B:232:ASP:HA	2.41	0.49
1:H:233:LEU:HG	1:H:251:GLU:OE2	2.12	0.49
1:F:233:LEU:O	2:P:109:LEU:CB	2.60	0.49
1:D:239:ASP:CG	1:D:240:ARG:H	2.16	0.49
1:I:63:ASP:HB2	1:I:65:ASN:HB2	1.94	0.49
1:F:78:LEU:HD12	1:F:252:THR:HG23	1.95	0.49
1:D:231:GLN:H	1:D:252:THR:HB	1.77	0.49
1:C:78:LEU:HD12	1:C:252:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:126:CYS:HB2	1:I:129:SER:OG	2.12	0.49
1:D:167:ILE:HG21	1:D:262:ALA:HA	1.94	0.49
2:N:111:ILE:C	2:N:112:ARG:HG2	2.33	0.49
1:F:231:GLN:H	1:F:252:THR:HB	1.78	0.49
1:G:250:THR:HG22	1:G:251:GLU:H	1.78	0.49
1:H:176:ASN:HD21	1:H:178:ASP:HB2	1.78	0.49
1:C:140:ARG:HH22	1:C:161:ILE:CG2	2.25	0.49
1:F:55:LEU:CD1	1:F:76:LEU:HB2	2.42	0.49
1:B:167:ILE:HG21	1:B:262:ALA:HA	1.94	0.49
1:A:239:ASP:CG	1:A:240:ARG:H	2.16	0.49
2:T:111:ILE:C	2:T:112:ARG:HG2	2.32	0.49
1:D:179:ARG:CG	1:D:179:ARG:HH11	2.26	0.49
1:F:158:ALA:HA	1:F:161:ILE:HD13	1.95	0.49
1:C:64:GLU:HA	1:C:69:LYS:HZ1	1.78	0.49
1:E:7:LEU:O	1:E:9:ARG:HG3	2.13	0.49
1:A:167:ILE:HG21	1:A:262:ALA:HA	1.95	0.49
1:F:187:GLU:OE2	1:J:189:GLY:HA3	2.13	0.49
1:J:55:LEU:HD12	1:J:76:LEU:HB2	1.95	0.48
1:G:81:LEU:HD23	1:G:81:LEU:C	2.33	0.48
1:B:179:ARG:HH11	1:B:179:ARG:CG	2.26	0.48
1:A:110:THR:O	1:A:114:VAL:HG23	2.13	0.48
1:E:89:LEU:C	1:E:91:GLU:H	2.16	0.48
1:B:129:SER:HB2	3:B:1013:HOH:O	2.14	0.48
1:C:7:LEU:O	1:C:9:ARG:HG3	2.13	0.48
1:F:152:LEU:HD12	1:F:200:CYS:SG	2.54	0.48
1:F:196:ARG:NH1	1:F:196:ARG:CG	2.62	0.48
1:G:158:ALA:HA	1:G:161:ILE:HD13	1.95	0.48
1:I:97:ARG:HD3	1:J:73:ARG:NH2	2.27	0.48
1:A:7:LEU:O	1:A:9:ARG:N	2.45	0.48
1:F:265:LEU:O	1:F:266:LEU:HD23	2.13	0.48
1:C:63:ASP:HB2	1:C:65:ASN:HB2	1.96	0.48
1:E:167:ILE:HG21	1:E:262:ALA:HA	1.95	0.48
1:I:214:ASP:OD2	1:I:267:LYS:HG2	2.13	0.48
1:C:205:LYS:HE2	1:C:220:GLU:OE1	2.13	0.48
1:J:7:LEU:O	1:J:9:ARG:N	2.45	0.48
1:D:90:TRP:O	1:D:90:TRP:CD1	2.67	0.48
2:S:111:ILE:HD12	2:S:111:ILE:N	2.28	0.48
1:D:233:LEU:O	2:N:109:LEU:HB2	2.14	0.48
1:B:233:LEU:HG	1:B:251:GLU:OE2	2.13	0.48
1:I:135:LEU:HD23	1:I:265:LEU:HD21	1.95	0.48
1:H:63:ASP:HB2	1:H:65:ASN:HB2	1.95	0.48
1:G:63:ASP:HB2	1:G:65:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:LEU:O	2:K:109:LEU:HB2	2.12	0.48
1:J:81:LEU:HD23	1:J:81:LEU:C	2.33	0.48
1:C:233:LEU:O	2:M:109:LEU:HB3	2.14	0.48
1:H:78:LEU:HD12	1:H:252:THR:HG22	1.96	0.48
1:G:28:GLU:O	1:G:31:LYS:HG2	2.13	0.48
1:F:145:GLY:HA3	1:F:150:ASP:HB3	1.96	0.48
1:I:28:GLU:O	1:I:31:LYS:HG2	2.14	0.48
2:M:111:ILE:C	2:M:112:ARG:HG2	2.33	0.47
2:N:111:ILE:N	2:N:111:ILE:HD12	2.29	0.47
1:I:176:ASN:HD22	1:I:179:ARG:N	1.96	0.47
1:B:81:LEU:O	1:B:81:LEU:HD23	2.14	0.47
1:F:63:ASP:HB2	1:F:65:ASN:HB2	1.96	0.47
1:G:233:LEU:HG	1:G:251:GLU:OE2	2.13	0.47
1:F:176:ASN:HD22	1:F:179:ARG:N	1.92	0.47
1:F:250:THR:HG22	1:F:251:GLU:N	2.30	0.47
1:D:229:LEU:CD1	1:D:232:ASP:HA	2.44	0.47
1:G:110:THR:O	1:G:114:VAL:HG23	2.14	0.47
1:B:7:LEU:O	1:B:9:ARG:N	2.45	0.47
1:H:233:LEU:O	2:R:109:LEU:HB2	2.14	0.47
1:J:214:ASP:OD2	1:J:267:LYS:HG2	2.14	0.47
1:H:55:LEU:HD11	1:H:76:LEU:HD12	1.96	0.47
1:E:63:ASP:HB2	1:E:65:ASN:HB2	1.96	0.47
1:B:176:ASN:HD21	1:B:178:ASP:HB2	1.79	0.47
1:F:73:ARG:HH21	1:J:97:ARG:CD	2.27	0.47
1:H:99:LYS:HA	1:H:100:PRO:HD3	1.74	0.47
1:H:215:ALA:HB3	1:H:266:LEU:HD12	1.96	0.47
1:G:112:ARG:O	1:G:116:GLU:HG3	2.14	0.47
1:B:179:ARG:NE	1:B:267:LYS:HE3	2.30	0.47
1:C:93:ASP:OD1	1:I:8:LYS:NZ	2.45	0.47
1:F:64:GLU:HA	1:F:69:LYS:HZ2	1.79	0.47
1:H:135:LEU:HD23	1:H:265:LEU:HD21	1.97	0.47
1:F:189:GLY:H	1:G:196:ARG:HH12	1.62	0.47
1:F:233:LEU:O	2:P:109:LEU:HB3	2.14	0.47
1:E:215:ALA:HB3	1:E:266:LEU:HD12	1.97	0.47
1:E:158:ALA:HA	1:E:161:ILE:HD13	1.95	0.47
1:H:126:CYS:CB	1:H:129:SER:OG	2.63	0.47
1:A:60:VAL:O	1:A:61:LEU:HD12	2.14	0.47
1:E:168:GLU:HA	1:E:171:TYR:OH	2.15	0.47
1:A:112:ARG:O	1:A:116:GLU:HG3	2.15	0.47
2:P:111:ILE:C	2:P:112:ARG:HG2	2.35	0.47
1:C:64:GLU:HA	1:C:69:LYS:HZ2	1.79	0.47
1:G:126:CYS:HB2	1:G:129:SER:OG	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:173:LEU:HB2	1:G:201:LEU:HD11	1.96	0.47
1:H:179:ARG:NE	1:H:267:LYS:HE3	2.30	0.47
1:C:173:LEU:HB2	1:C:201:LEU:HD11	1.96	0.47
1:B:12:ALA:HB2	1:B:237:TYR:CD1	2.50	0.47
1:I:7:LEU:O	1:I:9:ARG:N	2.46	0.47
1:H:140:ARG:HD3	1:H:263:LEU:O	2.15	0.47
1:B:158:ALA:HA	1:B:161:ILE:HD13	1.96	0.47
1:C:126:CYS:HB2	1:C:129:SER:OG	2.14	0.47
1:J:25:ARG:HA	1:J:25:ARG:HD2	1.57	0.47
1:C:89:LEU:C	1:C:91:GLU:H	2.19	0.46
1:B:169:GLY:HA3	1:B:221:ARG:HB3	1.97	0.46
1:I:239:ASP:CG	1:I:240:ARG:H	2.19	0.46
1:B:233:LEU:O	2:L:109:LEU:HB2	2.15	0.46
1:E:89:LEU:O	1:E:91:GLU:N	2.48	0.46
1:C:81:LEU:HD23	1:C:81:LEU:C	2.36	0.46
1:I:67:VAL:HG13	1:I:68:VAL:HG22	1.98	0.46
2:P:111:ILE:H	2:P:111:ILE:HD12	1.79	0.46
1:A:158:ALA:HA	1:A:161:ILE:HD13	1.97	0.46
1:E:140:ARG:HD3	1:E:263:LEU:O	2.16	0.46
1:B:78:LEU:HD12	1:B:252:THR:HG22	1.97	0.46
1:B:140:ARG:HH22	1:B:161:ILE:CG2	2.28	0.46
1:I:126:CYS:CB	1:I:129:SER:OG	2.64	0.46
1:J:7:LEU:O	1:J:9:ARG:HG3	2.16	0.46
1:J:63:ASP:HB2	1:J:65:ASN:HB2	1.96	0.46
1:B:67:VAL:HG13	1:B:68:VAL:HG22	1.98	0.46
1:J:155:ILE:HG22	1:J:156:VAL:N	2.30	0.46
1:F:233:LEU:HG	1:F:251:GLU:OE2	2.15	0.46
1:A:97:ARG:HD3	1:B:73:ARG:NH2	2.30	0.46
1:D:112:ARG:O	1:D:116:GLU:HG3	2.16	0.46
1:G:7:LEU:O	1:G:9:ARG:HG3	2.16	0.46
1:A:63:ASP:HB2	1:A:65:ASN:HB2	1.98	0.46
2:R:111:ILE:HD12	2:R:111:ILE:N	2.30	0.46
1:J:233:LEU:O	2:T:109:LEU:HB2	2.14	0.46
1:J:233:LEU:O	2:T:109:LEU:HB3	2.15	0.46
1:G:179:ARG:HH11	1:G:179:ARG:HG2	1.81	0.46
1:E:173:LEU:HB2	1:E:201:LEU:HD11	1.98	0.46
1:G:36:GLY:HA3	1:G:122:ILE:HD13	1.97	0.46
1:H:167:ILE:HG21	1:H:262:ALA:HA	1.97	0.46
1:E:25:ARG:HD2	1:E:25:ARG:HA	1.58	0.46
1:A:25:ARG:HA	1:A:25:ARG:HD2	1.60	0.46
1:B:189:GLY:H	1:C:196:ARG:HH12	1.63	0.46
1:C:55:LEU:HD12	1:C:76:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:55:LEU:HD12	1:I:76:LEU:HB2	1.96	0.46
1:G:7:LEU:O	1:G:9:ARG:N	2.46	0.46
