Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:40 pm BST

PDB ID	:	4RO0
Title	:	Crystal structure of MthK gating ring in a ligand-free form
Authors	:	Dong, W.; Guo, R.; Chai, H.; Chen, Z.; Cui, H.; Ren, Z.; Li, Y.; Ye, S.
Deposited on	:	2014-10-27
Resolution	:	3.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

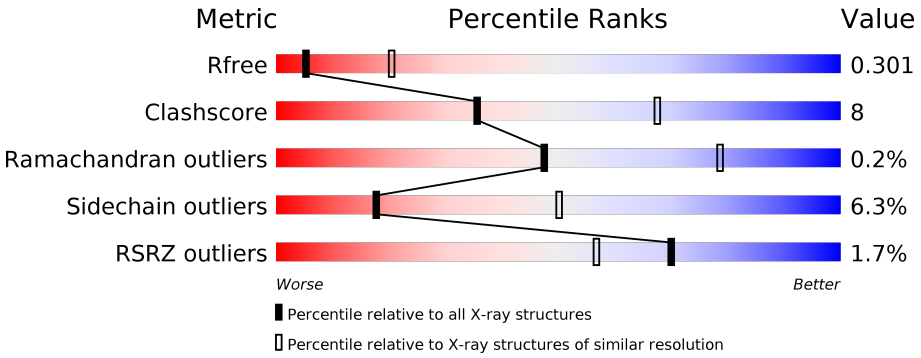
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	230	2% 60% 34%
1	B	230	64% 31%
1	C	230	63% 28% 5%
1	D	230	67% 25%
1	E	230	60% 31% 5%
1	F	230	62% 30%

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Mol	Chain	Length	Quality of chain
1	G	230	61% 32%
1	H	230	63% 29%
1	I	230	65% 29%
1	J	230	57% 36%
1	K	230	69% 24%
1	L	230	64% 30%
1	M	230	74% 20%
1	N	230	65% 27%
1	O	230	64% 26% 5%
1	P	230	67% 28%
1	Q	230	10% 66% 29%
1	R	230	3% 66% 28%
1	S	230	70% 23%
1	T	230	66% 27%
1	a	230	91% 5%
1	b	230	92%
1	c	230	90% 6%
1	d	230	91% 5%
1	e	230	91% 5%
1	f	230	91% 5%
1	g	230	3% 90% 6%
1	h	230	3% 91% 5%
1	i	230	93%
1	j	230	92%
1	k	230	90% 6%

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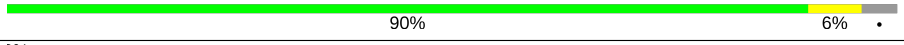
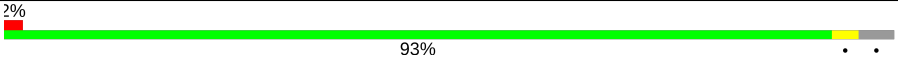
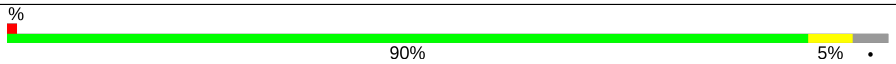
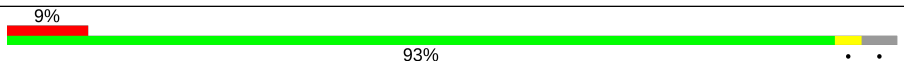
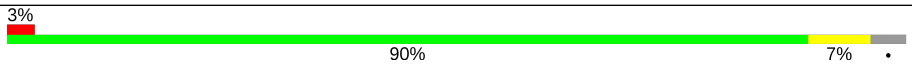
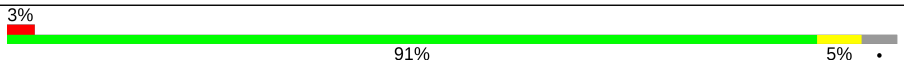
Mol	Chain	Length	Quality of chain
1	l	230	
1	m	230	
1	n	230	
1	o	230	
1	p	230	
1	q	230	
1	r	230	
1	s	230	
1	t	230	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 68748 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 Calcium-gated potassium channel MthK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	a	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	B	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	b	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	C	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	c	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	D	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	d	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	E	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	e	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	F	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	f	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	G	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	g	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	H	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	h	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	i	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	J	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	j	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	K	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	k	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	L	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	l	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	M	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	m	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	N	221	Total	C	N	O	S	0	0	0
			1713	1066	302	338	7			
1	n	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	O	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	o	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	P	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	p	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	Q	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	q	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	R	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	r	221	Total	C	N	O	S	0	0	0
			1713	1066	302	338	7			
1	S	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			

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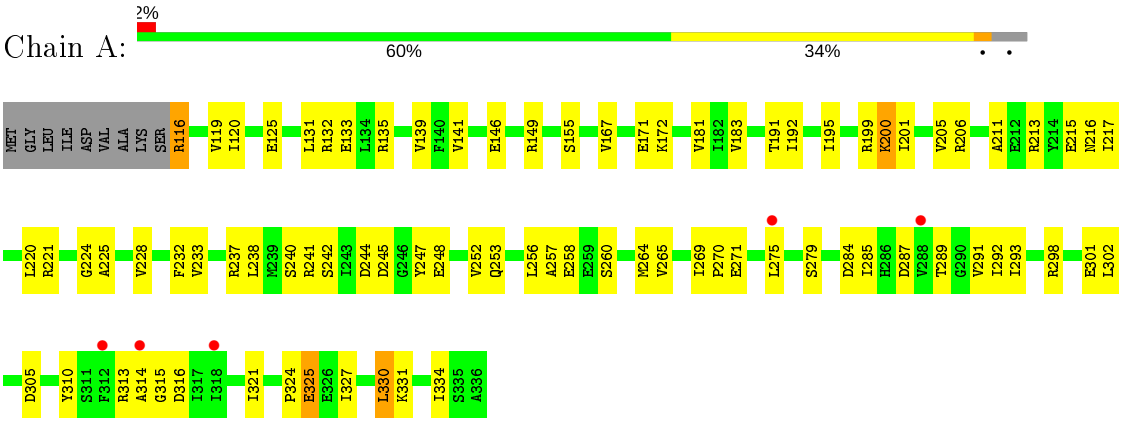
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	s	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	T	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	t	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			

3 Residue-property plots (i)

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

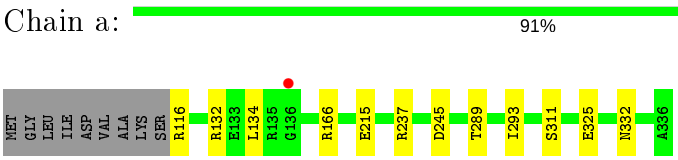
- Molecule 1: Calcium-gated potassium channel MthK

Chain A:



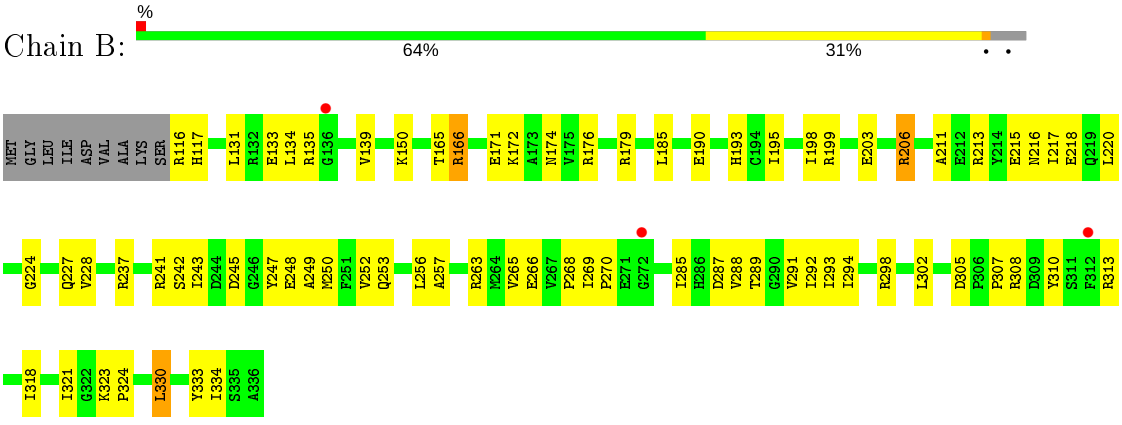
- Molecule 1: Calcium-gated potassium channel MthK

Chain a:



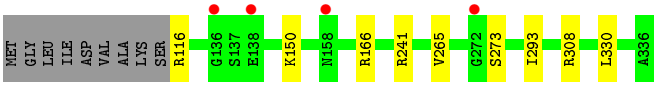
- Molecule 1: Calcium-gated potassium channel MthK

Chain B:



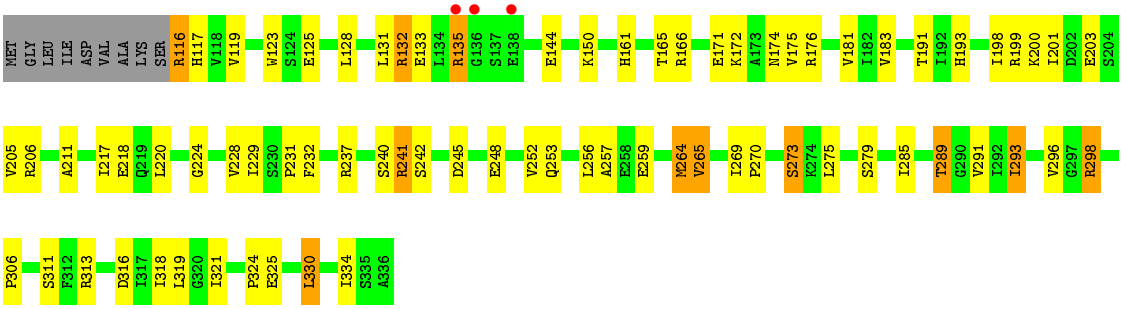
- Molecule 1: Calcium-gated potassium channel MthK

Chain b:



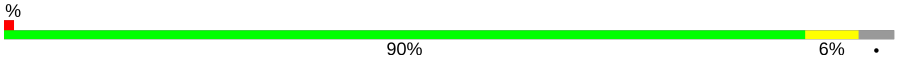
• Molecule 1: Calcium-gated potassium channel MthK

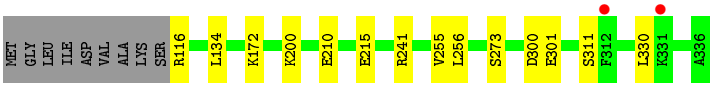
Chain C:



• Molecule 1: Calcium-gated potassium channel MthK

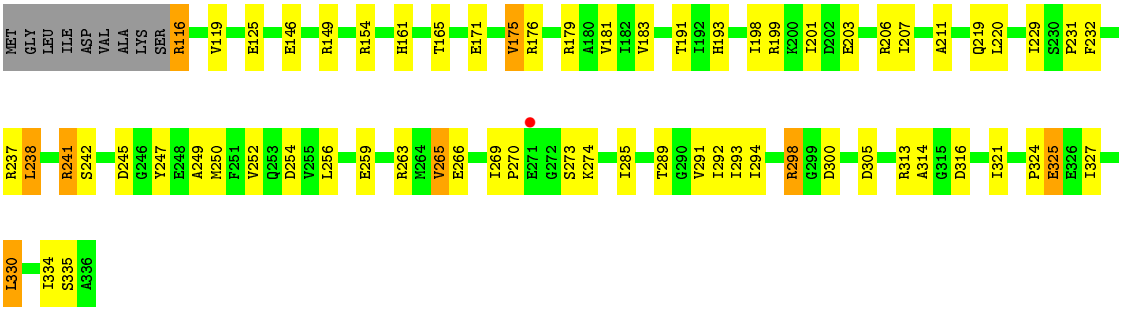
Chain c:





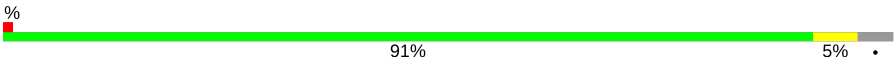
• Molecule 1: Calcium-gated potassium channel MthK

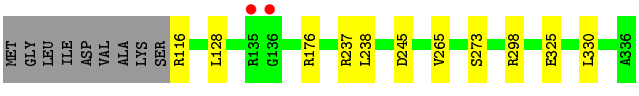
Chain D:



• Molecule 1: Calcium-gated potassium channel MthK

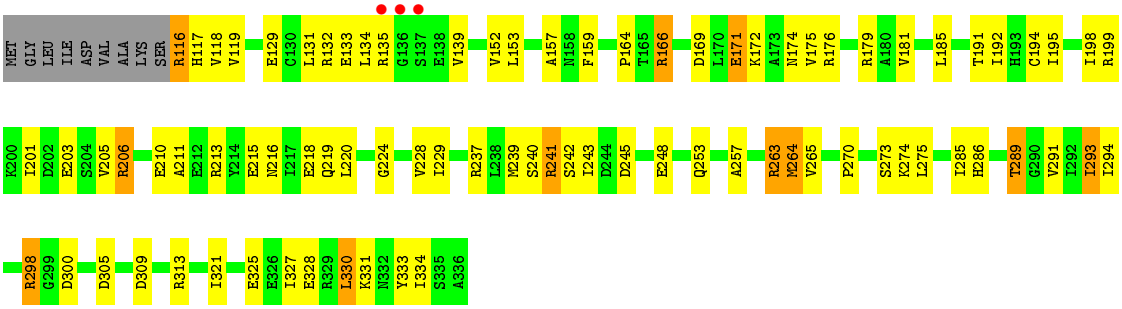
Chain d:





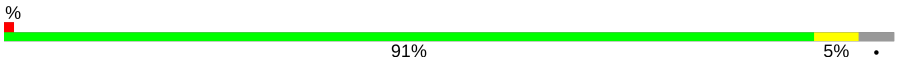
• Molecule 1: Calcium-gated potassium channel MthK

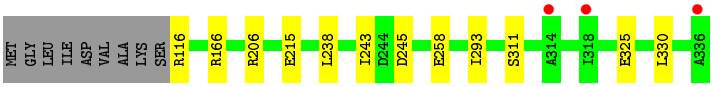
Chain E:



- Molecule 1: Calcium-gated potassium channel MthK

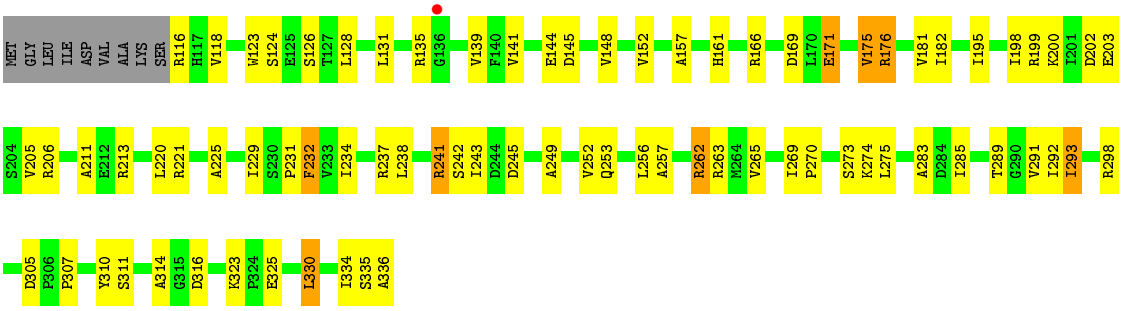
Chain e:





- Molecule 1: Calcium-gated potassium channel MthK

Chain F:

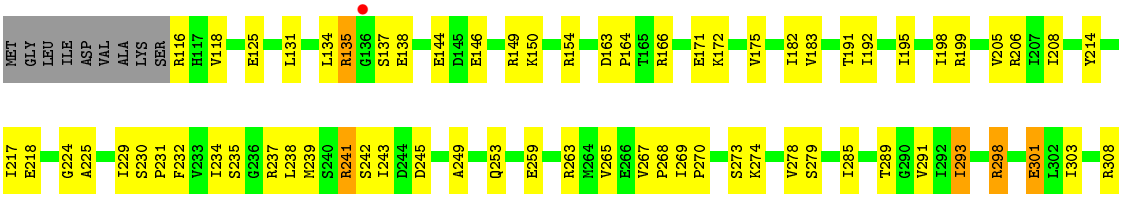


- Molecule 1: Calcium-gated potassium channel MthK

Chain f:

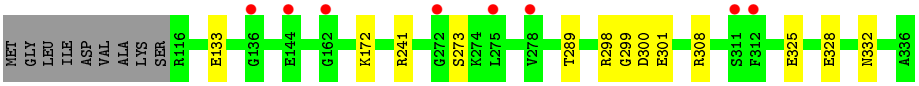
- Molecule 1: Calcium-gated potassium channel MthK

Chain G:



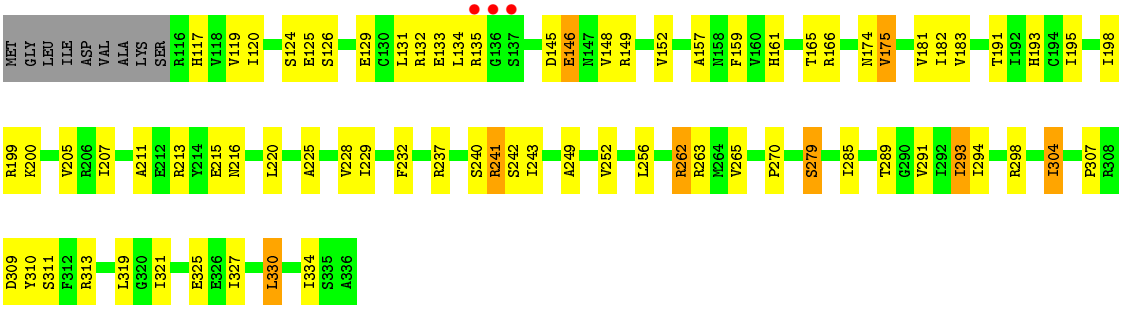
• Molecule 1: Calcium-gated potassium channel MthK

Chain g:



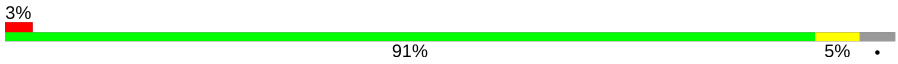
• Molecule 1: Calcium-gated potassium channel MthK

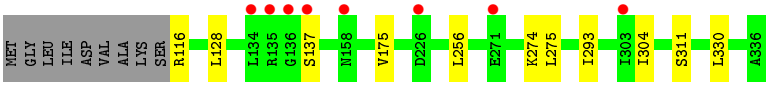
Chain H:



• Molecule 1: Calcium-gated potassium channel MthK

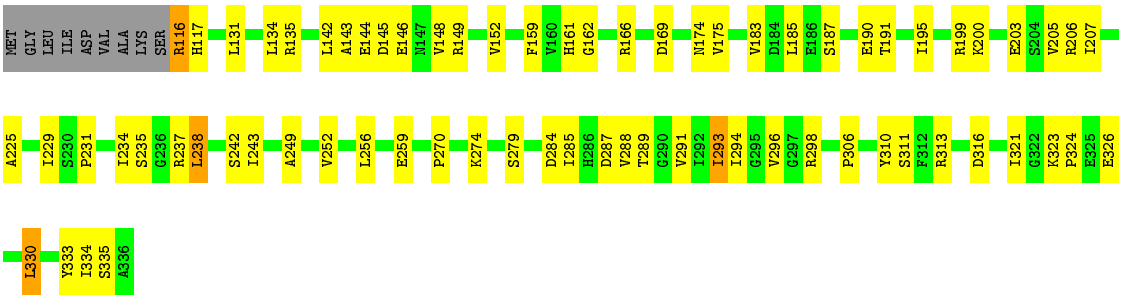
Chain h:





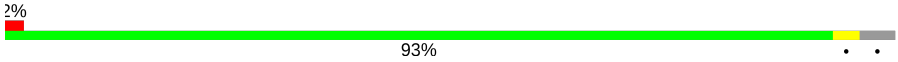
• Molecule 1: Calcium-gated potassium channel MthK

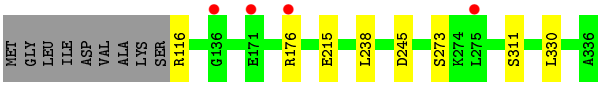
Chain I:



• Molecule 1: Calcium-gated potassium channel MthK

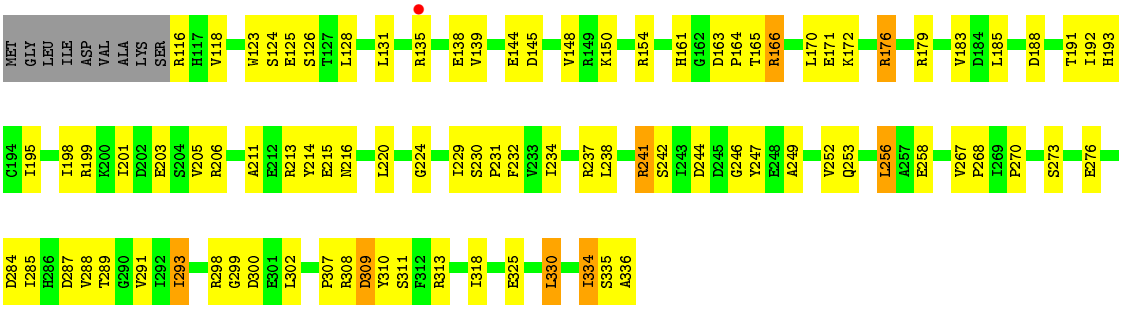
Chain i:





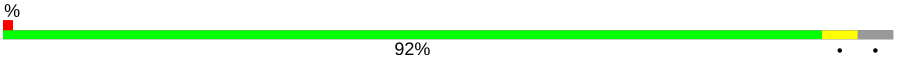
• Molecule 1: Calcium-gated potassium channel MthK

Chain J:



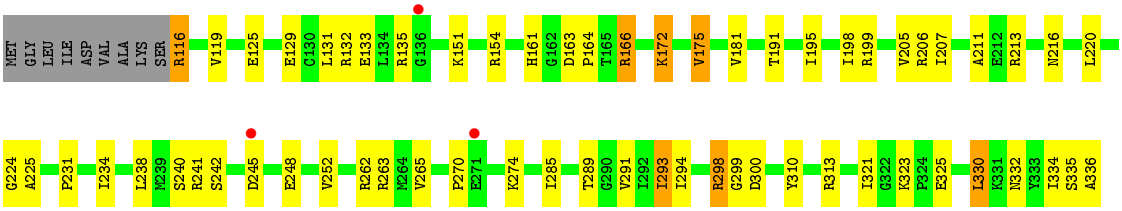
• Molecule 1: Calcium-gated potassium channel MthK

Chain j:



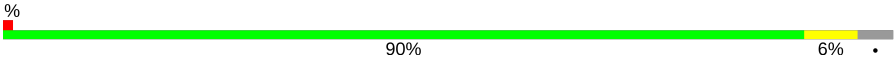
• Molecule 1: Calcium-gated potassium channel MthK

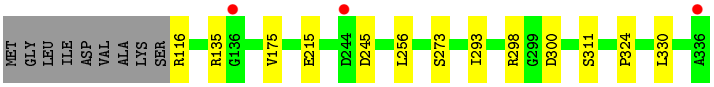
Chain K:



• Molecule 1: Calcium-gated potassium channel MthK

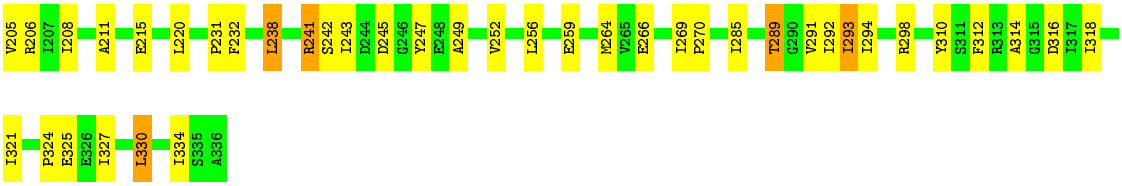
Chain k:





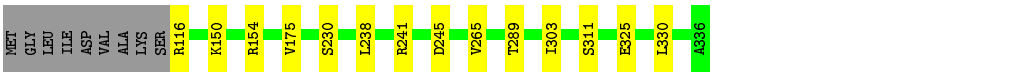
• Molecule 1: Calcium-gated potassium channel MthK

Chain L:



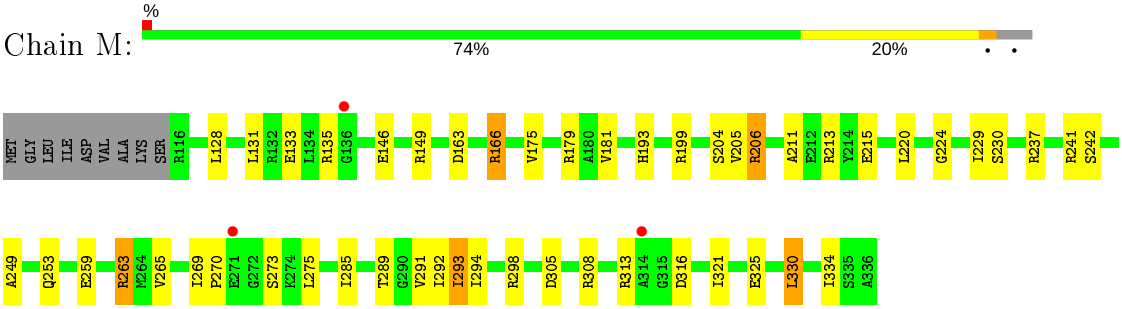
• Molecule 1: Calcium-gated potassium channel MthK

Chain l:



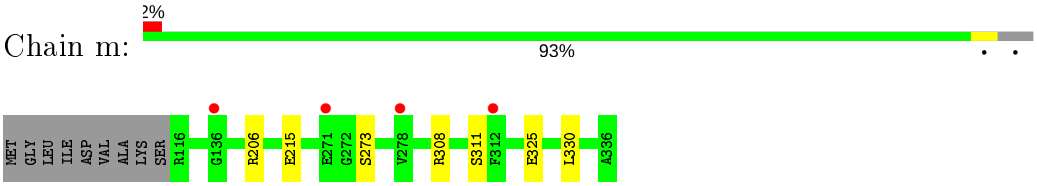
• Molecule 1: Calcium-gated potassium channel MthK

Chain M:



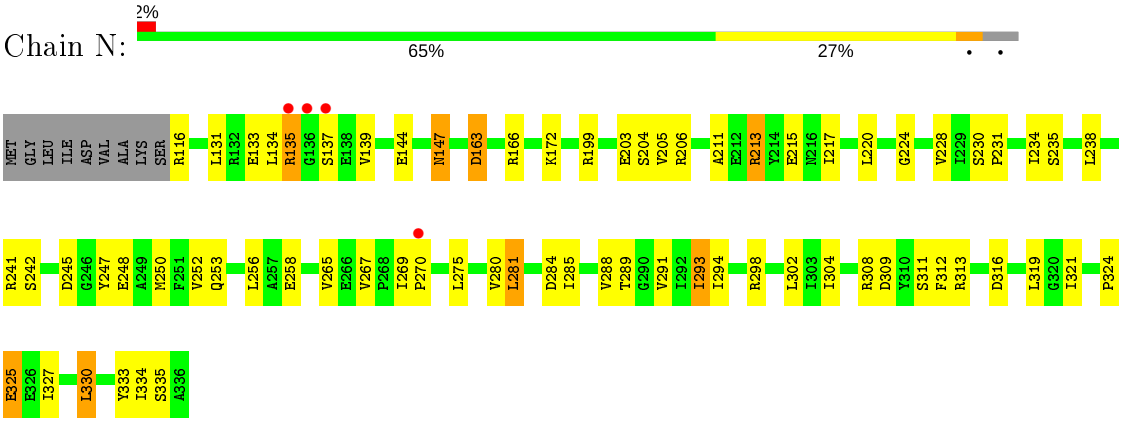
• Molecule 1: Calcium-gated potassium channel MthK

Chain m:



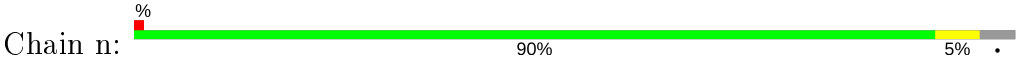
• Molecule 1: Calcium-gated potassium channel MthK

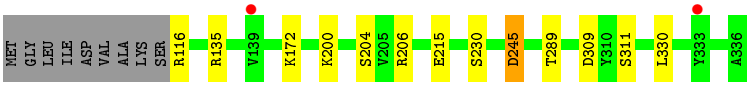
Chain N:



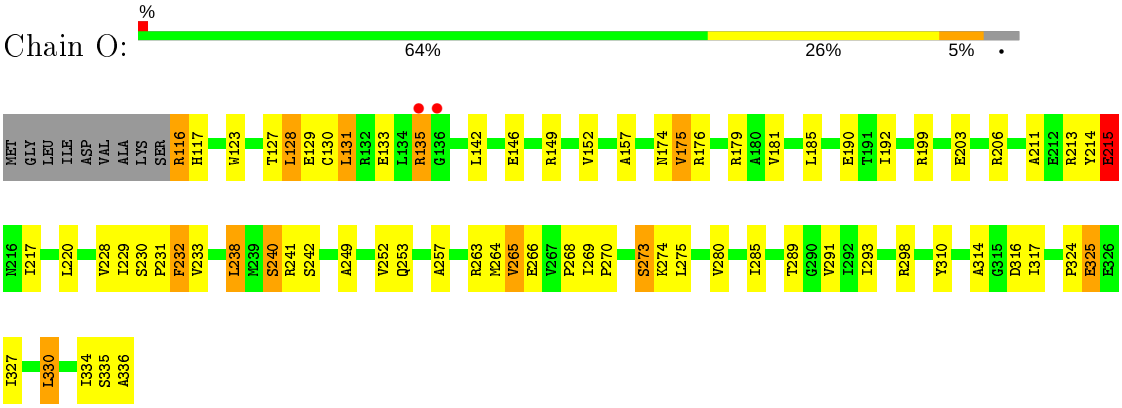
• Molecule 1: Calcium-gated potassium channel MthK

Chain n:

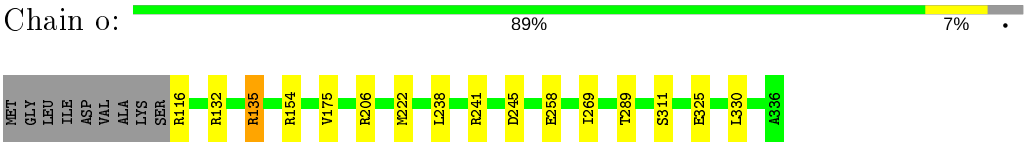




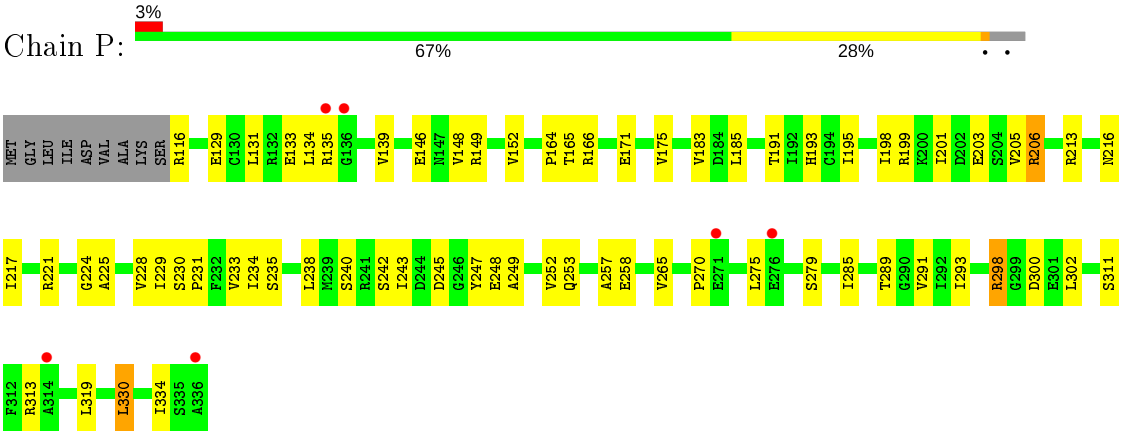
• Molecule 1: Calcium-gated potassium channel MthK



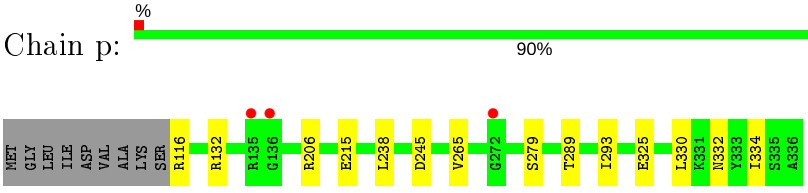
• Molecule 1: Calcium-gated potassium channel MthK



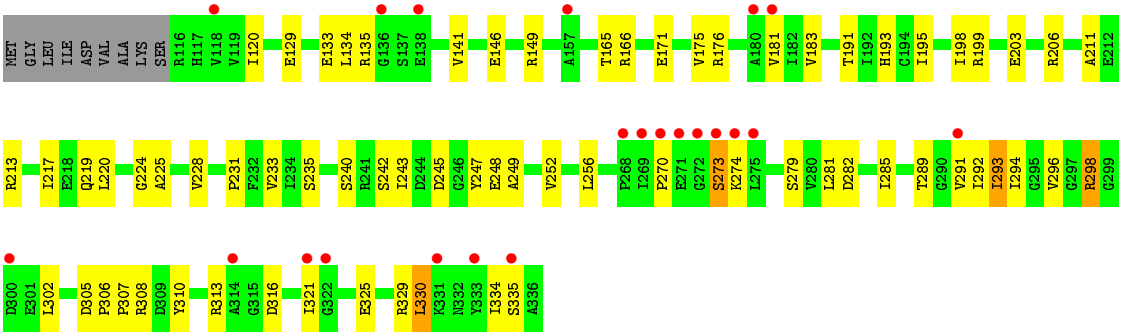
• Molecule 1: Calcium-gated potassium channel MthK