1:B:63:ASP:HB2	1:B:65:ASN:HB2	1.98	0.46
1:A:214:ASP:OD2	1:A:267:LYS:HG2	2.16	0.46
1:F:76:LEU:HA	1:F:77:PRO:HD2	1.73	0.46
1:I:189:GLY:O	1:J:190:HIS:HB2	2.16	0.46
1:E:85:PHE:CZ	1:E:107:LEU:HD13	2.51	0.46
1:E:239:ASP:CG	1:E:240:ARG:H	2.19	0.46
2:L:111:ILE:C	2:L:112:ARG:HG2	2.35	0.46
1:E:230:GLY:HA3	1:E:252:THR:HG22	1.98	0.46
1:I:89:LEU:C	1:I:91:GLU:H	2.19	0.46
1:D:64:GLU:HA	1:D:69:LYS:HZ1	1.79	0.46
1:D:69:LYS:HG2	1:D:69:LYS:H	1.58	0.46
1:H:7:LEU:O	1:H:9:ARG:N	2.47	0.46
1:I:87:LEU:HD23	1:I:87:LEU:HA	1.74	0.46
1:H:233:LEU:O	2:R:109:LEU:HB3	2.15	0.45
1:G:250:THR:HG22	1:G:251:GLU:N	2.31	0.45
1:H:176:ASN:HD22	1:H:179:ARG:N	1.97	0.45
1:J:140:ARG:HD3	1:J:263:LEU:O	2.16	0.45
1:G:140:ARG:HH22	1:G:161:ILE:CG2	2.29	0.45
1:J:89:LEU:C	1:J:91:GLU:H	2.19	0.45
1:E:64:GLU:HA	1:E:69:LYS:HZ1	1.80	0.45
1:A:152:LEU:HD12	1:A:200:CYS:SG	2.56	0.45
1:E:171:TYR:O	1:E:204:GLY:HA3	2.17	0.45
1:F:209:THR:HA	1:F:210:PRO:HD3	1.82	0.45
2:Q:109:LEU:HD12	2:Q:111:ILE:CD1	2.21	0.45
1:D:7:LEU:O	1:D:9:ARG:N	2.46	0.45
1:G:168:GLU:HA	1:G:171:TYR:OH	2.15	0.45
1:C:196:ARG:NH1	1:C:196:ARG:CG	2.61	0.45
1:J:176:ASN:HD21	1:J:178:ASP:HB2	1.81	0.45
1:D:214:ASP:OD2	1:D:267:LYS:HG2	2.16	0.45
1:C:158:ALA:HA	1:C:161:ILE:CD1	2.46	0.45
1:A:188:ALA:CB	1:B:149:LYS:HG2	2.45	0.45
1:F:149:LYS:HG3	1:F:149:LYS:H	1.55	0.45
1:C:69:LYS:HG2	1:C:69:LYS:H	1.59	0.45
1:D:173:LEU:HB2	1:D:201:LEU:HD11	1.98	0.45
1:F:7:LEU:O	1:F:9:ARG:N	2.47	0.45
1:J:167:ILE:HG21	1:J:262:ALA:HA	1.98	0.45
1:A:140:ARG:HD3	1:A:263:LEU:O	2.15	0.45
1:I:215:ALA:CB	1:I:266:LEU:HD12	2.47	0.45
1:J:112:ARG:O	1:J:116:GLU:HG3	2.16	0.45
1:I:233:LEU:O	2:S:109:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:149:LYS:HG3	1:G:149:LYS:H	1.57	0.45
1:F:89:LEU:C	1:F:91:GLU:H	2.19	0.45
1:J:126:CYS:CB	1:J:129:SER:OG	2.65	0.45
1:G:258:VAL:O	1:G:260:PRO:HD3	2.17	0.45
1:D:12:ALA:HB2	1:D:237:TYR:CD1	2.51	0.45
1:J:233:LEU:HG	1:J:251:GLU:OE2	2.17	0.45
1:F:176:ASN:HD21	1:F:178:ASP:HB2	1.81	0.45
1:E:231:GLN:HA	1:E:231:GLN:OE1	2.17	0.45
1:I:209:THR:HA	1:I:210:PRO:HD3	1.80	0.45
1:I:171:TYR:O	1:I:204:GLY:HA3	2.16	0.45
1:E:28:GLU:O	1:E:31:LYS:HG2	2.16	0.45
1:D:152:LEU:HD12	1:D:200:CYS:SG	2.57	0.45
1:B:36:GLY:HA3	1:B:122:ILE:HD13	1.99	0.45
1:C:179:ARG:NE	1:C:267:LYS:HE3	2.32	0.45
1:D:135:LEU:HD23	1:D:265:LEU:HD21	1.98	0.45
1:F:97:ARG:HD3	1:G:73:ARG:NH2	2.26	0.45
1:A:64:GLU:HA	1:A:69:LYS:HZ1	1.82	0.45
1:F:173:LEU:HB2	1:F:201:LEU:HD11	1.99	0.45
1:I:34:LEU:HD23	1:I:34:LEU:HA	1.79	0.45
1:C:155:ILE:HD11	1:C:197:VAL:HG13	1.99	0.45
1:B:170:PRO:HA	3:B:1008:HOH:O	2.17	0.45
1:H:25:ARG:HD2	1:H:25:ARG:HA	1.58	0.45
1:E:233:LEU:HG	1:E:251:GLU:OE2	2.16	0.45
1:I:7:LEU:O	1:I:9:ARG:HG3	2.16	0.45
1:I:239:ASP:HB3	1:I:246:ARG:NH2	2.32	0.45
1:D:155:ILE:HG22	1:D:156:VAL:N	2.32	0.45
1:D:117:PHE:O	1:D:120:GLU:HB2	2.16	0.45
1:F:12:ALA:HA	1:F:13:PRO:HD3	1.74	0.45
1:G:214:ASP:OD2	1:G:267:LYS:HG2	2.17	0.45
1:D:233:LEU:O	2:N:109:LEU:HB3	2.15	0.45
1:G:78:LEU:HD12	1:G:252:THR:HG22	1.98	0.45
1:I:258:VAL:O	1:I:260:PRO:HD3	2.17	0.45
1:F:7:LEU:O	1:F:9:ARG:HG3	2.18	0.45
1:G:117:PHE:O	1:G:120:GLU:HB2	2.17	0.45
1:J:152:LEU:HD12	1:J:200:CYS:SG	2.57	0.45
1:H:171:TYR:O	1:H:204:GLY:HA3	2.17	0.45
1:J:239:ASP:CG	1:J:240:ARG:H	2.19	0.45
1:D:176:ASN:HD21	1:D:178:ASP:HB2	1.82	0.44
1:J:140:ARG:HH22	1:J:161:ILE:CG2	2.30	0.44
1:A:155:ILE:HD11	1:A:197:VAL:HG13	1.99	0.44
1:I:135:LEU:HD11	1:I:212:ILE:HG22	1.98	0.44
1:A:7:LEU:O	1:A:9:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:169:GLY:HA3	1:C:221:ARG:HB3	2.00	0.44
1:D:36:GLY:HA3	1:D:122:ILE:CD1	2.47	0.44
1:D:179:ARG:NE	1:D:267:LYS:HE3	2.32	0.44
1:G:89:LEU:C	1:G:91:GLU:H	2.21	0.44
1:F:55:LEU:HD11	1:F:76:LEU:HD12	1.99	0.44
1:I:89:LEU:O	1:I:91:GLU:N	2.50	0.44
1:D:55:LEU:HD12	1:D:76:LEU:HB2	1.99	0.44
1:A:12:ALA:HB2	1:A:237:TYR:CD1	2.52	0.44
2:T:111:ILE:N	2:T:111:ILE:HD12	2.32	0.44
1:G:230:GLY:HA3	1:G:252:THR:HG22	1.99	0.44
1:B:64:GLU:HA	1:B:69:LYS:HZ2	1.81	0.44
1:G:126:CYS:CB	1:G:129:SER:OG	2.65	0.44
1:B:55:LEU:HD12	1:B:76:LEU:HB2	1.99	0.44
1:B:99:LYS:HA	1:B:100:PRO:HD3	1.82	0.44
1:C:135:LEU:HD23	1:C:265:LEU:HD21	1.99	0.44
1:C:25:ARG:HD2	1:C:25:ARG:HA	1.62	0.44
1:B:117:PHE:O	1:B:120:GLU:HB2	2.18	0.44
1:J:179:ARG:NE	1:J:267:LYS:HE3	2.32	0.44
1:J:265:LEU:O	1:J:266:LEU:HD23	2.17	0.44
1:D:99:LYS:HE3	1:E:57:GLU:OE1	2.18	0.44
1:G:233:LEU:O	2:Q:109:LEU:HB2	2.17	0.44
1:I:233:LEU:O	2:S:109:LEU:HB2	2.17	0.44
1:D:196:ARG:CG	1:D:196:ARG:NH1	2.66	0.44
1:J:179:ARG:HH11	1:J:179:ARG:CG	2.30	0.44
1:G:140:ARG:HD3	1:G:263:LEU:O	2.17	0.44
1:A:64:GLU:HA	1:A:69:LYS:HZ2	1.82	0.44
1:A:76:LEU:HA	1:A:77:PRO:HD2	1.78	0.44
1:I:233:LEU:HG	1:I:251:GLU:OE2	2.17	0.44
1:F:230:GLY:HA3	1:F:252:THR:HG22	2.00	0.44
1:D:78:LEU:HD12	1:D:252:THR:HG22	1.99	0.44
1:A:180:TRP:HH2	1:A:194:GLU:HG3	1.83	0.44
1:I:265:LEU:O	1:I:266:LEU:HD23	2.18	0.44
1:A:233:LEU:O	2:K:109:LEU:HB3	2.17	0.44
1:F:266:LEU:O	1:F:267:LYS:C	2.56	0.44
1:J:135:LEU:HD23	1:J:265:LEU:HD21	2.00	0.44
1:E:81:LEU:O	1:E:81:LEU:HD23	2.18	0.44
1:A:265:LEU:O	1:A:266:LEU:HD23	2.18	0.44
1:G:78:LEU:HD12	1:G:252:THR:HG23	2.00	0.44
1:J:173:LEU:HB2	1:J:201:LEU:HD11	2.00	0.44
1:E:126:CYS:HB2	1:E:129:SER:OG	2.17	0.44
1:A:12:ALA:HA	1:A:13:PRO:HD3	1.74	0.44
1:B:152:LEU:HD12	1:B:200:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:167:ILE:HG21	1:I:262:ALA:HA	2.00	0.44
1:C:87:LEU:HA	1:C:87:LEU:HD23	1.74	0.44
1:E:233:LEU:O	2:O:109:LEU:HB3	2.18	0.44
1:A:179:ARG:CG	1:A:179:ARG:HH11	2.29	0.44
1:C:140:ARG:HD3	1:C:263:LEU:O	2.18	0.44
1:F:190:HIS:HB2	1:J:189:GLY:O	2.18	0.44
1:H:265:LEU:O	1:H:266:LEU:HD23	2.17	0.44
1:B:155:ILE:HG22	1:B:156:VAL:N	2.33	0.44
1:J:258:VAL:O	1:J:260:PRO:HD3	2.18	0.44
1:D:176:ASN:HB3	1:D:179:ARG:HB2	1.99	0.43
1:I:152:LEU:HD12	1:I:200:CYS:SG	2.58	0.43
1:E:104:LEU:H	1:E:104:LEU:HD12	1.82	0.43