• Molecule 1: Calcium-gated potassium channel MthK

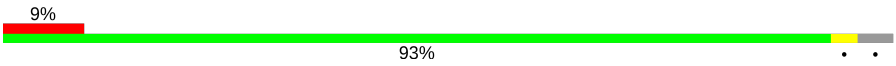


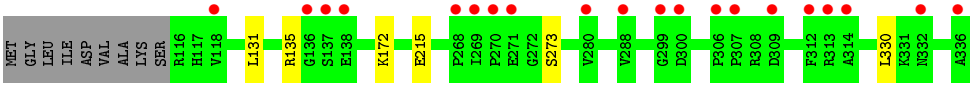
• Molecule 1: Calcium-gated potassium channel MthK



• Molecule 1: Calcium-gated potassium channel MthK

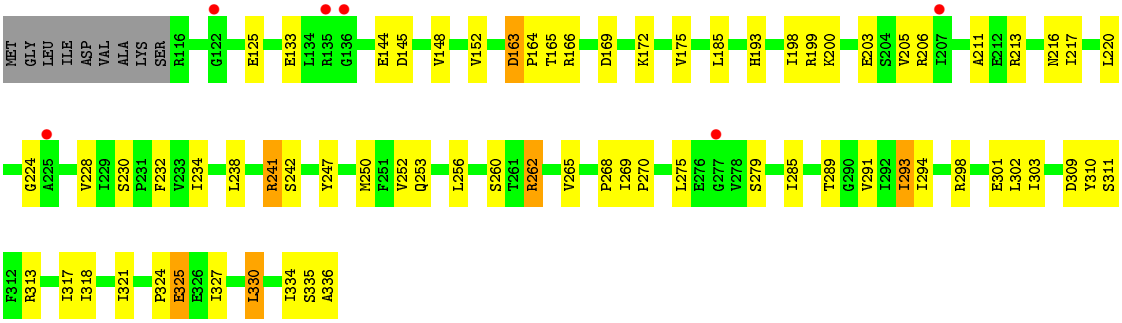
Chain q:





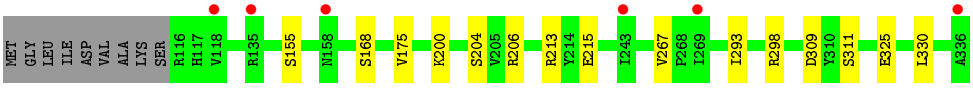
• Molecule 1: Calcium-gated potassium channel MthK

Chain R:



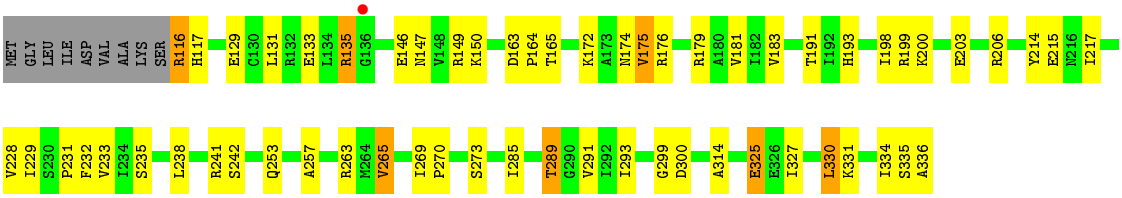
• Molecule 1: Calcium-gated potassium channel MthK

Chain r:



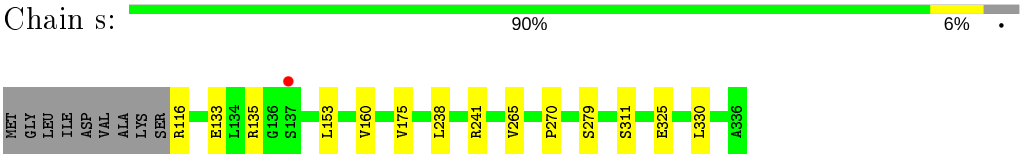
• Molecule 1: Calcium-gated potassium channel MthK

Chain S:



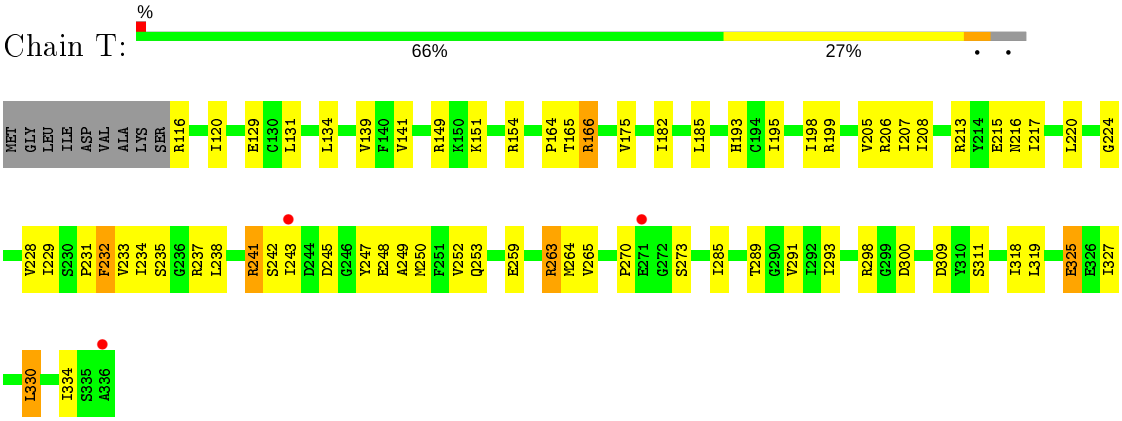
• Molecule 1: Calcium-gated potassium channel MthK

Chain s:



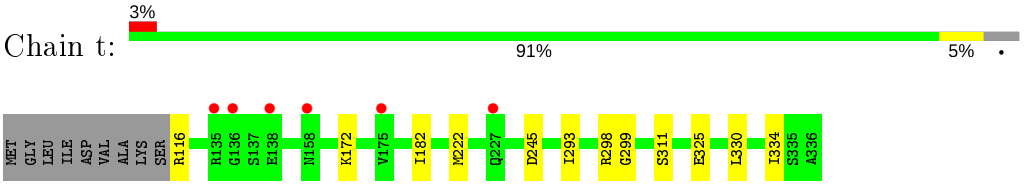
• Molecule 1: Calcium-gated potassium channel MthK

Chain T:



• Molecule 1: Calcium-gated potassium channel MthK

Chain t:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	166.34Å 231.68Å 197.98Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	49.26 – 3.18 49.21 – 3.18	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.26-3.18) 92.2 (49.21-3.18)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.263 , 0.301 0.263 , 0.301	Depositor DCC
R_{free} test set	2303 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	68748	wwPDB-VP
Average B, all atoms (Å^2)	79.0	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 54.89 % 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 3.4248e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/1740	0.61	0/2347
1	B	0.39	1/1740 (0.1%)	0.57	1/2347 (0.0%)
1	C	0.38	0/1740	0.60	0/2347
1	D	0.39	0/1740	0.60	0/2347
1	E	0.40	0/1740	0.61	0/2347
1	F	0.39	0/1740	0.59	0/2347
1	G	0.41	0/1740	0.60	1/2347 (0.0%)
1	H	0.39	0/1740	0.59	0/2347
1	I	0.35	0/1740	0.57	0/2347
1	J	0.38	0/1740	0.61	0/2347
1	K	0.37	0/1740	0.59	0/2347
1	L	0.43	0/1740	0.61	1/2347 (0.0%)
1	M	0.36	0/1740	0.56	0/2347
1	N	0.38	0/1734	0.59	0/2340
1	O	0.43	0/1740	0.63	1/2347 (0.0%)
1	P	0.35	0/1740	0.58	0/2347
1	Q	0.36	1/1740 (0.1%)	0.55	0/2347
1	R	0.38	0/1740	0.59	0/2347
1	S	0.37	0/1740	0.57	0/2347
1	T	0.37	0/1740	0.59	0/2347
1	a	0.40	0/1740	0.62	0/2347
1	b	0.36	0/1740	0.56	0/2347
1	c	0.39	0/1740	0.60	1/2347 (0.0%)
1	d	0.41	0/1740	0.64	0/2347
1	e	0.39	0/1740	0.60	0/2347
1	f	0.41	0/1740	0.61	0/2347
1	g	0.46	0/1740	0.64	1/2347 (0.0%)
1	h	0.37	0/1740	0.57	0/2347
1	i	0.39	0/1740	0.60	0/2347
1	j	0.40	0/1740	0.57	1/2347 (0.0%)
1	k	0.40	0/1740	0.63	0/2347
1	l	0.39	0/1740	0.60	0/2347
1	m	0.37	0/1740	0.57	0/2347
1	n	0.38	0/1740	0.63	1/2347 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	o	0.41	0/1740	0.61	0/2347
1	p	0.36	0/1740	0.57	0/2347
1	q	0.35	0/1740	0.54	0/2347
1	r	0.36	0/1734	0.58	0/2340
1	s	0.38	0/1740	0.59	0/2347
1	t	0.35	0/1740	0.56	0/2347
All	All	0.39	2/69588 (0.0%)	0.59	8/93866 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	GLU	CD-OE1	-5.19	1.20	1.25
1	Q	171	GLU	CD-OE1	-5.08	1.20	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	266	GLU	OE1-CD-OE2	-5.75	116.41	123.30
1	n	245	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	266	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	j	276	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	g	328	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	c	210	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	L	138	GLU	OE1-CD-OE2	-5.14	117.14	123.30
1	G	144	GLU	OE1-CD-OE2	-5.10	117.18	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1719	0	1726	81	0
1	B	1719	0	1726	46	0
1	C	1719	0	1726	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1719	0	1726	64	0
1	E	1719	0	1726	73	0
1	F	1719	0	1726	54	0
1	G	1719	0	1726	56	0
1	H	1719	0	1726	69	0
1	I	1719	0	1726	47	0
1	J	1719	0	1726	75	0
1	K	1719	0	1726	48	0
1	L	1719	0	1726	56	0
1	M	1719	0	1726	45	0
1	N	1713	0	1715	64	0
1	O	1719	0	1726	65	0
1	P	1719	0	1726	50	0
1	Q	1719	0	1726	52	0
1	R	1719	0	1726	59	0
1	S	1719	0	1726	53	0
1	T	1719	0	1726	47	0
1	a	1719	0	1726	0	0
1	b	1719	0	1726	0	0
1	c	1719	0	1726	0	0
1	d	1719	0	1726	0	0
1	e	1719	0	1726	0	0
1	f	1719	0	1726	0	0
1	g	1719	0	1726	0	0
1	h	1719	0	1726	0	0
1	i	1719	0	1726	0	0
1	j	1719	0	1726	0	0
1	k	1719	0	1726	0	0
1	l	1719	0	1726	0	0
1	m	1719	0	1726	0	0
1	n	1719	0	1726	0	0
1	o	1719	0	1726	0	0
1	p	1719	0	1726	0	0
1	q	1719	0	1726	0	0
1	r	1713	0	1715	0	0
1	s	1719	0	1726	0	0
1	t	1719	0	1726	0	0
All	All	68748	0	69018	1117	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 8.

All (1117) 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:I:324:PRO:HB2	1:S:325:GLU:HG2	36.68	1.12
1:M:298:ARG:HH22	1:M:313:ARG:HB2	1.94	1.12
1:A:116:ARG:HG2	1:A:116:ARG:HH21	2.96	1.08
1:O:116:ARG:HG3	1:O:116:ARG:HH21	1.51	1.07
1:J:298:ARG:HH22	1:J:313:ARG:HB2	1.15	1.06
1:C:132:ARG:HH11	1:C:132:ARG:HG3	1.16	1.06
1:D:116:ARG:HH21	1:D:116:ARG:HG3	1.20	1.05
1:C:298:ARG:NH1	1:C:313:ARG:NH1	2.04	1.05
1:M:308:ARG:HG2	1:M:308:ARG:HH11	3.26	1.04
1:A:298:ARG:NH2	1:A:313:ARG:HB2	3.35	1.04
1:D:325:GLU:HG2	1:R:324:PRO:HB2	38.63	1.03
1:S:116:ARG:HH21	1:S:116:ARG:HG3	3.27	1.03
1:A:298:ARG:HH22	1:A:313:ARG:HB2	2.65	1.01
1:I:324:PRO:HB2	1:S:325:GLU:CG	37.43	1.01
1:D:325:GLU:CG	1:N:324:PRO:HB2	1.91	1.00
1:D:325:GLU:HG2	1:N:324:PRO:HB2	1.01	1.00
1:A:132:ARG:HH11	1:A:132:ARG:HG3	3.60	0.99
1:C:324:PRO:HB3	1:S:325:GLU:HG2	38.96	0.99
1:I:298:ARG:HH22	1:I:313:ARG:HB2	2.64	0.99
1:J:176:ARG:HG3	1:J:176:ARG:HH21	1.28	0.98
1:D:325:GLU:CG	1:R:324:PRO:HB2	37.78	0.98
1:L:324:PRO:HB2	1:T:325:GLU:HG2	39.17	0.98
1:D:325:GLU:HG2	1:N:324:PRO:CB	1.93	0.97
1:A:298:ARG:HH22	1:A:313:ARG:CB	3.24	0.96
1:A:298:ARG:HH12	1:A:313:ARG:HD2	1.29	0.95
1:A:324:PRO:CB	1:O:325:GLU:HG2	73.61	0.94
1:J:188:ASP:HB3	1:J:216:ASN:HD22	1.33	0.93
1:A:324:PRO:HB3	1:O:325:GLU:HG2	73.53	0.92
1:O:298:ARG:NH2	1:O:316:ASP:OD2	2.01	0.92
1:D:298:ARG:HH12	1:D:313:ARG:NE	3.66	0.91
1:F:298:ARG:NH2	1:F:310:TYR:OH	2.39	0.91
1:D:324:PRO:HB2	1:R:325:GLU:HG2	36.84	0.91
1:O:133:GLU:OE1	1:O:241:ARG:NH1	27.17	0.90
1:E:298:ARG:CZ	1:E:313:ARG:HD2	2.01	0.90
1:L:285:ILE:HB	1:L:293:ILE:HD11	2.06	0.89
1:S:285:ILE:HB	1:S:293:ILE:HD11	1.55	0.89
1:C:298:ARG:HH22	1:C:313:ARG:HB2	3.59	0.88
1:I:206:ARG:NH1	1:I:242:SER:O	31.72	0.88
1:D:325:GLU:HG2	1:R:324:PRO:CB	39.51	0.88
1:H:285:ILE:O	1:H:289:THR:HG22	1.74	0.87
1:D:298:ARG:HH12	1:D:313:ARG:CZ	4.05	0.86
1:C:298:ARG:HH12	1:C:313:ARG:CZ	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:262:ARG:HH11	1:R:262:ARG:HG3	1.41	0.86
1:N:285:ILE:HB	1:N:293:ILE:HD11	2.14	0.85
1:Q:206:ARG:NH1	1:Q:242:SER:O	32.33	0.85
1:B:285:ILE:O	1:B:289:THR:HG22	1.81	0.85
1:S:285:ILE:O	1:S:289:THR:HG22	1.97	0.85
1:P:298:ARG:HH22	1:P:313:ARG:HG3	1.41	0.85
1:C:298:ARG:HH12	1:C:313:ARG:NH1	1.74	0.85
1:J:285:ILE:O	1:J:289:THR:HG22	1.77	0.84
1:D:285:ILE:O	1:D:289:THR:HG22	1.85	0.83
1:F:285:ILE:O	1:F:289:THR:HG22	1.78	0.83
1:A:285:ILE:O	1:A:289:THR:HG22	1.79	0.82
1:K:116:ARG:HB2	1:K:116:ARG:HH21	3.61	0.82
1:H:125:GLU:HB3	1:H:232:PHE:HD1	11.86	0.81
1:R:133:GLU:OE1	1:R:241:ARG:NH1	27.67	0.81
1:E:298:ARG:NH1	1:E:313:ARG:HD2	1.95	0.80
1:F:206:ARG:NH1	1:F:242:SER:O	32.63	0.80
1:L:131:LEU:HD21	1:L:139:VAL:HG11	1.63	0.80
1:J:188:ASP:HB3	1:J:216:ASN:ND2	1.97	0.80
1:A:116:ARG:HH21	1:A:116:ARG:HG3	1.46	0.80
1:Q:213:ARG:HG2	1:T:166:ARG:NH2	46.84	0.80
1:D:324:PRO:HB2	1:R:325:GLU:CG	37.50	0.79
1:C:248:GLU:HG3	1:C:264:MET:HG2	13.61	0.79
1:D:285:ILE:HB	1:D:293:ILE:HD11	1.90	0.78
1:R:217:ILE:HG23	1:R:228:VAL:HG11	1.65	0.78
1:M:206:ARG:NH1	1:M:242:SER:O	31.74	0.78
1:D:116:ARG:HG3	1:D:116:ARG:NH2	1.93	0.78
1:E:116:ARG:NH2	1:E:179:ARG:HD2	1.98	0.78
1:E:119:VAL:HB	1:E:181:VAL:HG13	1.67	0.77
1:B:298:ARG:NH1	1:B:313:ARG:NH1	3.24	0.77
1:M:308:ARG:CG	1:M:308:ARG:HH11	3.36	0.77
1:O:275:LEU:HD12	1:O:334:ILE:HG23	1.67	0.77
1:C:132:ARG:HG3	1:C:132:ARG:NH1	1.96	0.77
1:J:237:ARG:NH1	1:J:241:ARG:HE	1.82	0.77
1:J:176:ARG:HH21	1:J:176:ARG:CG	1.96	0.76
1:N:281:LEU:HD12	1:N:308:ARG:HB3	1.66	0.76
1:P:116:ARG:HH21	1:P:116:ARG:HG3	2.70	0.76
1:J:298:ARG:NH2	1:J:313:ARG:HB2	1.98	0.76
1:S:206:ARG:NH1	1:S:242:SER:O	33.12	0.76
1:M:285:ILE:O	1:M:289:THR:HG22	1.86	0.76
1:D:324:PRO:HB2	1:N:325:GLU:HG2	1.67	0.76
1:Q:298:ARG:NH2	1:Q:313:ARG:HB2	3.05	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:PRO:CB	1:S:325:GLU:HG2	39.60	0.76
1:J:188:ASP:CB	1:J:216:ASN:HD22	1.98	0.75
1:P:298:ARG:HH12	1:P:313:ARG:CD	2.00	0.74
1:N:144:GLU:OE2	1:N:163:ASP:HB2	1.86	0.74
1:A:248:GLU:HG3	1:A:264:MET:HG2	13.96	0.74
1:N:269:ILE:HD12	1:N:316:ASP:HB2	1.88	0.74
1:T:285:ILE:O	1:T:289:THR:HG22	2.05	0.74
1:L:324:PRO:HB2	1:T:325:GLU:CG	38.45	0.74
1:G:270:PRO:HD2	1:G:334:ILE:HG22	1.70	0.73
1:E:328:GLU:HA	1:E:331:LYS:HD3	5.67	0.73
1:R:285:ILE:O	1:R:289:THR:HG22	1.98	0.73
1:O:146:GLU:OE1	1:O:149:ARG:NH1	2.22	0.73
1:A:116:ARG:CG	1:A:116:ARG:HH21	2.24	0.73
1:T:116:ARG:HH21	1:T:116:ARG:HG3	2.58	0.73
1:O:298:ARG:HH21	1:O:316:ASP:CG	1.92	0.72
1:P:298:ARG:HH12	1:P:313:ARG:HD2	1.52	0.72
1:S:133:GLU:OE1	1:S:241:ARG:NH1	28.34	0.72
1:A:324:PRO:HB2	1:O:325:GLU:CG	73.68	0.72
1:C:116:ARG:HG3	1:C:116:ARG:HH21	3.06	0.72
1:Q:134:LEU:HD11	1:Q:243:ILE:HD11	34.27	0.72
1:T:285:ILE:HB	1:T:293:ILE:HD11	1.71	0.72
1:C:285:ILE:O	1:C:289:THR:HG22	2.40	0.72
1:N:147:ASN:HD22	1:N:147:ASN:H	1.38	0.72
1:H:298:ARG:HH12	1:H:313:ARG:HB2	1.54	0.71
1:E:199:ARG:HE	1:E:203:GLU:HA	1.54	0.71
1:P:171:GLU:HG3	1:P:201:ILE:HD13	2.75	0.71
1:F:298:ARG:NH2	1:F:316:ASP:OD2	2.22	0.71
1:E:285:ILE:O	1:E:289:THR:HG22	2.37	0.71
1:M:285:ILE:HB	1:M:293:ILE:HD11	1.73	0.71
1:I:285:ILE:O	1:I:289:THR:HG22	2.01	0.71
1:M:298:ARG:NH2	1:M:313:ARG:HB2	2.19	0.71
1:O:298:ARG:HH11	1:O:298:ARG:HG3	4.49	0.71
1:T:237:ARG:HG2	1:T:241:ARG:HH12	1.53	0.71
1:G:323:LYS:HB2	1:G:326:GLU:HG3	2.40	0.71
1:N:289:THR:HG23	1:N:291:VAL:H	1.56	0.71
1:E:298:ARG:HH12	1:E:313:ARG:NH1	1.88	0.70
1:G:199:ARG:NH2	1:G:205:VAL:O	2.23	0.70
1:E:263:ARG:NH1	1:E:265:VAL:HG12	2.07	0.70
1:H:270:PRO:HD2	1:H:334:ILE:HG22	1.72	0.70
1:Q:199:ARG:NH1	1:Q:224:GLY:O	2.49	0.70
1:Q:289:THR:HG21	1:Q:330:LEU:HG	1.83	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:285:ILE:O	1:O:289:THR:HG22	1.91	0.70
1:O:116:ARG:NH2	1:O:116:ARG:HG3	2.12	0.69
1:L:206:ARG:NH1	1:L:242:SER:O	33.08	0.69
1:A:116:ARG:HG2	1:A:116:ARG:NH2	3.67	0.69
1:Q:298:ARG:NH2	1:Q:316:ASP:OD2	2.22	0.69
1:C:298:ARG:NH1	1:C:313:ARG:CZ	2.52	0.69
1:C:298:ARG:NH1	1:C:313:ARG:HH11	1.91	0.69
1:R:206:ARG:NH1	1:R:242:SER:O	31.84	0.69
1:G:229:ILE:HG12	1:G:238:LEU:HD23	15.19	0.68
1:Q:166:ARG:HH21	1:R:213:ARG:HE	45.51	0.68
1:K:216:ASN:O	1:K:220:LEU:HD12	3.23	0.68
1:S:150:LYS:HA	1:S:150:LYS:HE2	2.10	0.68
1:N:288:VAL:HG11	1:N:333:TYR:CE1	2.67	0.68
1:S:270:PRO:HD2	1:S:334:ILE:HG22	2.22	0.68
1:C:324:PRO:HB3	1:S:325:GLU:CG	38.22	0.68
1:A:298:ARG:NH1	1:A:313:ARG:HD2	2.05	0.68
1:T:199:ARG:NH2	1:T:205:VAL:O	2.26	0.68
1:C:298:ARG:NH2	1:C:316:ASP:OD2	3.43	0.68
1:H:289:THR:HG23	1:H:291:VAL:H	1.60	0.67
1:O:289:THR:HG23	1:O:291:VAL:H	1.69	0.67
1:S:116:ARG:NH2	1:S:116:ARG:HG3	3.52	0.67
1:R:289:THR:HG23	1:R:291:VAL:H	1.59	0.67
1:P:116:ARG:HG3	1:P:116:ARG:NH2	3.17	0.67
1:J:199:ARG:NH2	1:J:205:VAL:O	2.27	0.67
1:J:211:ALA:HB2	1:J:220:LEU:HD22	1.83	0.67
1:A:324:PRO:CB	1:O:325:GLU:CG	72.79	0.67
1:C:183:VAL:HG12	1:C:191:THR:HG23	1.77	0.66
1:D:206:ARG:NH1	1:D:242:SER:O	33.21	0.66
1:E:206:ARG:NH1	1:E:242:SER:O	32.49	0.66
1:L:270:PRO:HD2	1:L:334:ILE:HG22	1.77	0.66
1:B:206:ARG:NH1	1:B:242:SER:O	31.43	0.66
1:E:117:HIS:HE1	1:E:174:ASN:HB3	1.61	0.66
1:E:298:ARG:HH22	1:E:313:ARG:NE	3.33	0.66
1:L:298:ARG:NH2	1:L:316:ASP:OD2	2.29	0.66
1:T:120:ILE:HG12	1:T:182:ILE:HB	1.77	0.66
1:E:298:ARG:HH22	1:E:313:ARG:CD	2.70	0.66
1:E:298:ARG:HH22	1:E:313:ARG:HH11	1.43	0.66
1:D:289:THR:HG23	1:D:291:VAL:H	1.61	0.66
1:G:131:LEU:O	1:G:135:ARG:HB2	2.54	0.66
1:D:298:ARG:NH1	1:D:313:ARG:CZ	4.41	0.66
1:J:176:ARG:HG3	1:J:176:ARG:NH2	2.02	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ARG:CZ	1:C:316:ASP:OD1	3.48	0.65
1:L:330:LEU:HD22	1:L:334:ILE:HD11	2.10	0.65
1:A:125:GLU:HB3	1:A:232:PHE:HD1	11.36	0.65
1:B:165:THR:HB	1:B:193:HIS:ND1	2.11	0.65
1:L:289:THR:HG23	1:L:291:VAL:H	1.60	0.65
1:J:237:ARG:HH11	1:J:241:ARG:HE	1.43	0.65
1:A:131:LEU:O	1:A:135:ARG:HB2	2.67	0.65
1:O:213:ARG:HB3	1:O:215:GLU:HG3	1.78	0.65
1:S:289:THR:HG23	1:S:291:VAL:H	1.66	0.65
1:I:270:PRO:HD2	1:I:334:ILE:HG22	1.78	0.65
1:A:292:ILE:HD11	1:A:305:ASP:HB2	11.87	0.65
1:K:133:GLU:OE1	1:K:241:ARG:NH1	27.33	0.65
1:S:146:GLU:OE1	1:S:149:ARG:NH1	2.50	0.65
1:H:125:GLU:HB3	1:H:232:PHE:CD1	11.00	0.65
1:E:286:HIS:HE1	1:E:305:ASP:OD1	12.38	0.64
1:G:285:ILE:O	1:G:289:THR:HG22	1.97	0.64
1:I:116:ARG:HH21	1:I:116:ARG:HG3	2.53	0.64
1:Q:285:ILE:O	1:Q:289:THR:HG22	2.02	0.64
1:D:324:PRO:HB2	1:N:325:GLU:CG	2.27	0.64
1:M:298:ARG:HH22	1:M:313:ARG:CB	2.59	0.64
1:B:294:ILE:HD11	1:B:321:ILE:HG13	1.79	0.64
1:C:269:ILE:HD12	1:C:316:ASP:HB2	1.79	0.64
1:E:117:HIS:CE1	1:E:174:ASN:HB3	2.32	0.64
1:D:292:ILE:HD11	1:D:305:ASP:HB2	12.23	0.64
1:H:165:THR:HB	1:H:193:HIS:ND1	2.13	0.64
1:K:294:ILE:HD11	1:K:321:ILE:HD11	2.38	0.64
1:D:270:PRO:HD2	1:D:273:SER:HB2	1.86	0.64
1:K:131:LEU:O	1:K:135:ARG:HB2	1.98	0.64
1:N:270:PRO:HD3	1:N:334:ILE:HG23	5.36	0.64
1:P:199:ARG:NH1	1:P:224:GLY:O	2.41	0.64
1:N:199:ARG:NH1	1:N:224:GLY:O	2.31	0.64
1:F:298:ARG:NH2	1:F:310:TYR:CZ	2.93	0.64
1:H:262:ARG:HH11	1:H:262:ARG:CG	2.11	0.64
1:I:285:ILE:HB	1:I:293:ILE:HD11	2.05	0.64
1:R:289:THR:HG21	1:R:330:LEU:HG	1.80	0.64
1:A:298:ARG:CZ	1:A:316:ASP:OD1	3.36	0.64
1:K:234:ILE:O	1:K:238:LEU:HB2	2.58	0.63
1:I:324:PRO:CB	1:S:325:GLU:HG2	35.86	0.63
1:C:324:PRO:CB	1:S:325:GLU:CG	38.84	0.63
1:F:274:LYS:HD3	1:F:335:SER:O	2.77	0.63
1:L:294:ILE:HD11	1:L:321:ILE:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:206:ARG:NH1	1:O:242:SER:O	32.14	0.63
1:H:262:ARG:HH11	1:H:262:ARG:HG3	1.62	0.63
1:C:132:ARG:HH11	1:C:132:ARG:CG	2.02	0.63
1:F:330:LEU:HD22	1:F:334:ILE:HD11	2.09	0.63
1:K:285:ILE:O	1:K:289:THR:HG22	2.04	0.63
1:M:213:ARG:HG2	1:P:166:ARG:NH2	47.25	0.63
1:B:133:GLU:OE1	1:B:241:ARG:NH1	26.77	0.63
1:F:131:LEU:HD21	1:F:139:VAL:HG11	1.82	0.62
1:G:285:ILE:HD12	1:G:293:ILE:HD11	3.71	0.62
1:H:262:ARG:NH1	1:H:304:ILE:HB	19.81	0.62
1:P:285:ILE:O	1:P:289:THR:HG22	2.00	0.62
1:I:199:ARG:HE	1:I:203:GLU:HA	1.64	0.62