1:F:239:ASP:HB3	1:F:246:ARG:NH2	2.33	0.43
1:G:158:ALA:HA	1:G:161:ILE:CD1	2.49	0.43
1:B:260:PRO:O	1:B:263:LEU:HB3	2.18	0.43
1:B:135:LEU:HD23	1:B:265:LEU:HD21	2.00	0.43
2:K:111:ILE:N	2:K:111:ILE:HD12	2.34	0.43
1:D:140:ARG:HD3	1:D:263:LEU:O	2.17	0.43
1:I:155:ILE:HD11	1:I:197:VAL:HG13	2.00	0.43
1:B:36:GLY:HA3	1:B:122:ILE:CD1	2.48	0.43
2:Q:111:ILE:N	2:Q:111:ILE:HD12	2.33	0.43
1:A:78:LEU:HD12	1:A:252:THR:HG22	1.98	0.43
1:J:89:LEU:O	1:J:91:GLU:N	2.51	0.43
1:B:8:LYS:HB3	1:B:11:PHE:CD1	2.54	0.43
1:A:180:TRP:CH2	1:A:194:GLU:HG3	2.54	0.43
1:F:53:HIS:ND1	1:F:228:ILE:HD13	2.33	0.43
1:B:155:ILE:HD11	1:B:197:VAL:HG13	2.01	0.43
1:F:168:GLU:HA	1:F:171:TYR:OH	2.19	0.43
1:F:25:ARG:HA	1:F:25:ARG:HD2	1.55	0.43
1:E:135:LEU:HD23	1:E:265:LEU:HD21	1.99	0.43
1:B:76:LEU:HA	1:B:77:PRO:HD2	1.76	0.43
1:A:215:ALA:HB3	1:A:266:LEU:HD12	2.01	0.43
1:I:169:GLY:HA3	1:I:221:ARG:HB3	2.00	0.43
1:H:180:TRP:HH2	1:H:194:GLU:HG3	1.84	0.43
1:D:12:ALA:HA	1:D:13:PRO:HD3	1.76	0.43
1:G:135:LEU:HD23	1:G:265:LEU:HD21	2.00	0.43
1:D:81:LEU:O	1:D:250:THR:HG23	2.19	0.43
1:D:89:LEU:O	1:D:91:GLU:N	2.51	0.43
1:F:89:LEU:O	1:F:91:GLU:N	2.51	0.43
1:A:155:ILE:HG22	1:A:156:VAL:N	2.33	0.43
1:G:87:LEU:HD23	1:G:87:LEU:HA	1.69	0.43
1:I:81:LEU:O	1:I:250:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:GLU:HA	1:B:171:TYR:OH	2.19	0.43
1:E:266:LEU:O	1:E:267:LYS:C	2.57	0.43
1:G:12:ALA:CB	1:G:237:TYR:CD1	3.01	0.43
1:D:64:GLU:HA	1:D:69:LYS:HZ2	1.81	0.43
1:E:119:ASP:OD2	1:E:211:ARG:NE	2.43	0.43
1:H:34:LEU:HD22	1:H:118:GLU:OE2	2.19	0.43
1:J:87:LEU:HD23	1:J:87:LEU:HA	1.73	0.43
1:D:231:GLN:OE1	1:D:231:GLN:HA	2.19	0.43
1:I:76:LEU:HA	1:I:77:PRO:HD2	1.78	0.43
1:H:155:ILE:HD11	1:H:197:VAL:HG13	2.00	0.43
1:C:36:GLY:HA3	1:C:122:ILE:CD1	2.49	0.43
1:E:152:LEU:O	1:E:156:VAL:HG13	2.19	0.43
1:H:250:THR:HG22	1:H:251:GLU:N	2.34	0.42
1:J:250:THR:HG22	1:J:251:GLU:N	2.33	0.42
1:I:158:ALA:HA	1:I:161:ILE:HD13	1.99	0.42
1:H:89:LEU:C	1:H:91:GLU:H	2.23	0.42
1:F:69:LYS:H	1:F:69:LYS:HG2	1.65	0.42
1:D:7:LEU:O	1:D:9:ARG:HG3	2.18	0.42
1:B:171:TYR:O	1:B:204:GLY:HA3	2.19	0.42
1:A:169:GLY:HA3	1:A:221:ARG:HB3	2.01	0.42
1:I:179:ARG:NE	1:I:267:LYS:HE3	2.34	0.42
1:A:147:THR:CG2	1:A:149:LYS:HE3	2.42	0.42
1:I:34:LEU:HD22	1:I:118:GLU:OE2	2.18	0.42
1:A:117:PHE:O	1:A:120:GLU:HB2	2.19	0.42
1:C:250:THR:HG22	1:C:251:GLU:N	2.34	0.42
1:B:87:LEU:HA	1:B:87:LEU:HD23	1.75	0.42
1:B:209:THR:HA	1:B:210:PRO:HD3	1.78	0.42
1:C:76:LEU:HA	1:C:77:PRO:HD2	1.79	0.42
1:H:169:GLY:HA3	1:H:221:ARG:HB3	2.01	0.42
1:G:155:ILE:HD11	1:G:197:VAL:HG13	2.01	0.42
1:C:147:THR:CG2	1:C:149:LYS:HE3	2.41	0.42
1:D:158:ALA:HA	1:D:161:ILE:CD1	2.49	0.42
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.80	0.42
1:E:87:LEU:HA	1:E:87:LEU:HD23	1.74	0.42
1:F:179:ARG:NE	1:F:267:LYS:HE3	2.34	0.42
1:G:64:GLU:HA	1:G:69:LYS:HZ2	1.81	0.42
1:F:155:ILE:HD11	1:F:197:VAL:HG13	2.00	0.42
1:I:173:LEU:HB2	1:I:201:LEU:HD11	2.01	0.42
1:F:126:CYS:CB	1:F:129:SER:OG	2.68	0.42
1:B:7:LEU:HB3	1:B:236:GLY:HA3	2.00	0.42
1:C:28:GLU:O	1:C:31:LYS:HG2	2.19	0.42
1:I:117:PHE:C	1:I:117:PHE:CD2	2.93	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:97:ARG:CD	1:G:73:ARG:HH21	2.29	0.42
1:B:89:LEU:C	1:B:91:GLU:H	2.22	0.42
1:I:152:LEU:O	1:I:156:VAL:HG13	2.20	0.42
1:F:239:ASP:CG	1:F:240:ARG:H	2.23	0.42
1:E:152:LEU:HD12	1:E:200:CYS:SG	2.59	0.42
1:H:239:ASP:CG	1:H:240:ARG:H	2.23	0.42
1:B:239:ASP:CG	1:B:240:ARG:H	2.20	0.42
1:A:43:GLU:O	1:A:44:GLY:O	2.37	0.42
1:G:189:GLY:HA3	1:H:187:GLU:OE2	2.20	0.42
1:H:117:PHE:CD2	1:H:117:PHE:C	2.93	0.42
1:B:250:THR:HG22	1:B:251:GLU:N	2.35	0.42
1:J:176:ASN:HD22	1:J:179:ARG:N	1.94	0.42
1:C:89:LEU:O	1:C:91:GLU:N	2.53	0.42
1:D:153:GLU:O	1:D:156:VAL:HG22	2.19	0.42
1:I:124:ARG:NH2	1:I:211:ARG:O	2.51	0.42
1:J:117:PHE:O	1:J:120:GLU:HB2	2.20	0.42
1:A:36:GLY:HA3	1:A:122:ILE:CD1	2.49	0.42
1:G:99:LYS:HA	1:G:100:PRO:HD3	1.79	0.42
1:J:142:ILE:HD12	1:J:142:ILE:HA	1.95	0.42
1:D:170:PRO:HA	3:D:1009:HOH:O	2.20	0.42
1:B:233:LEU:O	2:L:109:LEU:HB3	2.19	0.42
1:I:140:ARG:HD2	1:I:260:PRO:O	2.20	0.42
1:G:85:PHE:CE1	1:G:107:LEU:HB2	2.54	0.42
1:D:112:ARG:NE	1:E:164:LYS:O	2.51	0.42
1:F:171:TYR:O	1:F:204:GLY:HA3	2.20	0.42
1:C:104:LEU:H	1:C:104:LEU:HD12	1.84	0.42
1:D:142:ILE:HA	1:D:142:ILE:HD12	1.93	0.42
1:G:104:LEU:H	1:G:104:LEU:HD12	1.84	0.42
1:A:176:ASN:HB3	1:A:179:ARG:HB2	2.01	0.42
1:J:78:LEU:HD12	1:J:252:THR:HG22	2.01	0.42
1:F:216:LEU:HA	1:F:216:LEU:HD12	1.77	0.42
1:C:89:LEU:C	1:C:91:GLU:N	2.73	0.42
1:B:85:PHE:CE1	1:B:107:LEU:HB2	2.55	0.42
1:I:31:LYS:NZ	3:I:1049:HOH:O	2.53	0.42
1:E:117:PHE:C	1:E:117:PHE:CD2	2.93	0.42
1:E:89:LEU:C	1:E:91:GLU:N	2.73	0.42
1:B:126:CYS:CB	1:B:129:SER:OG	2.67	0.42
1:C:209:THR:HA	1:C:210:PRO:HD3	1.80	0.42
1:F:31:LYS:NZ	3:F:1010:HOH:O	2.53	0.42
1:F:140:ARG:HH22	1:F:161:ILE:CG2	2.33	0.41
1:E:6:PHE:O	1:E:8:LYS:CG	2.67	0.41
1:H:12:ALA:CB	1:H:237:TYR:CD1	3.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:155:ILE:HD11	1:J:197:VAL:HG13	2.01	0.41
1:A:168:GLU:HA	1:A:171:TYR:OH	2.20	0.41
1:J:169:GLY:HA3	1:J:221:ARG:HB3	2.01	0.41
1:E:112:ARG:O	1:E:116:GLU:HG3	2.20	0.41
1:J:168:GLU:HA	1:J:171:TYR:OH	2.20	0.41
1:H:87:LEU:HD23	1:H:87:LEU:HA	1.75	0.41
1:F:34:LEU:HA	1:F:34:LEU:HD23	1.87	0.41
1:G:184:LEU:HD22	1:G:184:LEU:HA	1.95	0.41
1:I:25:ARG:HA	1:I:25:ARG:HD2	1.56	0.41
1:F:81:LEU:HD23	1:F:81:LEU:C	2.40	0.41
1:D:198:GLU:HG2	1:D:204:GLY:O	2.20	0.41
1:G:55:LEU:HD11	1:G:76:LEU:HD12	2.02	0.41
1:E:126:CYS:CB	1:E:129:SER:OG	2.68	0.41
1:G:36:GLY:HA3	1:G:122:ILE:CD1	2.50	0.41
1:H:7:LEU:O	1:H:9:ARG:HG3	2.20	0.41
1:C:117:PHE:O	1:C:120:GLU:HB2	2.20	0.41
1:F:117:PHE:CD2	1:F:117:PHE:C	2.94	0.41
1:B:179:ARG:NH1	1:B:179:ARG:CG	2.83	0.41
1:I:161:ILE:HG22	1:I:161:ILE:O	2.19	0.41
1:C:239:ASP:CG	1:C:240:ARG:N	2.73	0.41
1:G:7:LEU:HG	1:G:7:LEU:H	1.75	0.41
1:C:258:VAL:O	1:C:260:PRO:HD3	2.20	0.41
1:H:117:PHE:O	1:H:120:GLU:HB2	2.19	0.41
1:A:171:TYR:O	1:A:204:GLY:HA3	2.20	0.41
1:J:171:TYR:O	1:J:204:GLY:HA3	2.20	0.41
1:C:145:GLY:HA3	1:C:150:ASP:HB3	2.02	0.41
1:G:239:ASP:HB3	1:G:246:ARG:NH2	2.35	0.41
2:Q:111:ILE:H	2:Q:111:ILE:HD12	1.84	0.41
1:B:140:ARG:HD2	1:B:260:PRO:O	2.21	0.41
1:A:126:CYS:CB	1:A:129:SER:OG	2.68	0.41
1:D:97:ARG:CD	1:E:73:ARG:HH21	2.34	0.41
1:H:69:LYS:HG2	1:H:69:LYS:H	1.60	0.41
1:D:7:LEU:HB3	1:D:236:GLY:HA3	2.02	0.41
1:D:155:ILE:CD1	1:D:197:VAL:HG13	2.50	0.41
1:D:117:PHE:C	1:D:117:PHE:CD2	2.93	0.41
1:H:180:TRP:CH2	1:H:194:GLU:HG3	2.56	0.41
1:G:265:LEU:O	1:G:266:LEU:HD23	2.21	0.41
1:F:170:PRO:HA	3:F:1003:HOH:O	2.21	0.41
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.90	0.41
1:D:266:LEU:O	1:D:267:LYS:C	2.59	0.41
1:B:231:GLN:HA	1:B:231:GLN:OE1	2.21	0.41
1:C:69:LYS:HB3	1:C:69:LYS:HE3	1.94	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:152:LEU:HD12	1:H:200:CYS:SG	2.60	0.41
1:G:179:ARG:NE	1:G:267:LYS:HE3	2.35	0.41
1:F:59:GLU:O	1:F:61:LEU:HD13	2.20	0.41
1:D:97:ARG:HD3	1:E:73:ARG:NH2	2.36	0.41
1:G:169:GLY:HA3	1:G:221:ARG:HB3	2.02	0.41
1:C:180:TRP:HH2	1:C:194:GLU:HG3	1.85	0.41
1:D:34:LEU:HD22	1:D:118:GLU:OE2	2.20	0.41
1:F:250:THR:HG22	1:F:251:GLU:H	1.85	0.41
1:E:135:LEU:HD11	1:E:212:ILE:HG22	2.03	0.41
1:J:266:LEU:O	1:J:267:LYS:C	2.59	0.41
1:D:265:LEU:O	1:D:266:LEU:HD23	2.21	0.41
1:I:140:ARG:HD3	1:I:263:LEU:O	2.21	0.41
1:D:72:LEU:HD11	1:I:129:SER:HB3	2.03	0.41
1:A:250:THR:HG22	1:A:251:GLU:H	1.85	0.41
1:D:155:ILE:HD11	1:D:197:VAL:HG13	2.01	0.41
1:J:28:GLU:O	1:J:31:LYS:HG2	2.21	0.41
1:D:169:GLY:HA3	1:D:221:ARG:HB3	2.01	0.41
1:H:209:THR:HA	1:H:210:PRO:HD3	1.84	0.41
1:G:176:ASN:HD21	1:G:178:ASP:HB2	1.85	0.41
1:C:176:ASN:HD21	1:C:178:ASP:HB2	1.85	0.41
1:J:215:ALA:HB3	1:J:266:LEU:HD12	2.03	0.41
1:D:179:ARG:NH1	1:D:179:ARG:CG	2.83	0.41
1:H:78:LEU:HD12	1:H:252:THR:HG23	2.01	0.41
1:D:140:ARG:HD2	1:D:260:PRO:O	2.21	0.41
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.90	0.41
1:G:89:LEU:O	1:G:91:GLU:N	2.54	0.41
1:D:89:LEU:C	1:D:91:GLU:H	2.23	0.41
1:J:89:LEU:C	1:J:91:GLU:N	2.74	0.41
1:I:89:LEU:C	1:I:91:GLU:N	2.75	0.41
1:B:173:LEU:HB2	1:B:201:LEU:HD11	2.02	0.41
1:I:152:LEU:HD22	1:I:152:LEU:N	2.35	0.41
1:C:126:CYS:CB	1:C:129:SER:OG	2.68	0.41
1:E:7:LEU:HG	1:E:7:LEU:H	1.75	0.41
1:D:81:LEU:C	1:D:81:LEU:HD23	2.41	0.41
1:H:34:LEU:HA	1:H:34:LEU:HD23	1.91	0.41
1:E:209:THR:HA	1:E:210:PRO:HD3	1.80	0.41
1:E:169:GLY:HA3	1:E:221:ARG:HB3	2.01	0.41
1:F:67:VAL:HG13	1:F:68:VAL:HG22	2.03	0.41
1:I:196:ARG:NH1	1:I:196:ARG:CG	2.65	0.41
2:K:111:ILE:C	2:K:112:ARG:HG2	2.40	0.41
1:D:161:ILE:H	1:D:161:ILE:HD12	1.86	0.41
1:B:89:LEU:HD12	1:B:245:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:53:HIS:ND1	1:G:228:ILE:HD13	2.36	0.41
1:A:173:LEU:HB2	1:A:201:LEU:HD11	2.02	0.41
1:I:218:VAL:HA	1:I:262:ALA:O	2.21	0.41
1:G:193:LEU:O	1:G:194:GLU:C	2.60	0.41
1:H:140:ARG:HH22	1:H:161:ILE:CG2	2.34	0.40
1:A:97:ARG:CD	1:B:73:ARG:HH21	2.35	0.40
1:A:55:LEU:HD11	1:A:76:LEU:HD12	2.04	0.40
1:J:36:GLY:HA3	1:J:122:ILE:CD1	2.51	0.40
1:E:176:ASN:HD22	1:E:179:ARG:N	1.97	0.40
1:J:149:LYS:H	1:J:149:LYS:HG3	1.54	0.40
1:D:215:ALA:HB3	1:D:266:LEU:HD12	2.03	0.40
1:D:126:CYS:CB	1:D:129:SER:OG	2.69	0.40
1:A:175:ILE:HD12	1:A:180:TRP:HB2	2.04	0.40
1:D:171:TYR:O	1:D:204:GLY:HA3	2.21	0.40
1:C:171:TYR:O	1:C:204:GLY:HA3	2.21	0.40
1:D:145:GLY:HA3	1:D:150:ASP:HB3	2.04	0.40
1:F:218:VAL:HA	1:F:262:ALA:O	2.22	0.40
1:H:189:GLY:HA3	1:I:187:GLU:OE2	2.21	0.40
1:D:51:ALA:HB2	1:I:54:PRO:HB3	2.02	0.40
1:A:179:ARG:NE	1:A:267:LYS:HE3	2.36	0.40
1:E:176:ASN:HD21	1:E:178:ASP:HB2	1.86	0.40
1:H:140:ARG:HD2	1:H:260:PRO:O	2.21	0.40
1:G:216:LEU:HD12	1:G:216:LEU:HA	1.83	0.40
1:H:12:ALA:HA	1:H:13:PRO:HD3	1.73	0.40
1:J:117:PHE:CD2	1:J:117:PHE:C	2.95	0.40
1:H:28:GLU:O	1:H:31:LYS:HG2	2.21	0.40
1:J:184:LEU:HA	1:J:184:LEU:HD22	1.95	0.40
1:D:87:LEU:HD23	1:D:87:LEU:HA	1.76	0.40
1:F:169:GLY:HA3	1:F:221:ARG:HB3	2.02	0.40
1:F:214:ASP:OD2	1:F:267:LYS:HG2	2.20	0.40
1:H:230:GLY:HA3	1:H:252:THR:HG22	2.04	0.40
1:D:140:ARG:HH22	1:D:161:ILE:CG2	2.34	0.40
1:F:89:LEU:C	1:F:91:GLU:N	2.74	0.40
1:D:76:LEU:HA	1:D:77:PRO:HD2	1.79	0.40
1:G:171:TYR:O	1:G:204:GLY:HA3	2.22	0.40
1:D:152:LEU:O	1:D:156:VAL:HG13	2.21	0.40
1:G:117:PHE:C	1:G:117:PHE:CD2	2.95	0.40
1:J:99:LYS:HA	1:J:100:PRO:HD3	1.79	0.40
1:H:145:GLY:HA3	1:H:150:ASP:OD2	2.21	0.40
1:D:67:VAL:HG13	1:D:68:VAL:HG22	2.03	0.40
2:S:111:ILE:O	2:S:112:ARG:CB	2.69	0.40
1:F:140:ARG:HD2	1:F:260:PRO:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:156:VAL:HG21	1:J:181:ILE:HG12	2.04	0.40
1:B:7:LEU:O	1:B:9:ARG:HG3	2.22	0.40
1:D:181:ILE:HG12	1:E:156:VAL:HG21	2.04	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	262/265 (99%)	232 (88%)	26 (10%)	4 (2%)	15	57
1	B	262/265 (99%)	233 (89%)	24 (9%)	5 (2%)	12	51
1	C	262/265 (99%)	232 (88%)	27 (10%)	3 (1%)	21	65
1	D	262/265 (99%)	231 (88%)	26 (10%)	5 (2%)	12	51
1	E	262/265 (99%)	232 (88%)	24 (9%)	6 (2%)	10	45
1	F	262/265 (99%)	235 (90%)	22 (8%)	5 (2%)	12	51
1	G	262/265 (99%)	231 (88%)	26 (10%)	5 (2%)	12	51
1	H	262/265 (99%)	232 (88%)	26 (10%)	4 (2%)	15	57
1	I	262/265 (99%)	234 (89%)	23 (9%)	5 (2%)	12	51
1	J	262/265 (99%)	233 (89%)	24 (9%)	5 (2%)	12	51
2	K	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	L	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	M	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	N	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	O	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	P	6/8 (75%)	3 (50%)	1 (17%)	2 (33%)	0	0
2	Q	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	R	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	S	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
All	All	2680/2730 (98%)	2355 (88%)	267 (10%)	58 (2%)	10	46