1:K:116:ARG:NH2	1:K:116:ARG:HB2	3.58	0.62
1:K:161:HIS:O	1:L:154:ARG:NH1	29.82	0.62
1:S:183:VAL:HG12	1:S:191:THR:HG23	1.80	0.62
1:L:298:ARG:NH2	1:L:310:TYR:OH	3.01	0.61
1:N:289:THR:HG21	1:N:330:LEU:HG	2.29	0.61
1:N:298:ARG:NH1	1:N:313:ARG:NH1	2.48	0.61
1:H:237:ARG:HH11	1:H:241:ARG:HH22	1.49	0.61
1:D:211:ALA:HB2	1:D:220:LEU:HD22	1.83	0.61
1:I:284:ASP:OD1	1:I:287:ASP:HB2	2.95	0.61
1:N:280:VAL:HG22	1:N:312:PHE:HE1	4.30	0.61
1:Q:294:ILE:HD11	1:Q:321:ILE:HD11	1.82	0.61
1:A:237:ARG:HH11	1:A:241:ARG:HD3	3.70	0.61
1:G:270:PRO:HD2	1:G:334:ILE:CG2	2.30	0.61
1:K:199:ARG:NH2	1:K:205:VAL:O	2.49	0.61
1:F:270:PRO:HD2	1:F:334:ILE:HG22	1.83	0.60
1:K:289:THR:HG23	1:K:291:VAL:H	1.66	0.60
1:P:289:THR:HG21	1:P:330:LEU:HG	1.82	0.60
1:J:330:LEU:HD22	1:J:334:ILE:HD11	3.09	0.60
1:M:308:ARG:NH1	1:M:308:ARG:HG2	3.52	0.60
1:T:289:THR:HG21	1:T:330:LEU:HG	1.82	0.60
1:C:298:ARG:NH2	1:C:316:ASP:OD1	4.00	0.60
1:Q:294:ILE:HD11	1:Q:321:ILE:HG13	2.53	0.60
1:J:289:THR:HG23	1:J:291:VAL:H	1.67	0.60
1:N:133:GLU:OE1	1:N:241:ARG:NH1	27.54	0.60
1:Q:298:ARG:NE	1:Q:316:ASP:OD1	2.37	0.60
1:C:131:LEU:O	1:C:135:ARG:HB2	2.02	0.60
1:N:294:ILE:HD11	1:N:321:ILE:HG13	2.72	0.60
1:C:270:PRO:HD3	1:C:334:ILE:HG21	1.82	0.60
1:O:116:ARG:HD2	1:O:179:ARG:HG2	3.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:199:ARG:NH1	1:T:224:GLY:O	2.35	0.60
1:A:298:ARG:CZ	1:A:313:ARG:HD2	2.77	0.60
1:P:206:ARG:NH1	1:P:242:SER:O	31.70	0.60
1:R:285:ILE:HG21	1:R:293:ILE:HD11	4.34	0.60
1:E:171:GLU:OE2	1:E:176:ARG:NH2	2.67	0.60
1:G:263:ARG:HH21	1:G:265:VAL:HG12	3.95	0.60
1:I:199:ARG:NH1	1:I:207:ILE:HD12	2.16	0.60
1:A:132:ARG:NH1	1:A:132:ARG:HG3	3.84	0.60
1:B:287:ASP:OD1	1:B:308:ARG:NH2	10.95	0.60
1:T:259:GLU:HG2	1:T:263:ARG:HB2	1.84	0.60
1:I:134:LEU:HD11	1:I:243:ILE:HD11	34.11	0.59
1:L:176:ARG:HD2	1:S:299:GLY:HA3	106.71	0.59
1:H:131:LEU:O	1:H:135:ARG:HB2	2.01	0.59
1:J:131:LEU:O	1:J:135:ARG:HB2	2.02	0.59
1:R:145:ASP:HB3	1:R:148:VAL:HG23	1.85	0.59
1:E:275:LEU:HD12	1:E:334:ILE:HG23	1.84	0.59
1:H:330:LEU:HD22	1:H:334:ILE:HD11	1.85	0.59
1:C:298:ARG:HH22	1:C:313:ARG:CB	3.78	0.59
1:H:134:LEU:HD11	1:H:243:ILE:HD11	33.74	0.59
1:P:270:PRO:HD2	1:P:334:ILE:HG22	1.84	0.59
1:E:199:ARG:NH2	1:E:205:VAL:O	2.71	0.59
1:R:335:SER:O	1:R:336:ALA:HB2	3.50	0.59
1:O:217:ILE:HG23	1:O:228:VAL:HG11	1.83	0.59
1:E:263:ARG:HH11	1:E:265:VAL:HG12	1.66	0.59
1:F:211:ALA:HB2	1:F:220:LEU:HD22	2.16	0.59
1:R:262:ARG:NH1	1:R:262:ARG:HG3	2.12	0.59
1:F:289:THR:HG23	1:F:291:VAL:H	1.71	0.59
1:F:195:ILE:HA	1:F:198:ILE:HD12	2.29	0.58
1:G:265:VAL:HG11	1:G:327:ILE:HG12	2.37	0.58
1:S:270:PRO:CD	1:S:334:ILE:HG22	2.96	0.58
1:B:211:ALA:HB2	1:B:220:LEU:HD22	2.04	0.58
1:J:307:PRO:HG2	1:J:310:TYR:HB2	2.06	0.58
1:N:206:ARG:NH1	1:N:242:SER:O	31.97	0.58
1:Q:219:GLN:HE21	1:R:200:LYS:HE2	40.59	0.58
1:F:335:SER:O	1:F:336:ALA:HB2	2.04	0.58
1:E:270:PRO:HD2	1:E:334:ILE:HG22	1.95	0.58
1:J:234:ILE:HG22	1:J:238:LEU:HD13	1.86	0.58
1:P:298:ARG:HH12	1:P:313:ARG:NE	2.00	0.58
1:N:199:ARG:NH2	1:N:205:VAL:O	2.61	0.58
1:G:134:LEU:O	1:G:137:SER:HB2	2.03	0.58
1:J:242:SER:OG	1:J:249:ALA:HB2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:298:ARG:HH22	1:Q:313:ARG:HD2	3.41	0.58
1:H:252:VAL:HA	1:H:256:LEU:HD23	1.85	0.58
1:I:143:ALA:HB3	1:I:159:PHE:HE1	2.45	0.58
1:I:298:ARG:HH12	1:I:313:ARG:HD2	1.69	0.58
1:P:298:ARG:HH12	1:P:313:ARG:CZ	2.35	0.58
1:S:335:SER:O	1:S:336:ALA:CB	2.51	0.58
1:L:146:GLU:OE1	1:L:149:ARG:NH1	2.41	0.57
1:E:298:ARG:NH2	1:E:313:ARG:HD2	2.19	0.57
1:H:294:ILE:HD11	1:H:321:ILE:CD1	2.33	0.57
1:L:285:ILE:O	1:L:289:THR:HG22	2.03	0.57
1:M:298:ARG:NH2	1:M:313:ARG:HD2	2.41	0.57
1:O:265:VAL:HG11	1:O:327:ILE:HG12	1.86	0.57
1:G:289:THR:HG21	1:G:330:LEU:HG	1.86	0.57
1:N:147:ASN:N	1:N:147:ASN:HD22	2.02	0.57
1:O:330:LEU:O	1:O:334:ILE:HG13	2.15	0.57
1:F:199:ARG:NH2	1:F:205:VAL:O	2.40	0.57
1:I:131:LEU:O	1:I:135:ARG:HB2	4.45	0.57
1:T:164:PRO:HG3	1:T:185:LEU:HD21	1.85	0.57
1:I:289:THR:HG23	1:I:291:VAL:H	1.78	0.57
1:M:270:PRO:HD2	1:M:334:ILE:HG22	1.86	0.57
1:R:279:SER:HA	1:R:310:TYR:O	2.34	0.57
1:S:270:PRO:HD3	1:S:334:ILE:HG21	2.70	0.57
1:A:253:GLN:O	1:A:257:ALA:HB3	2.21	0.57
1:F:229:ILE:O	1:F:231:PRO:HD3	2.52	0.57
1:I:166:ARG:HB3	1:I:169:ASP:HB2	1.85	0.57
1:J:237:ARG:HH11	1:J:241:ARG:NE	2.03	0.57
1:K:206:ARG:NH1	1:K:242:SER:O	31.16	0.57
1:O:335:SER:O	1:O:336:ALA:CB	2.52	0.57
1:F:171:GLU:OE2	1:F:176:ARG:NH2	2.89	0.57
1:H:211:ALA:HB2	1:H:220:LEU:HD22	1.86	0.57
1:E:298:ARG:NH2	1:E:313:ARG:HB2	2.19	0.57
1:N:302:LEU:HG	1:N:304:ILE:HG13	1.86	0.57
1:L:298:ARG:HH21	1:L:316:ASP:CG	2.08	0.56
1:E:164:PRO:HG2	1:E:185:LEU:HD21	1.85	0.56
1:T:120:ILE:HB	1:T:141:VAL:HG22	2.32	0.56
1:B:298:ARG:HH12	1:B:313:ARG:CZ	3.57	0.56
1:I:199:ARG:NH2	1:I:205:VAL:O	2.37	0.56
1:G:118:VAL:HG21	1:G:243:ILE:HD13	38.28	0.56
1:H:242:SER:OG	1:H:249:ALA:HB2	2.30	0.56
1:N:285:ILE:O	1:N:289:THR:HG22	2.05	0.56
1:S:285:ILE:HD12	1:S:293:ILE:HD11	2.56	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:203:GLU:HG2	1:S:300:ASP:OD2	106.19	0.56
1:T:237:ARG:HG2	1:T:241:ARG:NH1	2.20	0.56
1:N:270:PRO:HD3	1:N:334:ILE:CG2	4.54	0.56
1:P:289:THR:HG23	1:P:291:VAL:H	1.71	0.56
1:F:175:VAL:HG13	1:F:198:ILE:HG23	2.64	0.56
1:I:289:THR:HG21	1:I:330:LEU:HG	1.86	0.56
1:N:131:LEU:O	1:N:135:ARG:HB2	2.79	0.56
1:G:242:SER:OG	1:G:249:ALA:HB2	2.06	0.55
1:L:206:ARG:NH1	1:L:208:ILE:HD11	4.21	0.55
1:J:298:ARG:NH1	1:J:313:ARG:HD2	2.22	0.55
1:K:298:ARG:NH2	1:K:313:ARG:HG3	2.21	0.55
1:M:289:THR:HG21	1:M:330:LEU:HG	1.90	0.55
1:N:284:ASP:O	1:N:288:VAL:HG23	2.79	0.55
1:N:294:ILE:HD11	1:N:321:ILE:CD1	2.77	0.55
1:O:131:LEU:O	1:O:135:ARG:HB2	3.14	0.55
1:R:247:TYR:HB3	1:R:302:LEU:HD13	22.78	0.55
1:C:298:ARG:NH2	1:C:316:ASP:CG	4.13	0.55
1:M:330:LEU:HD22	1:M:334:ILE:HD11	1.98	0.55
1:C:298:ARG:HH11	1:C:313:ARG:NH1	1.95	0.55
1:F:232:PHE:H	1:F:232:PHE:HD2	1.53	0.55
1:Q:281:LEU:HD13	1:Q:308:ARG:HE	2.31	0.55
1:F:200:LYS:HE3	1:G:218:GLU:HG2	58.92	0.55
1:K:298:ARG:NH2	1:K:313:ARG:HB2	2.19	0.55
1:B:330:LEU:O	1:B:334:ILE:HG13	2.06	0.55
1:J:171:GLU:HG3	1:J:201:ILE:HD13	1.87	0.55
1:M:292:ILE:HD11	1:M:305:ASP:HB2	12.24	0.54
1:A:298:ARG:NH2	1:A:316:ASP:OD1	3.37	0.54
1:K:199:ARG:NH1	1:K:224:GLY:O	2.39	0.54
1:C:211:ALA:HB2	1:C:220:LEU:HD22	2.05	0.54
1:D:199:ARG:HE	1:D:203:GLU:HA	1.82	0.54
1:M:294:ILE:HD11	1:M:321:ILE:HD11	1.89	0.54
1:E:248:GLU:HG3	1:E:264:MET:HG2	14.11	0.54
1:J:318:ILE:HD12	1:J:334:ILE:HD11	1.88	0.54
1:M:146:GLU:OE1	1:M:149:ARG:NH1	2.47	0.54
1:O:175:VAL:HG22	1:O:181:VAL:HG21	2.73	0.54
1:O:192:ILE:HG13	1:O:220:LEU:HD12	2.65	0.54
1:O:330:LEU:HD22	1:O:334:ILE:HD11	1.89	0.54
1:E:289:THR:HG23	1:E:291:VAL:H	1.83	0.54
1:J:188:ASP:CB	1:J:216:ASN:ND2	2.64	0.54
1:O:116:ARG:HD2	1:O:179:ARG:HG3	1.88	0.54
1:F:335:SER:O	1:F:336:ALA:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:298:ARG:HH12	1:H:313:ARG:CB	2.21	0.54
1:J:237:ARG:O	1:J:241:ARG:HD3	2.07	0.54
1:K:211:ALA:HB2	1:K:220:LEU:HD22	1.88	0.54
1:L:199:ARG:HE	1:L:203:GLU:HA	1.73	0.54
1:Q:217:ILE:HG23	1:Q:228:VAL:HG11	2.11	0.54
1:Q:298:ARG:CZ	1:Q:310:TYR:OH	2.56	0.54
1:L:145:ASP:HB3	1:L:148:VAL:HG23	1.89	0.54
1:A:146:GLU:OE1	1:A:149:ARG:NH1	2.55	0.54
1:M:298:ARG:CZ	1:M:316:ASP:OD1	3.12	0.54
1:R:330:LEU:O	1:R:334:ILE:HG13	2.07	0.54
1:O:285:ILE:HG21	1:O:293:ILE:HD11	1.90	0.53
1:A:269:ILE:HD12	1:A:316:ASP:HB2	1.95	0.53
1:C:171:GLU:HG3	1:C:201:ILE:HD13	3.15	0.53
1:A:217:ILE:HG23	1:A:228:VAL:HG11	1.91	0.53
1:B:298:ARG:HH12	1:B:313:ARG:HD2	1.73	0.53
1:E:263:ARG:HG3	1:E:264:MET:N	2.24	0.53
1:E:213:ARG:HG2	1:H:166:ARG:NH2	46.57	0.53
1:J:166:ARG:HH22	1:K:213:ARG:HG2	46.51	0.53
1:A:324:PRO:HB2	1:O:325:GLU:HG3	73.95	0.53
1:S:270:PRO:CD	1:S:334:ILE:CG2	3.50	0.53
1:B:268:PRO:O	1:B:270:PRO:HD3	2.07	0.53
1:H:240:SER:HA	1:H:243:ILE:HD12	2.82	0.53
1:J:242:SER:HA	1:J:246:GLY:HA3	2.16	0.53
1:A:116:ARG:NH2	1:A:116:ARG:HG3	2.21	0.53
1:D:247:TYR:H	1:D:266:GLU:CD	25.43	0.53
1:E:237:ARG:HH11	1:E:241:ARG:NH2	3.16	0.53
1:P:247:TYR:HB3	1:P:302:LEU:HD13	22.77	0.53
1:D:294:ILE:HD11	1:D:321:ILE:HD11	1.90	0.53
1:J:284:ASP:OD1	1:J:287:ASP:HB2	2.09	0.53
1:M:289:THR:HG23	1:M:291:VAL:H	1.74	0.53
1:F:118:VAL:HB	1:F:139:VAL:HG22	1.90	0.53
1:N:211:ALA:HB2	1:N:220:LEU:HD22	1.90	0.53
1:P:270:PRO:HD2	1:P:334:ILE:CG2	2.37	0.53
1:F:237:ARG:O	1:F:241:ARG:HB2	2.09	0.53
1:G:270:PRO:O	1:G:273:SER:HB2	2.09	0.53
1:L:166:ARG:HB3	1:L:169:ASP:HB2	1.91	0.53
1:A:171:GLU:HG3	1:A:201:ILE:HD13	1.91	0.53
1:F:285:ILE:HD12	1:F:293:ILE:HD11	3.65	0.53
1:J:229:ILE:HG12	1:J:238:LEU:HD23	14.57	0.53
1:J:154:ARG:HE	1:K:172:LYS:NZ	2.06	0.53
1:T:165:THR:HB	1:T:193:HIS:ND1	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ARG:HD2	1:A:241:ARG:NH1	3.11	0.53
1:A:298:ARG:NH1	1:A:313:ARG:HH11	2.06	0.53
1:A:298:ARG:NH2	1:A:313:ARG:HD2	2.79	0.53
1:G:206:ARG:NH1	1:G:242:SER:O	31.95	0.53
1:I:279:SER:HA	1:I:310:TYR:O	2.36	0.53
1:N:298:ARG:HH22	1:N:313:ARG:HB2	1.72	0.53
1:R:298:ARG:HH22	1:R:313:ARG:HB2	1.74	0.53
1:E:131:LEU:HD21	1:E:139:VAL:HG11	1.91	0.52
1:F:166:ARG:HB3	1:F:169:ASP:HB2	2.01	0.52
1:N:247:TYR:HA	1:N:250:MET:HG2	4.40	0.52
1:E:253:GLN:O	1:E:257:ALA:HB3	2.44	0.52
1:L:133:GLU:OE1	1:L:241:ARG:NH1	28.22	0.52
1:O:152:VAL:HG13	1:O:157:ALA:HB3	2.42	0.52
1:R:309:ASP:N	1:R:309:ASP:OD1	2.61	0.52
1:O:335:SER:O	1:O:336:ALA:HB2	2.34	0.52
1:P:131:LEU:O	1:P:135:ARG:HB2	2.09	0.52
1:F:232:PHE:N	1:F:232:PHE:CD2	2.77	0.52
1:Q:298:ARG:HE	1:Q:316:ASP:CG	2.12	0.52
1:D:146:GLU:OE1	1:D:149:ARG:NH1	2.42	0.52
1:G:146:GLU:O	1:G:149:ARG:HB3	2.97	0.52
1:H:307:PRO:HG2	1:H:310:TYR:HB2	1.91	0.52
1:O:117:HIS:CE1	1:O:174:ASN:HB3	3.46	0.52
1:O:229:ILE:HG22	1:O:231:PRO:HD3	1.92	0.52
1:Q:289:THR:HG23	1:Q:291:VAL:H	1.74	0.52
1:B:298:ARG:HH12	1:B:313:ARG:NH1	3.21	0.52
1:E:211:ALA:HB2	1:E:220:LEU:HD22	1.90	0.52
1:H:237:ARG:NH1	1:H:241:ARG:HH12	2.07	0.52
1:J:199:ARG:NH1	1:J:224:GLY:O	2.48	0.52
1:A:133:GLU:OE1	1:A:241:ARG:NH1	26.86	0.52
1:B:292:ILE:HD11	1:B:305:ASP:HB2	11.73	0.52
1:A:211:ALA:HB2	1:A:220:LEU:HD22	1.92	0.52
1:Q:248:GLU:O	1:Q:252:VAL:HG23	2.10	0.52
1:D:183:VAL:HG12	1:D:191:THR:HG23	1.91	0.52
1:K:270:PRO:HD3	1:K:334:ILE:HG21	1.92	0.52
1:P:298:ARG:NH1	1:P:313:ARG:HD2	2.22	0.52
1:D:298:ARG:HG3	1:D:316:ASP:OD1	5.37	0.51
1:G:263:ARG:NH2	1:G:327:ILE:HD13	2.25	0.51
1:H:199:ARG:NH1	1:H:207:ILE:HD12	2.25	0.51
1:J:285:ILE:HB	1:J:293:ILE:HD11	1.91	0.51
1:L:231:PRO:HG2	1:L:232:PHE:CD2	2.45	0.51
1:B:116:ARG:HB3	1:B:179:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:THR:HG23	1:C:291:VAL:H	1.79	0.51
1:D:300:ASP:OD2	1:O:203:GLU:HG2	46.11	0.51
1:G:285:ILE:HD12	1:G:293:ILE:CD1	3.51	0.51
1:I:146:GLU:OE1	1:I:149:ARG:NH1	2.43	0.51
1:K:298:ARG:HH22	1:K:313:ARG:HG3	1.75	0.51
1:P:131:LEU:HD21	1:P:139:VAL:HG11	1.92	0.51
1:R:294:ILE:HD11	1:R:321:ILE:HD11	2.48	0.51
1:T:175:VAL:HG11	1:T:198:ILE:HG23	1.92	0.51
1:C:298:ARG:HH12	1:C:313:ARG:CD	2.22	0.51
1:G:263:ARG:NH2	1:G:265:VAL:HG12	3.29	0.51
1:Q:274:LYS:HD3	1:Q:335:SER:O	2.10	0.51
1:E:330:LEU:O	1:E:334:ILE:HG13	2.11	0.51
1:G:289:THR:HG23	1:G:291:VAL:H	1.76	0.51
1:K:133:GLU:HG3	1:K:240:SER:OG	28.01	0.51
1:K:195:ILE:HA	1:K:198:ILE:HD12	1.92	0.51
1:E:131:LEU:O	1:E:135:ARG:HB2	2.11	0.51
1:I:183:VAL:HG12	1:I:191:THR:HG23	2.28	0.51
1:S:265:VAL:HG21	1:S:327:ILE:HG12	1.92	0.51
1:H:199:ARG:NH2	1:H:205:VAL:O	2.48	0.51
1:L:171:GLU:OE2	1:L:176:ARG:NH2	2.43	0.51
1:R:125:GLU:HB3	1:R:232:PHE:HD1	11.85	0.51
1:B:242:SER:OG	1:B:249:ALA:HB2	2.14	0.51
1:C:171:GLU:OE2	1:C:176:ARG:NH2	3.14	0.51
1:J:145:ASP:HB3	1:J:148:VAL:HG23	2.45	0.51
1:M:298:ARG:HH21	1:M:316:ASP:CG	2.13	0.51
1:O:232:PHE:N	1:O:232:PHE:CD2	2.79	0.51
1:Q:146:GLU:OE1	1:Q:149:ARG:NH1	2.47	0.51
1:A:131:LEU:CD1	1:A:155:SER:HB3	3.30	0.51
1:L:270:PRO:HD2	1:L:334:ILE:CG2	2.47	0.51
1:F:242:SER:OG	1:F:249:ALA:HB2	2.11	0.51
1:S:270:PRO:HD3	1:S:334:ILE:CG2	3.11	0.51
1:A:221:ARG:NH2	1:A:258:GLU:OE2	26.03	0.50
1:E:206:ARG:HG2	1:E:206:ARG:HH11	1.75	0.50
1:I:231:PRO:HB3	1:I:235:SER:HB2	5.58	0.50
1:A:270:PRO:HD2	1:A:334:ILE:HG22	1.93	0.50
1:B:131:LEU:O	1:B:135:ARG:HB2	2.12	0.50
1:B:199:ARG:HE	1:B:203:GLU:HA	1.87	0.50
1:D:119:VAL:HB	1:D:181:VAL:HG22	2.00	0.50
1:H:195:ILE:HA	1:H:198:ILE:HD12	2.60	0.50
1:L:292:ILE:HD12	1:L:321:ILE:HB	1.93	0.50
1:J:230:SER:H	1:J:253:GLN:HE22	13.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:298:ARG:NH2	1:K:313:ARG:CG	2.74	0.50
1:M:211:ALA:HB2	1:M:220:LEU:HD22	1.93	0.50
1:R:268:PRO:HA	1:R:317:ILE:HD13	1.93	0.50
1:C:119:VAL:HB	1:C:181:VAL:HG22	2.09	0.50
1:C:298:ARG:HH12	1:C:313:ARG:NE	2.07	0.50
1:D:125:GLU:HB3	1:D:232:PHE:HD1	11.47	0.50
1:H:146:GLU:OE1	1:H:149:ARG:NH1	3.09	0.50
1:J:116:ARG:HB2	1:J:179:ARG:HG3	1.93	0.50
1:P:242:SER:OG	1:P:249:ALA:HB2	2.11	0.50
1:T:175:VAL:CG1	1:T:198:ILE:HG23	2.41	0.50
1:E:199:ARG:NH1	1:E:224:GLY:O	2.44	0.50
1:H:265:VAL:HG11	1:H:327:ILE:CG2	2.83	0.50
1:L:232:PHE:H	1:L:232:PHE:HD2	1.60	0.50
1:L:238:LEU:HD21	1:L:252:VAL:HG21	2.07	0.50
1:A:275:LEU:HD12	1:A:334:ILE:HG13	3.64	0.50
1:M:308:ARG:NH1	1:M:308:ARG:CG	3.74	0.50
1:S:199:ARG:HE	1:S:203:GLU:HA	1.77	0.50
1:A:213:ARG:NE	1:B:166:ARG:HH12	23.65	0.50
1:B:199:ARG:NH1	1:B:224:GLY:O	2.45	0.50
1:M:131:LEU:O	1:M:135:ARG:HB2	2.12	0.50
1:A:265:VAL:HG11	1:A:327:ILE:CG2	2.42	0.49
1:A:269:ILE:HG22	1:A:314:ALA:HA	1.94	0.49
1:D:242:SER:OG	1:D:249:ALA:HB2	2.11	0.49
1:G:234:ILE:O	1:G:238:LEU:HB2	2.12	0.49
1:N:230:SER:H	1:N:253:GLN:HE22	13.41	0.49
1:H:175:VAL:HG22	1:H:181:VAL:HG21	1.93	0.49
1:D:229:ILE:HG22	1:D:231:PRO:HD3	2.20	0.49
1:E:171:GLU:HG3	1:E:201:ILE:HD13	2.46	0.49
1:F:213:ARG:HG2	1:G:166:ARG:HH22	23.21	0.49
1:F:269:ILE:HG22	1:F:314:ALA:HA	2.16	0.49
1:J:231:PRO:HG2	1:J:232:PHE:CD2	2.47	0.49
1:P:229:ILE:HG22	1:P:231:PRO:HD3	1.94	0.49
1:F:175:VAL:CG1	1:F:198:ILE:HG23	3.06	0.49
1:K:125:GLU:CD	1:L:166:ARG:HH22	2.15	0.49
1:K:289:THR:HG21	1:K:330:LEU:HG	2.18	0.49
1:L:206:ARG:HH11	1:L:208:ILE:HD11	4.17	0.49
1:T:242:SER:OG	1:T:249:ALA:HB2	2.12	0.49
1:A:131:LEU:HD12	1:A:155:SER:HB3	3.49	0.49
1:D:294:ILE:HD11	1:D:321:ILE:HG13	2.39	0.49
1:E:116:ARG:HH21	1:E:179:ARG:HD2	1.76	0.49
1:F:195:ILE:HD13	1:F:225:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:142:LEU:HD11	1:I:162:GLY:HA3	2.78	0.49
1:J:123:TRP:HZ2	1:J:128:LEU:HD12	2.16	0.49
1:G:183:VAL:HG12	1:G:191:THR:HG23	2.30	0.49
1:N:252:VAL:HA	1:N:256:LEU:HD23	5.84	0.49
1:O:129:GLU:HG3	1:O:233:VAL:HA	17.10	0.49
1:S:217:ILE:HG23	1:S:228:VAL:HG11	1.94	0.49
1:A:284:ASP:OD2	1:A:287:ASP:HB2	2.13	0.49
1:O:253:GLN:O	1:O:257:ALA:HB3	2.12	0.49
1:J:298:ARG:CZ	1:J:313:ARG:HD2	2.42	0.49
1:L:144:GLU:O	1:L:161:HIS:NE2	3.12	0.49
1:O:270:PRO:HD2	1:O:273:SER:HB2	1.95	0.49
1:O:285:ILE:HG13	1:O:293:ILE:HD11	4.09	0.49
1:R:301:GLU:OE1	1:R:301:GLU:HA	4.27	0.49
1:T:217:ILE:HG23	1:T:228:VAL:HG11	1.95	0.49
1:C:199:ARG:NH1	1:C:224:GLY:O	2.46	0.49
1:D:330:LEU:O	1:D:334:ILE:HG13	2.13	0.49
1:J:298:ARG:HH12	1:J:313:ARG:HD2	1.89	0.49
1:R:247:TYR:HA	1:R:250:MET:HG2	2.12	0.49
1:A:216:ASN:O	1:A:220:LEU:HD13	2.13	0.49
1:E:117:HIS:H	1:E:117:HIS:CD2	2.31	0.49
1:J:165:THR:HB	1:J:193:HIS:ND1	2.49	0.49
1:A:289:THR:HG23	1:A:291:VAL:H	1.78	0.48
1:E:330:LEU:HD22	1:E:334:ILE:HD11	1.96	0.48
1:F:175:VAL:HG22	1:F:181:VAL:HG21	1.95	0.48
1:F:263:ARG:NH1	1:F:265:VAL:HG12	2.28	0.48
1:J:252:VAL:HA	1:J:256:LEU:HD23	1.94	0.48
1:N:134:LEU:O	1:N:137:SER:N	2.70	0.48
1:Q:298:ARG:HG3	1:Q:316:ASP:OD1	2.13	0.48
1:R:144:GLU:OE2	1:R:163:ASP:HB2	2.13	0.48
1:R:291:VAL:HG21	1:R:330:LEU:HD12	2.16	0.48
1:B:217:ILE:HG23	1:B:228:VAL:HG11	2.05	0.48
1:D:237:ARG:HD2	1:D:241:ARG:NH2	2.28	0.48
1:S:129:GLU:HG3	1:S:233:VAL:HA	17.14	0.48
1:A:200:LYS:HD2	1:D:219:GLN:HE21	41.04	0.48
1:H:145:ASP:HB3	1:H:148:VAL:HG23	2.46	0.48
1:O:280:VAL:HG23	1:O:310:TYR:HB3	2.71	0.48
1:A:248:GLU:CG	1:A:264:MET:HG2	14.53	0.48
1:C:117:HIS:HE1	1:C:174:ASN:O	2.73	0.48
1:E:117:HIS:HE1	1:E:174:ASN:O	2.61	0.48
1:K:211:ALA:HB2	1:K:220:LEU:HD13	3.05	0.48
1:L:293:ILE:HG23	1:L:318:ILE:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:330:LEU:O	1:M:334:ILE:HG13	2.38	0.48
1:H:129:GLU:O	1:H:132:ARG:HB2	2.70	0.48
1:J:298:ARG:HH22	1:J:313:ARG:CB	2.05	0.48
1:A:125:GLU:HB3	1:A:232:PHE:CD1	10.63	0.48
1:A:331:LYS:O	1:A:334:ILE:HG22	5.63	0.48
1:B:195:ILE:HA	1:B:198:ILE:HD12	1.96	0.48
1:E:294:ILE:HD11	1:E:321:ILE:HG13	2.94	0.48
1:J:179:ARG:NH2	1:J:244:ASP:OD1	43.88	0.48
1:K:270:PRO:HD3	1:K:334:ILE:CG2	2.44	0.48
1:Q:134:LEU:HD11	1:Q:243:ILE:CD1	34.91	0.48
1:E:263:ARG:HG3	1:E:264:MET:O	2.14	0.48
1:H:294:ILE:HD11	1:H:321:ILE:HG13	1.96	0.48
1:S:165:THR:HB	1:S:193:HIS:ND1	2.40	0.48
1:Q:330:LEU:O	1:Q:334:ILE:HG13	2.15	0.48
1:E:195:ILE:HA	1:E:198:ILE:HD12	1.96	0.48
1:R:199:ARG:HE	1:R:203:GLU:HA	2.26	0.48
1:B:270:PRO:HD2	1:B:334:ILE:HG22	2.03	0.48
1:C:270:PRO:HD3	1:C:334:ILE:CG2	2.43	0.48
1:H:293:ILE:H	1:H:293:ILE:HG13	1.75	0.48
1:J:289:THR:HG21	1:J:330:LEU:HG	2.03	0.48
1:N:144:GLU:OE2	1:N:163:ASP:CB	2.59	0.48
1:P:116:ARG:CG	1:P:116:ARG:HH21	3.12	0.48
1:Q:270:PRO:O	1:Q:273:SER:HB3	2.14	0.48
1:T:116:ARG:NH2	1:T:116:ARG:HG3	3.09	0.48
1:F:152:VAL:HG13	1:F:157:ALA:HB3	2.28	0.47
1:G:268:PRO:O	1:G:270:PRO:HD3	2.13	0.47
1:I:274:LYS:HE2	1:I:335:SER:O	2.14	0.47
1:Q:292:ILE:HD11	1:Q:305:ASP:HB2	12.28	0.47
1:I:288:VAL:HG11	1:I:333:TYR:CE1	2.49	0.47
1:P:275:LEU:HD12	1:P:334:ILE:HG13	3.47	0.47
1:Q:199:ARG:HE	1:Q:203:GLU:HA	1.78	0.47
1:A:265:VAL:HG11	1:A:327:ILE:HG23	1.97	0.47
1:A:270:PRO:HD2	1:A:334:ILE:CG2	2.44	0.47
1:D:199:ARG:HH12	1:D:207:ILE:HG13	2.48	0.47
1:F:335:SER:O	1:F:336:ALA:HB3	2.60	0.47
1:M:269:ILE:HD12	1:M:316:ASP:HB2	2.21	0.47
1:T:129:GLU:HG3	1:T:233:VAL:HA	17.04	0.47
1:K:274:LYS:HD3	1:K:335:SER:O	2.14	0.47
1:M:298:ARG:NH2	1:M:316:ASP:OD1	2.65	0.47
1:P:195:ILE:HD13	1:P:225:ALA:HB2	2.04	0.47
1:G:166:ARG:HH22	1:H:213:ARG:HG2	46.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:217:ILE:HG23	1:N:228:VAL:HG11	2.14	0.47
1:Q:213:ARG:HG2	1:R:166:ARG:NH2	23.47	0.47
1:E:265:VAL:HG11	1:E:327:ILE:HG23	2.84	0.47
1:F:285:ILE:CD1	1:F:293:ILE:HD11	4.29	0.47
1:H:182:ILE:HD11	1:H:243:ILE:HD11	32.01	0.47
1:H:199:ARG:HE	1:H:199:ARG:HA	2.34	0.47
1:M:263:ARG:CZ	1:M:265:VAL:HG12	2.45	0.47
1:P:133:GLU:HG3	1:P:240:SER:OG	28.03	0.47
1:S:270:PRO:HD2	1:S:334:ILE:CG2	2.95	0.47
1:E:298:ARG:HH12	1:E:313:ARG:HD2	1.93	0.47
1:T:289:THR:HG23	1:T:291:VAL:H	1.80	0.47
1:A:167:VAL:HG13	1:A:201:ILE:HD11	2.28	0.47
1:A:247:TYR:HB3	1:A:302:LEU:HD13	22.59	0.47
1:D:241:ARG:NH2	1:D:259:GLU:OE2	22.17	0.47
1:D:274:LYS:HD2	1:D:335:SER:O	2.14	0.47
1:N:234:ILE:O	1:N:238:LEU:HB2	2.55	0.47
1:O:231:PRO:HG2	1:O:232:PHE:CD2	2.50	0.47
1:M:193:HIS:NE2	1:P:216:ASN:OD1	31.85	0.47
1:A:199:ARG:NH2	1:A:205:VAL:O	2.44	0.47
1:C:291:VAL:HG21	1:C:330:LEU:HD12	2.34	0.47
1:E:213:ARG:HG2	1:H:166:ARG:HH22	46.45	0.47
1:I:252:VAL:HA	1:I:256:LEU:HD23	2.34	0.47
1:J:270:PRO:HD2	1:J:334:ILE:HG22	3.44	0.47
1:L:176:ARG:HD2	1:S:299:GLY:CA	106.03	0.47
1:Q:213:ARG:HG2	1:T:166:ARG:HH21	47.62	0.47
1:F:252:VAL:HG13	1:F:256:LEU:HD12	5.22	0.47
1:K:298:ARG:NH2	1:K:310:TYR:OH	3.47	0.47
1:D:175:VAL:HG22	1:D:181:VAL:HG21	2.09	0.47
1:F:283:ALA:HB1	1:F:285:ILE:HG13	2.42	0.47
1:R:175:VAL:HG11	1:R:198:ILE:HG23	2.22	0.47
1:T:309:ASP:N	1:T:309:ASP:OD1	2.48	0.47
1:A:279:SER:HA	1:A:310:TYR:O	2.32	0.46
1:F:275:LEU:HD12	1:F:334:ILE:HG12	1.97	0.46
1:H:298:ARG:HH12	1:H:313:ARG:CG	2.27	0.46
1:I:234:ILE:O	1:I:238:LEU:HB2	2.58	0.46
1:J:214:TYR:C	1:J:216:ASN:H	2.18	0.46
1:M:237:ARG:HD2	1:M:259:GLU:OE2	22.30	0.46
1:P:293:ILE:H	1:P:293:ILE:HG13	2.87	0.46
1:T:131:LEU:HD21	1:T:139:VAL:HG11	2.06	0.46
1:D:116:ARG:HH21	1:D:116:ARG:CG	2.08	0.46
1:G:182:ILE:HA	1:G:208:ILE:O	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:268:PRO:HA	1:O:317:ILE:HD13	1.97	0.46