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLY
1	B	44	GLY
1	C	44	GLY
1	D	44	GLY
1	F	44	GLY
1	G	44	GLY
1	J	44	GLY
1	E	44	GLY
1	H	44	GLY
1	I	44	GLY
2	K	112	ARG
2	L	112	ARG
2	M	112	ARG
2	N	112	ARG
2	O	112	ARG
2	P	112	ARG
2	Q	112	ARG
2	R	112	ARG
2	S	112	ARG
2	T	112	ARG
1	A	242	LYS
1	E	242	LYS
1	F	242	LYS
1	B	242	LYS
1	C	242	LYS
1	D	90	TRP
1	D	242	LYS
1	E	90	TRP
1	F	90	TRP
1	G	242	LYS
1	H	242	LYS
1	I	90	TRP
1	I	242	LYS
1	J	242	LYS
1	E	7	LEU
1	G	7	LEU

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Mol	Chain	Res	Type
1	J	90	TRP
2	P	109	LEU
1	A	100	PRO
1	B	100	PRO
1	B	210	PRO
1	F	100	PRO
1	G	100	PRO
1	J	100	PRO
1	C	100	PRO
1	D	100	PRO
1	D	210	PRO
1	F	210	PRO
1	H	100	PRO
1	H	210	PRO
1	I	100	PRO
1	A	210	PRO
1	B	155	ILE
1	E	100	PRO
1	G	210	PRO
1	J	210	PRO
1	E	210	PRO
1	I	155	ILE

### 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	233/234 (100%)	192 (82%)	41 (18%)	3	10
1	B	233/234 (100%)	192 (82%)	41 (18%)	3	10
1	C	233/234 (100%)	189 (81%)	44 (19%)	2	9
1	D	233/234 (100%)	192 (82%)	41 (18%)	3	10
1	E	233/234 (100%)	189 (81%)	44 (19%)	2	9
1	F	233/234 (100%)	187 (80%)	46 (20%)	2	8
1	G	233/234 (100%)	191 (82%)	42 (18%)	2	10
1	H	233/234 (100%)	189 (81%)	44 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	233/234 (100%)	190 (82%)	43 (18%)	2	9
1	J	233/234 (100%)	190 (82%)	43 (18%)	2	9
2	K	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	L	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	M	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	N	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	O	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	P	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	Q	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	R	5/5 (100%)	4 (80%)	1 (20%)	2	8
2	S	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	T	5/5 (100%)	2 (40%)	3 (60%)	0	0
All	All	2380/2390 (100%)	1925 (81%)	455 (19%)	2	9

All (455) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	GLU
1	A	7	LEU
1	A	10	SER
1	A	16	GLU
1	A	17	LYS
1	A	41	ASP
1	A	55	LEU
1	A	58	VAL
1	A	60	VAL
1	A	68	VAL
1	A	69	LYS
1	A	73	ARG
1	A	81	LEU
1	A	82	ARG
1	A	84	THR
1	A	89	LEU
1	A	96	GLU
1	A	104	LEU
1	A	106	SER
1	A	124	ARG