1:O:274:LYS:HD2	1:O:336:ALA:HB3	2.53	0.46
1:Q:120:ILE:HB	1:Q:141:VAL:HG22	1.98	0.46
1:S:231:PRO:HG2	1:S:232:PHE:CD2	2.49	0.46
1:C:229:ILE:HG22	1:C:231:PRO:HD3	2.22	0.46
1:C:270:PRO:CD	1:C:334:ILE:CG2	2.92	0.46
1:N:324:PRO:HA	1:N:327:ILE:HD12	2.58	0.46
1:R:148:VAL:HG12	1:R:152:VAL:HG23	2.26	0.46
1:L:117:HIS:H	1:L:117:HIS:CD2	2.33	0.46
1:N:265:VAL:O	1:N:319:LEU:HA	2.31	0.46
1:P:217:ILE:HG23	1:P:228:VAL:HG11	2.51	0.46
1:P:234:ILE:O	1:P:238:LEU:HB2	2.25	0.46
1:Q:285:ILE:HG21	1:Q:293:ILE:HD11	3.99	0.46
1:G:298:ARG:NE	1:G:310:TYR:OH	4.10	0.46
1:H:330:LEU:O	1:H:334:ILE:HG13	2.15	0.46
1:Q:296:VAL:HG23	1:Q:306:PRO:HG3	1.98	0.46
1:R:293:ILE:H	1:R:293:ILE:HG13	1.49	0.46
1:S:253:GLN:O	1:S:257:ALA:HB3	2.15	0.46
1:T:182:ILE:HG13	1:T:208:ILE:HB	2.83	0.46
1:C:264:MET:CE	1:C:321:ILE:HG12	2.46	0.46
1:F:237:ARG:HH11	1:F:237:ARG:HG2	1.81	0.46
1:K:285:ILE:HB	1:K:293:ILE:HD11	2.30	0.46
1:L:232:PHE:N	1:L:232:PHE:CD2	2.83	0.46
1:L:269:ILE:HG22	1:L:314:ALA:HA	1.98	0.46
1:N:265:VAL:HG11	1:N:327:ILE:HG12	2.40	0.46
1:N:294:ILE:HD11	1:N:321:ILE:CG1	3.23	0.46
1:Q:252:VAL:HA	1:Q:256:LEU:HD13	3.72	0.46
1:A:248:GLU:HG3	1:A:264:MET:CG	13.23	0.46
1:D:165:THR:HB	1:D:193:HIS:ND1	2.42	0.46
1:F:199:ARG:HE	1:F:203:GLU:HA	1.81	0.46
1:G:253:GLN:NE2	1:G:253:GLN:HA	2.58	0.46
1:I:145:ASP:HB3	1:I:148:VAL:HG23	1.98	0.46
1:O:123:TRP:CZ2	1:O:128:LEU:HD12	2.68	0.46
1:R:164:PRO:HG2	1:R:185:LEU:HD21	1.98	0.46
1:R:330:LEU:HD22	1:R:334:ILE:HD11	1.96	0.46
1:R:335:SER:O	1:R:336:ALA:CB	3.09	0.46
1:T:270:PRO:HD2	1:T:273:SER:HB2	2.69	0.46
1:E:309:ASP:OD1	1:E:309:ASP:N	2.61	0.46
1:O:211:ALA:HB2	1:O:220:LEU:HD22	2.50	0.46
1:T:134:LEU:HD11	1:T:243:ILE:CD1	34.98	0.46
1:A:119:VAL:HB	1:A:181:VAL:HG22	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD13	1:B:190:GLU:HB3	1.97	0.46
1:C:298:ARG:HG3	1:C:316:ASP:OD1	2.15	0.46
1:E:133:GLU:HG3	1:E:240:SER:OG	27.98	0.46
1:G:199:ARG:NH1	1:G:224:GLY:O	2.56	0.46
1:P:248:GLU:O	1:P:252:VAL:HG23	2.40	0.46
1:G:279:SER:HA	1:G:310:TYR:O	2.37	0.46
1:I:134:LEU:HD11	1:I:243:ILE:CD1	34.40	0.46
1:R:125:GLU:HB3	1:R:232:PHE:CD1	11.00	0.46
1:B:247:TYR:HB3	1:B:302:LEU:HD13	22.19	0.45
1:C:289:THR:HG21	1:C:330:LEU:HG	2.02	0.45
1:E:237:ARG:NH1	1:E:241:ARG:NH2	3.78	0.45
1:G:237:ARG:HG2	1:G:241:ARG:HH11	1.81	0.45
1:J:195:ILE:HA	1:J:198:ILE:HD12	2.55	0.45
1:P:298:ARG:HH12	1:P:313:ARG:NH2	3.34	0.45
1:R:298:ARG:NH1	1:R:313:ARG:HD2	2.31	0.45
1:B:307:PRO:HG2	1:B:310:TYR:HB2	3.12	0.45
1:G:182:ILE:HD13	1:G:239:MET:HB3	26.07	0.45
1:L:120:ILE:HG12	1:L:182:ILE:HB	2.24	0.45
1:O:298:ARG:NH2	1:O:310:TYR:OH	2.50	0.45
1:S:175:VAL:CG1	1:S:198:ILE:HG23	2.66	0.45
1:T:232:PHE:H	1:T:232:PHE:HD2	1.64	0.45
1:A:289:THR:HG21	1:A:330:LEU:HG	1.98	0.45
1:C:237:ARG:HH21	1:C:241:ARG:NH1	2.14	0.45
1:F:292:ILE:HD11	1:F:305:ASP:HB2	12.36	0.45
1:I:237:ARG:HD2	1:I:259:GLU:OE1	20.22	0.45
1:J:287:ASP:HA	1:J:308:ARG:NH2	15.98	0.45
1:O:232:PHE:N	1:O:232:PHE:HD2	2.14	0.45
1:P:164:PRO:HG3	1:P:185:LEU:HD21	1.99	0.45
1:P:199:ARG:NH2	1:P:205:VAL:O	2.42	0.45
1:C:206:ARG:NH1	1:C:242:SER:O	32.05	0.45
1:G:335:SER:O	1:G:336:ALA:HB3	2.17	0.45
1:H:298:ARG:HH22	1:H:313:ARG:HB2	2.42	0.45
1:J:237:ARG:HG2	1:J:237:ARG:HH11	1.81	0.45
1:J:298:ARG:NH2	1:J:313:ARG:HD2	2.32	0.45
1:J:166:ARG:NH2	1:K:213:ARG:HG2	46.85	0.45
1:K:270:PRO:CD	1:K:334:ILE:HG22	2.46	0.45
1:B:131:LEU:HD21	1:B:139:VAL:HG11	1.99	0.45
1:H:213:ARG:HD2	1:H:216:ASN:ND2	2.31	0.45
1:N:309:ASP:OD1	1:N:309:ASP:N	2.55	0.45
1:Q:183:VAL:HG12	1:Q:191:THR:HG23	1.98	0.45
1:S:330:LEU:HD22	1:S:334:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:216:ASN:O	1:T:220:LEU:HD13	2.22	0.45
1:C:273:SER:HB2	1:C:334:ILE:HG22	2.89	0.45
1:J:125:GLU:HB3	1:J:232:PHE:HD1	10.90	0.45
1:O:269:ILE:HA	1:O:270:PRO:HD3	1.80	0.45
1:O:269:ILE:HG22	1:O:314:ALA:HA	2.09	0.45
1:Q:175:VAL:HG13	1:Q:181:VAL:HG21	2.41	0.45
1:R:199:ARG:HG3	1:R:224:GLY:HA3	1.98	0.45
1:G:163:ASP:HA	1:G:164:PRO:HD3	2.42	0.45
1:H:265:VAL:O	1:H:319:LEU:HA	2.26	0.45
1:I:296:VAL:HG23	1:I:306:PRO:HG3	2.85	0.45
1:T:330:LEU:HD22	1:T:334:ILE:HD11	1.98	0.45
1:D:237:ARG:O	1:D:241:ARG:HB2	2.17	0.45
1:E:166:ARG:HB3	1:E:169:ASP:HB2	2.25	0.45
1:E:263:ARG:HG2	1:E:265:VAL:HG13	1.99	0.45
1:E:293:ILE:HG13	1:E:293:ILE:H	1.49	0.45
1:F:124:SER:OG	1:F:126:SER:HB2	2.17	0.45
1:H:252:VAL:O	1:H:256:LEU:HB2	2.16	0.45
1:H:298:ARG:NH1	1:H:313:ARG:HD2	2.60	0.45
1:K:129:GLU:OE1	1:K:132:ARG:HD2	2.17	0.45
1:K:248:GLU:O	1:K:252:VAL:HG23	2.34	0.45
1:Q:165:THR:HB	1:Q:193:HIS:ND1	2.32	0.45
1:Q:166:ARG:HH21	1:R:213:ARG:NE	45.39	0.45
1:S:263:ARG:NH1	1:S:265:VAL:HG12	3.88	0.45
1:A:252:VAL:HG13	1:A:256:LEU:HD12	1.99	0.45
1:D:171:GLU:HG2	1:D:201:ILE:HD13	2.09	0.45
1:E:289:THR:HG21	1:E:330:LEU:HG	2.11	0.45
1:K:270:PRO:HD2	1:K:334:ILE:HG22	1.99	0.45
1:P:134:LEU:HD21	1:P:243:ILE:HD13	36.89	0.45
1:C:237:ARG:HD2	1:C:259:GLU:OE1	21.31	0.45
1:F:270:PRO:HD2	1:F:334:ILE:CG2	2.53	0.45
1:J:176:ARG:CG	1:J:176:ARG:NH2	2.66	0.45
1:L:119:VAL:HB	1:L:181:VAL:HG22	1.99	0.45
1:M:242:SER:OG	1:M:249:ALA:HB2	2.29	0.45
1:M:298:ARG:CZ	1:M:313:ARG:HD2	2.97	0.45
1:O:298:ARG:HH11	1:O:298:ARG:CG	4.01	0.45
1:P:221:ARG:NH2	1:P:258:GLU:OE1	26.84	0.45
1:Q:133:GLU:HB2	1:Q:240:SER:HB2	31.15	0.45
1:S:269:ILE:HG22	1:S:314:ALA:HA	1.99	0.45
1:E:219:GLN:NE2	1:H:200:LYS:HD3	54.32	0.44
1:M:229:ILE:HA	1:M:253:GLN:NE2	15.32	0.44
1:O:133:GLU:HG3	1:O:240:SER:OG	28.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:242:SER:OG	1:O:249:ALA:HB2	2.31	0.44
1:Q:285:ILE:HB	1:Q:293:ILE:HD11	1.99	0.44
1:T:151:LYS:O	1:T:154:ARG:HB2	2.17	0.44
1:K:175:VAL:HG22	1:K:181:VAL:HG21	2.42	0.44
1:L:211:ALA:HB2	1:L:220:LEU:HD22	2.57	0.44
1:M:308:ARG:H	1:M:308:ARG:HD2	4.76	0.44
1:P:146:GLU:OE1	1:P:149:ARG:NH1	2.60	0.44
1:R:275:LEU:HD12	1:R:334:ILE:HG23	1.98	0.44
1:C:172:LYS:HE3	1:D:154:ARG:HH11	33.34	0.44
1:E:152:VAL:HG11	1:E:159:PHE:HB2	1.98	0.44
1:F:221:ARG:HH22	1:F:253:GLN:HG2	23.76	0.44
1:G:175:VAL:CG1	1:G:198:ILE:HG23	2.48	0.44
1:H:232:PHE:N	1:H:232:PHE:CD2	2.88	0.44
1:H:285:ILE:HB	1:H:293:ILE:HD11	1.98	0.44
1:I:291:VAL:HG21	1:I:330:LEU:HD12	2.11	0.44
1:O:238:LEU:HD21	1:O:252:VAL:HG21	1.98	0.44
1:O:263:ARG:NH1	1:O:265:VAL:HG12	2.65	0.44
1:C:193:HIS:HD2	1:C:193:HIS:O	1.99	0.44
1:G:231:PRO:HB3	1:G:235:SER:HB2	5.65	0.44
1:E:192:ILE:HD12	1:H:193:HIS:CD2	41.97	0.44
1:K:330:LEU:O	1:K:334:ILE:HG13	2.36	0.44
1:R:211:ALA:HB2	1:R:220:LEU:HD22	2.09	0.44
1:T:263:ARG:HE	1:T:327:ILE:HD13	1.82	0.44
1:A:293:ILE:H	1:A:293:ILE:HG13	1.71	0.44
1:B:323:LYS:HB3	1:B:324:PRO:HD2	2.39	0.44
1:D:116:ARG:HB2	1:D:179:ARG:HB2	2.40	0.44
1:D:263:ARG:NH1	1:D:265:VAL:HG12	3.33	0.44
1:E:116:ARG:HH22	1:E:179:ARG:HD2	1.77	0.44
1:E:275:LEU:HD21	1:E:333:TYR:CE2	2.53	0.44
1:H:120:ILE:HG12	1:H:182:ILE:HB	2.00	0.44
1:H:195:ILE:HD13	1:H:225:ALA:HB2	2.43	0.44
1:I:187:SER:OG	1:I:190:GLU:HG3	3.52	0.44
1:J:231:PRO:HG2	1:J:232:PHE:HD2	1.83	0.44
1:N:131:LEU:HD21	1:N:139:VAL:HG11	2.06	0.44
1:N:280:VAL:HG22	1:N:312:PHE:CE1	4.19	0.44
1:A:116:ARG:CG	1:A:116:ARG:NH2	2.84	0.44
1:A:330:LEU:O	1:A:334:ILE:HG13	2.18	0.44
1:C:237:ARG:NH2	1:C:248:GLU:OE2	3.62	0.44
1:E:117:HIS:N	1:E:117:HIS:CD2	2.86	0.44
1:H:279:SER:HA	1:H:310:TYR:O	2.17	0.44
1:K:195:ILE:HD11	1:K:220:LEU:HD23	3.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:324:PRO:HA	1:L:327:ILE:HD12	1.98	0.44
1:M:298:ARG:NH2	1:M:316:ASP:OD2	2.49	0.44
1:N:275:LEU:HD12	1:N:334:ILE:HG12	5.29	0.44
1:D:298:ARG:HB2	1:S:176:ARG:NH1	2.33	0.44
1:S:335:SER:O	1:S:336:ALA:HB2	2.16	0.44
1:C:217:ILE:HG23	1:C:228:VAL:HG11	1.98	0.44
1:Q:298:ARG:NH2	1:Q:313:ARG:HD2	3.33	0.44
1:T:234:ILE:O	1:T:238:LEU:HB2	2.18	0.44
1:F:231:PRO:HG2	1:F:232:PHE:CD2	2.53	0.44
1:H:298:ARG:NH2	1:H:313:ARG:HD2	2.53	0.44
1:J:270:PRO:CD	1:J:334:ILE:HG23	2.48	0.44
1:M:166:ARG:NH2	1:N:213:ARG:HG2	46.67	0.44
1:N:134:LEU:O	1:N:137:SER:HB2	2.64	0.44
1:N:252:VAL:O	1:N:256:LEU:HB2	2.34	0.44
1:P:129:GLU:HG3	1:P:233:VAL:HA	17.00	0.44
1:A:199:ARG:NH1	1:A:224:GLY:O	2.66	0.44
1:G:267:VAL:HG21	1:G:330:LEU:HD22	4.24	0.44
1:I:229:ILE:HG12	1:I:238:LEU:HD23	13.44	0.44
1:K:163:ASP:HA	1:K:164:PRO:HD3	1.92	0.44
1:R:298:ARG:O	1:R:298:ARG:HG3	4.33	0.44
1:C:275:LEU:HD12	1:C:334:ILE:HG12	2.10	0.43
1:G:301:GLU:OE1	1:G:303:ILE:HD11	2.18	0.43
1:J:309:ASP:N	1:J:309:ASP:OD1	2.45	0.43
1:J:125:GLU:CD	1:K:166:ARG:HH22	2.22	0.43
1:M:175:VAL:HG13	1:M:181:VAL:HG21	2.68	0.43
1:N:293:ILE:HG13	1:N:293:ILE:H	1.56	0.43
1:O:199:ARG:HE	1:O:203:GLU:HA	1.88	0.43
1:A:133:GLU:HG3	1:A:240:SER:OG	27.09	0.43
1:F:234:ILE:HG13	1:F:257:ALA:HB2	11.25	0.43
1:G:308:ARG:H	1:G:308:ARG:HG2	3.86	0.43
1:H:262:ARG:NH1	1:H:262:ARG:CG	2.76	0.43
1:K:119:VAL:HB	1:K:181:VAL:HG13	2.00	0.43
1:K:262:ARG:NH2	1:K:323:LYS:HE3	2.57	0.43
1:M:133:GLU:OE1	1:M:241:ARG:NH1	26.97	0.43
1:N:147:ASN:N	1:N:147:ASN:ND2	2.65	0.43
1:N:253:GLN:HG3	1:N:258:GLU:OE1	2.18	0.43
1:D:231:PRO:HB2	1:D:231:PRO:HB2	0.00	0.43
1:E:153:LEU:HD23	1:E:157:ALA:O	2.96	0.43
1:H:262:ARG:HD3	1:H:321:ILE:CG2	3.44	0.43
1:K:298:ARG:NH2	1:K:313:ARG:CB	2.80	0.43
1:O:123:TRP:HZ2	1:O:128:LEU:HD12	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:HIS:CE1	1:B:174:ASN:HB2	2.75	0.43
1:C:150:LYS:HD3	1:D:161:HIS:CE1	2.53	0.43
1:F:176:ARG:HB2	1:F:202:ASP:HB2	3.23	0.43
1:H:262:ARG:HG3	1:H:304:ILE:HD13	18.31	0.43
1:K:207:ILE:HB	1:K:225:ALA:HA	2.00	0.43
1:B:248:GLU:O	1:B:252:VAL:HG23	2.18	0.43
1:H:220:LEU:HD23	1:H:228:VAL:HG13	2.93	0.43
1:K:231:PRO:HB2	1:K:231:PRO:HB2	0.00	0.43
1:L:118:VAL:HG21	1:L:243:ILE:HD13	38.31	0.43
1:L:242:SER:OG	1:L:249:ALA:HB2	2.19	0.43
1:O:335:SER:O	1:O:336:ALA:HB3	2.18	0.43
1:R:234:ILE:O	1:R:238:LEU:HB2	2.66	0.43
1:B:150:LYS:HG2	1:B:150:LYS:H	2.39	0.43
1:C:199:ARG:NH2	1:C:205:VAL:O	2.57	0.43
1:I:148:VAL:HG12	1:I:152:VAL:HG23	2.00	0.43
1:J:144:GLU:O	1:J:161:HIS:NE2	2.74	0.43
1:J:164:PRO:HG2	1:J:185:LEU:HD21	2.00	0.43