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Mol	Chain	Res	Type
1	A	131	VAL
1	A	139	GLU
1	A	140	ARG
1	A	143	GLU
1	A	147	THR
1	A	153	GLU
1	A	159	LEU
1	A	172	THR
1	A	173	LEU
1	A	175	ILE
1	A	179	ARG
1	A	184	LEU
1	A	196	ARG
1	A	229	LEU
1	A	234	SER
1	A	240	ARG
1	A	243	ASP
1	A	261	GLU
1	A	265	LEU
1	A	267	LYS
1	B	4	MET
1	B	5	GLU
1	B	7	LEU
1	B	10	SER
1	B	16	GLU
1	B	17	LYS
1	B	41	ASP
1	B	55	LEU
1	B	58	VAL
1	B	68	VAL
1	B	69	LYS
1	B	73	ARG
1	B	81	LEU
1	B	82	ARG
1	B	84	THR
1	B	89	LEU
1	B	96	GLU
1	B	104	LEU
1	B	106	SER
1	B	124	ARG
1	B	131	VAL
1	B	139	GLU

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Mol	Chain	Res	Type
1	B	140	ARG
1	B	147	THR
1	B	153	GLU
1	B	159	LEU
1	B	172	THR
1	B	173	LEU
1	B	175	ILE
1	B	179	ARG
1	B	184	LEU
1	B	196	ARG
1	B	219	SER
1	B	229	LEU
1	B	234	SER
1	B	240	ARG
1	B	243	ASP
1	B	252	THR
1	B	261	GLU
1	B	265	LEU
1	B	267	LYS
1	C	4	MET
1	C	5	GLU
1	C	7	LEU
1	C	10	SER
1	C	16	GLU
1	C	17	LYS
1	C	41	ASP
1	C	55	LEU
1	C	58	VAL
1	C	67	VAL
1	C	68	VAL
1	C	69	LYS
1	C	73	ARG
1	C	78	LEU
1	C	81	LEU
1	C	82	ARG
1	C	84	THR
1	C	89	LEU
1	C	96	GLU
1	C	104	LEU
1	C	106	SER
1	C	124	ARG
1	C	126	CYS

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Mol	Chain	Res	Type
1	C	131	VAL
1	C	139	GLU
1	C	140	ARG
1	C	147	THR
1	C	153	GLU
1	C	159	LEU
1	C	172	THR
1	C	173	LEU
1	C	175	ILE
1	C	179	ARG
1	C	184	LEU
1	C	196	ARG
1	C	214	ASP
1	C	219	SER
1	C	229	LEU
1	C	234	SER
1	C	240	ARG
1	C	243	ASP
1	C	261	GLU
1	C	265	LEU
1	C	267	LYS
1	D	4	MET
1	D	5	GLU
1	D	7	LEU
1	D	10	SER
1	D	16	GLU
1	D	17	LYS
1	D	41	ASP
1	D	55	LEU
1	D	58	VAL
1	D	60	VAL
1	D	68	VAL
1	D	69	LYS
1	D	73	ARG
1	D	81	LEU
1	D	82	ARG
1	D	84	THR
1	D	89	LEU
1	D	96	GLU
1	D	104	LEU
1	D	124	ARG
1	D	131	VAL

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Mol	Chain	Res	Type
1	D	139	GLU
1	D	140	ARG
1	D	147	THR
1	D	153	GLU
1	D	159	LEU
1	D	172	THR
1	D	173	LEU
1	D	175	ILE
1	D	179	ARG
1	D	184	LEU
1	D	196	ARG
1	D	229	LEU
1	D	234	SER
1	D	237	TYR
1	D	240	ARG
1	D	243	ASP
1	D	252	THR
1	D	261	GLU
1	D	265	LEU
1	D	267	LYS
1	E	4	MET
1	E	5	GLU
1	E	7	LEU
1	E	10	SER
1	E	16	GLU
1	E	17	LYS
1	E	41	ASP
1	E	55	LEU
1	E	58	VAL
1	E	60	VAL
1	E	68	VAL
1	E	69	LYS
1	E	73	ARG
1	E	81	LEU
1	E	82	ARG
1	E	84	THR
1	E	89	LEU
1	E	96	GLU
1	E	104	LEU
1	E	106	SER
1	E	124	ARG
1	E	126	CYS

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Mol	Chain	Res	Type
1	E	131	VAL
1	E	139	GLU
1	E	140	ARG
1	E	147	THR
1	E	153	GLU
1	E	159	LEU
1	E	172	THR
1	E	173	LEU
1	E	175	ILE
1	E	179	ARG
1	E	184	LEU
1	E	196	ARG
1	E	219	SER
1	E	229	LEU
1	E	234	SER
1	E	237	TYR
1	E	240	ARG
1	E	243	ASP
1	E	252	THR
1	E	261	GLU
1	E	265	LEU
1	E	267	LYS
1	F	4	MET
1	F	5	GLU
1	F	7	LEU
1	F	10	SER
1	F	16	GLU
1	F	17	LYS
1	F	41	ASP
1	F	55	LEU
1	F	58	VAL
1	F	60	VAL
1	F	68	VAL
1	F	69	LYS
1	F	73	ARG
1	F	78	LEU
1	F	81	LEU
1	F	82	ARG
1	F	84	THR
1	F	89	LEU
1	F	96	GLU
1	F	104	LEU

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Mol	Chain	Res	Type
1	F	106	SER
1	F	124	ARG
1	F	126	CYS
1	F	131	VAL
1	F	139	GLU
1	F	140	ARG
1	F	143	GLU
1	F	147	THR
1	F	153	GLU
1	F	159	LEU
1	F	172	THR
1	F	173	LEU
1	F	175	ILE
1	F	179	ARG
1	F	184	LEU
1	F	196	ARG
1	F	214	ASP
1	F	219	SER
1	F	229	LEU
1	F	234	SER
1	F	240	ARG
1	F	243	ASP
1	F	252	THR
1	F	261	GLU
1	F	265	LEU
1	F	267	LYS
1	G	4	MET
1	G	5	GLU
1	G	7	LEU
1	G	10	SER
1	G	16	GLU
1	G	17	LYS
1	G	41	ASP
1	G	55	LEU
1	G	58	VAL
1	G	60	VAL
1	G	68	VAL
1	G	69	LYS
1	G	73	ARG
1	G	78	LEU
1	G	81	LEU
1	G	82	ARG

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Mol	Chain	Res	Type
1	G	84	THR
1	G	89	LEU
1	G	96	GLU
1	G	104	LEU
1	G	106	SER
1	G	124	ARG
1	G	126	CYS
1	G	131	VAL
1	G	139	GLU
1	G	140	ARG
1	G	147	THR
1	G	153	GLU
1	G	159	LEU
1	G	172	THR
1	G	173	LEU
1	G	175	ILE
1	G	184	LEU
1	G	196	ARG
1	G	229	LEU
1	G	234	SER
1	G	237	TYR
1	G	240	ARG
1	G	243	ASP
1	G	261	GLU
1	G	265	LEU
1	G	267	LYS
1	H	4	MET
1	H	5	GLU
1	H	7	LEU
1	H	10	SER
1	H	16	GLU
1	H	17	LYS
1	H	41	ASP
1	H	55	LEU
1	H	58	VAL
1	H	60	VAL
1	H	68	VAL
1	H	69	LYS
1	H	73	ARG
1	H	78	LEU
1	H	81	LEU
1	H	82	ARG

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Mol	Chain	Res	Type
1	H	84	THR
1	H	89	LEU
1	H	96	GLU
1	H	104	LEU
1	H	106	SER
1	H	124	ARG
1	H	126	CYS
1	H	131	VAL
1	H	139	GLU
1	H	140	ARG
1	H	147	THR
1	H	153	GLU
1	H	159	LEU
1	H	172	THR
1	H	173	LEU
1	H	175	ILE
1	H	179	ARG
1	H	184	LEU
1	H	196	ARG
1	H	214	ASP
1	H	219	SER
1	H	229	LEU
1	H	234	SER
1	H	240	ARG
1	H	243	ASP
1	H	261	GLU
1	H	265	LEU
1	H	267	LYS
1	I	4	MET
1	I	5	GLU
1	I	7	LEU
1	I	10	SER
1	I	16	GLU
1	I	17	LYS
1	I	41	ASP
1	I	55	LEU
1	I	58	VAL
1	I	60	VAL
1	I	68	VAL
1	I	69	LYS
1	I	73	ARG
1	I	81	LEU

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Mol	Chain	Res	Type
1	I	82	ARG
1	I	84	THR
1	I	89	LEU
1	I	96	GLU
1	I	104	LEU
1	I	106	SER
1	I	124	ARG
1	I	126	CYS
1	I	131	VAL
1	I	139	GLU
1	I	140	ARG
1	I	147	THR
1	I	153	GLU
1	I	159	LEU
1	I	172	THR
1	I	173	LEU
1	I	175	ILE
1	I	184	LEU
1	I	196	ARG
1	I	214	ASP
1	I	219	SER
1	I	229	LEU
1	I	234	SER
1	I	240	ARG
1	I	243	ASP
1	I	252	THR
1	I	261	GLU
1	I	265	LEU
1	I	267	LYS
1	J	4	MET
1	J	5	GLU
1	J	7	LEU
1	J	10	SER
1	J	16	GLU
1	J	17	LYS
1	J	41	ASP
1	J	55	LEU
1	J	58	VAL
1	J	60	VAL
1	J	68	VAL
1	J	69	LYS
1	J	73	ARG

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Mol	Chain	Res	Type
1	J	81	LEU
1	J	82	ARG
1	J	84	THR
1	J	89	LEU
1	J	96	GLU
1	J	104	LEU
1	J	106	SER
1	J	124	ARG
1	J	126	CYS
1	J	131	VAL
1	J	139	GLU
1	J	140	ARG
1	J	147	THR
1	J	153	GLU
1	J	159	LEU
1	J	172	THR
1	J	173	LEU
1	J	175	ILE
1	J	179	ARG
1	J	184	LEU
1	J	196	ARG
1	J	219	SER
1	J	229	LEU
1	J	234	SER
1	J	237	TYR
1	J	240	ARG
1	J	243	ASP
1	J	261	GLU
1	J	265	LEU
1	J	267	LYS
2	K	109	LEU
2	K	111	ILE
2	L	109	LEU
2	L	111	ILE
2	L	112	ARG
2	M	109	LEU
2	M	111	ILE
2	M	112	ARG
2	N	109	LEU
2	N	111	ILE
2	O	109	LEU
2	O	111	ILE

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Mol	Chain	Res	Type
2	O	112	ARG
2	P	109	LEU
2	P	111	ILE
2	P	112	ARG
2	Q	109	LEU
2	Q	111	ILE
2	Q	112	ARG
2	R	109	LEU
2	S	109	LEU
2	S	111	ILE
2	S	112	ARG
2	T	109	LEU
2	T	111	ILE
2	T	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	B	176	ASN
1	C	176	ASN
1	D	176	ASN
1	E	176	ASN
1	F	176	ASN
1	G	176	ASN
1	H	176	ASN
1	I	176	ASN
1	J	176	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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, 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	264/265 (99%)	-0.26	0 100 100	99, 128, 173, 221	0
1	B	264/265 (99%)	-0.29	0 100 100	94, 128, 173, 228	0
1	C	264/265 (99%)	-0.32	0 100 100	89, 123, 172, 232	0
1	D	264/265 (99%)	-0.27	0 100 100	95, 126, 173, 232	0
1	E	264/265 (99%)	-0.30	0 100 100	97, 128, 175, 230	0
1	F	264/265 (99%)	-0.35	0 100 100	76, 108, 161, 226	0
1	G	264/265 (99%)	-0.31	0 100 100	89, 119, 166, 226	0
1	H	264/265 (99%)	-0.31	0 100 100	94, 123, 166, 209	0
1	I	264/265 (99%)	-0.35	0 100 100	86, 117, 166, 219	0
1	J	264/265 (99%)	-0.31	0 100 100	82, 115, 166, 222	0
2	K	8/8 (100%)	0.30	0 100 100	133, 150, 185, 199	0
2	L	8/8 (100%)	0.34	0 100 100	130, 150, 180, 193	0
2	M	8/8 (100%)	0.17	0 100 100	125, 139, 185, 191	0
2	N	8/8 (100%)	0.12	0 100 100	122, 146, 191, 200	0
2	O	8/8 (100%)	0.70	0 100 100	132, 153, 185, 201	0
2	P	8/8 (100%)	0.18	0 100 100	123, 135, 189, 211	0
2	Q	8/8 (100%)	0.16	0 100 100	129, 148, 177, 187	0
2	R	8/8 (100%)	0.17	0 100 100	129, 142, 172, 197	0
2	S	8/8 (100%)	0.06	0 100 100	116, 139, 177, 190	0
2	T	8/8 (100%)	0.22	0 100 100	119, 141, 183, 193	0
All	All	2720/2730 (99%)	-0.29	0 100 100	76, 123, 174, 232	0

There are no RSRZ outliers to report.

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.