1:J:188:ASP:O	1:J:192:ILE:HG13	2.45	0.43
1:J:284:ASP:O	1:J:288:VAL:HG23	2.32	0.43
1:T:232:PHE:N	1:T:232:PHE:CD2	2.87	0.43
1:C:289:THR:CG2	1:C:291:VAL:H	2.32	0.43
1:J:270:PRO:HD2	1:J:334:ILE:HG23	2.00	0.43
1:N:147:ASN:H	1:N:147:ASN:ND2	2.13	0.43
1:B:288:VAL:HG11	1:B:333:TYR:CE1	2.71	0.43
1:D:294:ILE:HD11	1:D:321:ILE:CD1	2.48	0.43
1:H:152:VAL:HG13	1:H:157:ALA:HB3	2.00	0.43
1:H:191:THR:HG22	1:H:220:LEU:HD11	3.98	0.43
1:N:270:PRO:HG2	1:N:335:SER:HA	3.04	0.43
1:O:185:LEU:HD13	1:O:190:GLU:HB3	2.23	0.43
1:Q:211:ALA:HB2	1:Q:220:LEU:HD22	1.99	0.43
1:R:285:ILE:HD12	1:R:293:ILE:HD12	3.89	0.43
1:R:298:ARG:HH12	1:R:313:ARG:HD2	1.81	0.43
1:B:253:GLN:O	1:B:257:ALA:HB3	2.27	0.43
1:C:175:VAL:HG11	1:C:198:ILE:HG23	2.00	0.43
1:G:172:LYS:HB3	1:G:172:LYS:HE2	4.33	0.43
1:G:278:VAL:O	1:G:312:PHE:HD1	2.72	0.43
1:G:330:LEU:O	1:G:334:ILE:HG13	2.19	0.43
1:H:159:PHE:HE2	1:H:161:HIS:HB2	1.83	0.43
1:L:163:ASP:HA	1:L:164:PRO:HD3	1.86	0.43
1:O:298:ARG:NH1	1:O:298:ARG:HG3	4.68	0.43
1:R:269:ILE:HA	1:R:270:PRO:HD3	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:HG12	1:A:191:THR:HG23	2.00	0.43
1:A:325:GLU:HG2	1:O:324:PRO:HB3	74.65	0.43
1:B:134:LEU:HD21	1:B:243:ILE:HD13	35.05	0.43
1:B:263:ARG:NH1	1:B:265:VAL:HG12	2.34	0.43
1:L:170:LEU:HA	1:L:170:LEU:HD23	1.93	0.43
1:P:148:VAL:HG12	1:P:152:VAL:HG23	2.82	0.43
1:B:285:ILE:H	1:B:285:ILE:HG13	1.62	0.42
1:D:250:MET:O	1:D:254:ASP:OD2	2.36	0.42
1:F:145:ASP:HB3	1:F:148:VAL:HG23	2.00	0.42
1:I:330:LEU:O	1:I:334:ILE:HG13	2.44	0.42
1:L:294:ILE:HD11	1:L:321:ILE:CG1	2.48	0.42
1:Q:252:VAL:HG13	1:Q:256:LEU:HD12	2.01	0.42
1:Q:293:ILE:HG13	1:Q:293:ILE:H	1.68	0.42
1:A:192:ILE:HD12	1:B:193:HIS:CD2	31.52	0.42
1:C:144:GLU:O	1:C:161:HIS:NE2	3.05	0.42
1:E:213:ARG:HB2	1:E:216:ASN:HD22	1.84	0.42
1:S:117:HIS:CE1	1:S:174:ASN:HB3	3.78	0.42
1:A:131:LEU:HD21	1:A:139:VAL:HG11	2.01	0.42
1:B:213:ARG:HD2	1:B:216:ASN:ND2	2.34	0.42
1:J:170:LEU:HD13	1:J:198:ILE:HG13	2.01	0.42
1:K:263:ARG:NH2	1:K:265:VAL:HG12	2.33	0.42
1:M:230:SER:H	1:M:253:GLN:HE22	13.59	0.42
1:P:175:VAL:CG1	1:P:198:ILE:HG23	2.49	0.42
1:P:265:VAL:O	1:P:319:LEU:HA	2.40	0.42
1:T:263:ARG:HG2	1:T:264:MET:N	2.95	0.42
1:C:298:ARG:NH2	1:C:313:ARG:HB2	3.66	0.42
1:E:134:LEU:HD21	1:E:243:ILE:HD12	35.57	0.42
1:G:125:GLU:HB3	1:G:232:PHE:HD1	11.09	0.42
1:H:270:PRO:HD2	1:H:334:ILE:CG2	2.45	0.42
1:M:273:SER:HB2	1:M:334:ILE:O	3.31	0.42
1:R:213:ARG:HB2	1:R:216:ASN:HD22	1.85	0.42
1:R:293:ILE:HD13	1:R:318:ILE:CG2	6.48	0.42
1:S:175:VAL:HG11	1:S:198:ILE:HG23	2.37	0.42
1:D:252:VAL:HA	1:D:256:LEU:HD23	5.29	0.42
1:D:274:LYS:HD3	1:D:335:SER:O	2.78	0.42
1:G:269:ILE:HG23	1:G:273:SER:CB	2.65	0.42
1:G:274:LYS:HE2	1:G:274:LYS:HB3	4.30	0.42
1:I:323:LYS:HB2	1:I:326:GLU:HG3	2.97	0.42
1:J:118:VAL:HB	1:J:139:VAL:HG22	2.38	0.42
1:M:199:ARG:NH2	1:M:205:VAL:O	2.62	0.42
1:P:175:VAL:HG11	1:P:198:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ARG:NH2	1:D:259:GLU:OE1	23.90	0.42
1:E:298:ARG:HH12	1:E:313:ARG:CZ	2.31	0.42
1:G:289:THR:HG22	1:G:291:VAL:H	2.82	0.42
1:G:309:ASP:N	1:G:309:ASP:OD1	2.49	0.42
1:J:183:VAL:HG12	1:J:191:THR:HG23	2.01	0.42
1:M:294:ILE:HD11	1:M:321:ILE:HG13	2.29	0.42
1:N:267:VAL:CG1	1:N:334:ILE:HD11	2.49	0.42
1:O:127:THR:O	1:O:130:CYS:HB3	2.36	0.42
1:O:214:TYR:HD1	1:O:233:VAL:HG11	1.84	0.42
1:Q:247:TYR:HB3	1:Q:302:LEU:HD13	22.78	0.42
1:R:265:VAL:HG11	1:R:327:ILE:HG21	2.01	0.42
1:S:131:LEU:O	1:S:135:ARG:HB2	2.20	0.42
1:A:195:ILE:HD13	1:A:225:ALA:HB2	2.11	0.42
1:A:253:GLN:HA	1:A:253:GLN:NE2	2.73	0.42
1:C:125:GLU:HB3	1:C:232:PHE:CD1	10.74	0.42
1:D:265:VAL:HG21	1:D:327:ILE:HG12	2.02	0.42
1:H:119:VAL:HB	1:H:181:VAL:HG22	2.46	0.42
1:J:267:VAL:HA	1:J:268:PRO:HD3	1.89	0.42
1:M:199:ARG:NH1	1:M:224:GLY:O	2.51	0.42
1:A:233:VAL:O	1:A:237:ARG:HB2	2.23	0.42
1:B:289:THR:HG23	1:B:291:VAL:H	1.84	0.42
1:L:264:MET:HE2	1:L:321:ILE:HG12	2.31	0.42
1:O:116:ARG:CG	1:O:116:ARG:HH21	2.26	0.42
1:S:116:ARG:HD2	1:S:179:ARG:HG2	4.16	0.42
1:G:237:ARG:HD2	1:G:259:GLU:OE2	20.47	0.42
1:L:247:TYR:H	1:L:266:GLU:CD	25.34	0.42
1:N:231:PRO:HG3	1:N:235:SER:HB2	6.95	0.42
1:N:275:LEU:HD21	1:N:333:TYR:CE2	2.90	0.42
1:S:229:ILE:HG22	1:S:231:PRO:HD3	2.38	0.42
1:A:285:ILE:HG13	1:A:285:ILE:H	1.83	0.42
1:E:228:VAL:C	1:E:229:ILE:HG13	2.40	0.42
1:G:335:SER:O	1:G:336:ALA:CB	2.68	0.42
1:I:144:GLU:O	1:I:161:HIS:NE2	2.51	0.42
1:J:298:ARG:HH22	1:J:313:ARG:HD2	2.00	0.42
1:S:181:VAL:HG11	1:S:198:ILE:HD13	2.01	0.42
1:A:206:ARG:NH1	1:A:242:SER:O	31.73	0.41
1:C:125:GLU:HB3	1:C:232:PHE:HD1	11.51	0.41
1:D:238:LEU:HA	1:D:238:LEU:HD12	1.96	0.41
1:H:263:ARG:CZ	1:H:265:VAL:HG12	2.50	0.41
1:P:330:LEU:O	1:P:334:ILE:HG13	2.20	0.41
1:B:237:ARG:HH11	1:B:241:ARG:CZ	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:PRO:HG2	1:F:310:TYR:HB2	2.02	0.41
1:G:195:ILE:HD13	1:G:225:ALA:HB2	2.00	0.41
1:J:335:SER:O	1:J:336:ALA:HB3	2.20	0.41
1:K:191:THR:O	1:K:195:ILE:HG13	2.73	0.41
1:L:150:LYS:HG2	1:L:150:LYS:H	2.10	0.41
1:N:199:ARG:HE	1:N:203:GLU:HA	2.23	0.41
1:N:269:ILE:HD11	1:N:312:PHE:HD2	2.55	0.41
1:P:199:ARG:HE	1:P:203:GLU:HA	2.17	0.41
1:Q:129:GLU:HG3	1:Q:233:VAL:HA	17.09	0.41
1:R:252:VAL:HG13	1:R:256:LEU:HD12	2.40	0.41
1:C:324:PRO:HB2	1:S:325:GLU:HG3	38.72	0.41
1:J:247:TYR:HB3	1:J:302:LEU:HD13	22.52	0.41
1:L:148:VAL:HG12	1:L:152:VAL:HG23	2.02	0.41
1:N:270:PRO:CD	1:N:334:ILE:HG23	5.89	0.41
1:Q:195:ILE:HA	1:Q:198:ILE:HD12	2.01	0.41
1:C:296:VAL:HG23	1:C:306:PRO:HG3	2.02	0.41
1:D:237:ARG:HH11	1:D:241:ARG:HE	1.67	0.41
1:E:118:VAL:HG21	1:E:243:ILE:HD13	38.37	0.41
1:L:117:HIS:CE1	1:L:174:ASN:HB2	2.56	0.41
1:M:275:LEU:HD12	1:M:334:ILE:HG23	3.48	0.41
1:T:195:ILE:HG23	1:T:207:ILE:HD13	2.31	0.41
1:T:265:VAL:O	1:T:319:LEU:HA	2.37	0.41
1:B:227:GLN:OE1	1:B:250:MET:HB3	25.02	0.41
1:B:330:LEU:HD22	1:B:334:ILE:HD11	2.02	0.41
1:C:133:GLU:HB2	1:C:240:SER:HB2	30.95	0.41
1:C:265:VAL:O	1:C:319:LEU:HA	2.20	0.41
1:D:116:ARG:CG	1:D:116:ARG:NH2	2.73	0.41
1:E:129:GLU:O	1:E:132:ARG:HB2	2.20	0.41
1:K:335:SER:O	1:K:336:ALA:HB3	2.25	0.41
1:M:163:ASP:OD2	1:P:213:ARG:NH2	25.93	0.41
1:N:281:LEU:HB2	1:N:308:ARG:HB3	3.39	0.41
1:Q:242:SER:OG	1:Q:249:ALA:HB2	2.39	0.41
1:Q:298:ARG:NH2	1:Q:316:ASP:OD1	3.46	0.41
1:T:247:TYR:HA	1:T:250:MET:HG2	2.02	0.41
1:E:210:GLU:HB2	1:E:239:MET:CE	16.43	0.41
1:E:270:PRO:HD2	1:E:334:ILE:CG2	2.50	0.41
1:I:195:ILE:HD13	1:I:225:ALA:HB2	2.05	0.41
1:J:330:LEU:O	1:J:334:ILE:HG13	3.80	0.41
1:O:263:ARG:CG	1:O:264:MET:N	2.84	0.41
1:Q:231:PRO:HB3	1:Q:235:SER:HB2	5.85	0.41
1:S:231:PRO:HB3	1:S:235:SER:HB2	5.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HD12	1:A:321:ILE:HB	3.24	0.41
1:C:248:GLU:O	1:C:252:VAL:HG23	2.20	0.41
1:F:141:VAL:HG11	1:F:152:VAL:HG21	2.03	0.41
1:L:199:ARG:NH2	1:L:205:VAL:O	2.55	0.41
1:O:238:LEU:HD12	1:O:238:LEU:HA	1.85	0.41
1:T:229:ILE:HA	1:T:253:GLN:NE2	15.23	0.41
1:C:199:ARG:HE	1:C:203:GLU:HA	1.84	0.41
1:D:198:ILE:H	1:D:198:ILE:HG13	2.01	0.41
1:E:194:CYS:SG	1:E:198:ILE:HD11	2.61	0.41
1:H:232:PHE:HD2	1:H:232:PHE:N	2.21	0.41
1:L:238:LEU:HA	1:L:238:LEU:HD12	1.81	0.41
1:L:241:ARG:NH2	1:L:259:GLU:OE2	22.53	0.41
1:M:213:ARG:CG	1:P:166:ARG:NH2	47.21	0.41
1:Q:195:ILE:HD13	1:Q:225:ALA:HB2	2.33	0.41
1:R:230:SER:H	1:R:253:GLN:HE22	13.57	0.41
1:C:285:ILE:HB	1:C:293:ILE:HD11	2.15	0.41
1:G:214:TYR:CD1	1:G:217:ILE:HD12	3.42	0.41
1:I:285:ILE:H	1:I:285:ILE:HG13	1.86	0.41
1:I:298:ARG:CZ	1:I:316:ASP:OD1	3.58	0.41
1:J:163:ASP:HA	1:J:164:PRO:HD2	2.62	0.41
1:P:183:VAL:HG12	1:P:191:THR:HG23	2.29	0.41
1:T:195:ILE:HA	1:T:198:ILE:HD12	2.41	0.41
1:T:182:ILE:HA	1:T:208:ILE:O	2.50	0.41
1:T:231:PRO:HB3	1:T:235:SER:HB2	5.85	0.41
1:A:133:GLU:HB2	1:A:240:SER:HB2	30.32	0.41
1:C:165:THR:HB	1:C:193:HIS:ND1	2.98	0.41
1:F:182:ILE:HD11	1:F:243:ILE:HD11	31.55	0.41
1:H:159:PHE:CE2	1:H:161:HIS:HB2	2.56	0.41
1:O:231:PRO:HG2	1:O:232:PHE:HD2	1.84	0.41
1:R:166:ARG:HB3	1:R:169:ASP:HB2	2.52	0.41
1:R:165:THR:HB	1:R:193:HIS:CE1	2.56	0.41
1:R:199:ARG:NH1	1:R:224:GLY:O	2.60	0.41
1:T:265:VAL:HG11	1:T:327:ILE:HG12	2.17	0.41
1:B:203:GLU:HG2	1:B:203:GLU:H	1.81	0.41
1:C:298:ARG:HH22	1:C:313:ARG:HG3	1.86	0.41
1:H:124:SER:OG	1:H:126:SER:HB2	2.46	0.41
1:J:124:SER:OG	1:J:126:SER:HB2	2.48	0.41
1:L:252:VAL:HG13	1:L:256:LEU:HD12	2.02	0.41
1:N:269:ILE:HA	1:N:270:PRO:HD3	1.90	0.41
1:R:199:ARG:NH2	1:R:205:VAL:O	2.54	0.41
1:B:269:ILE:HD11	1:B:318:ILE:HD11	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:ILE:HD12	1:H:193:HIS:CD2	32.84	0.40
1:P:253:GLN:O	1:P:257:ALA:HB3	2.21	0.40
1:S:200:LYS:O	1:S:200:LYS:HG2	4.11	0.40
1:A:120:ILE:HB	1:A:141:VAL:HG22	2.45	0.40
1:A:221:ARG:HH22	1:A:258:GLU:CD	25.98	0.40
1:C:123:TRP:HZ2	1:C:128:LEU:HD12	2.00	0.40
1:C:269:ILE:HD11	1:C:318:ILE:HD11	2.52	0.40
1:F:123:TRP:HZ2	1:F:128:LEU:HD12	1.86	0.40
1:F:144:GLU:O	1:F:161:HIS:NE2	2.78	0.40
1:F:262:ARG:HG3	1:F:323:LYS:HG3	2.02	0.40
1:G:230:SER:H	1:G:253:GLN:HE22	12.98	0.40
1:H:133:GLU:HB2	1:H:240:SER:HB2	30.95	0.40
1:J:203:GLU:HG2	1:J:203:GLU:H	1.75	0.40
1:L:292:ILE:HG13	1:L:292:ILE:H	1.70	0.40
1:T:248:GLU:O	1:T:252:VAL:HG23	2.34	0.40
1:A:132:ARG:NH1	1:A:132:ARG:CG	3.96	0.40
1:C:116:ARG:CG	1:C:116:ARG:HH21	3.25	0.40
1:C:132:ARG:CG	1:C:132:ARG:NH1	2.71	0.40
1:E:175:VAL:HG11	1:E:198:ILE:HG23	2.01	0.40
1:E:298:ARG:HH22	1:E:313:ARG:CG	2.60	0.40
1:I:242:SER:OG	1:I:249:ALA:HB2	2.30	0.40
1:I:294:ILE:HD11	1:I:321:ILE:CD1	2.67	0.40
1:J:125:GLU:HB3	1:J:232:PHE:CD1	10.20	0.40
1:L:285:ILE:HD11	1:L:312:PHE:CZ	2.56	0.40
1:N:248:GLU:O	1:N:252:VAL:HG23	2.43	0.40
1:P:231:PRO:HB3	1:P:235:SER:HB2	5.61	0.40
1:R:232:PHE:N	1:R:232:PHE:CD2	3.20	0.40
1:A:269:ILE:O	1:A:315:GLY:N	2.52	0.40
1:B:218:GLU:HG2	1:C:200:LYS:NZ	40.54	0.40
1:C:253:GLN:O	1:C:257:ALA:HB3	2.21	0.40
1:D:269:ILE:HG22	1:D:314:ALA:HA	2.12	0.40
1:D:269:ILE:HA	1:D:270:PRO:HD3	1.94	0.40
1:E:191:THR:O	1:E:195:ILE:HG13	2.22	0.40
1:H:263:ARG:NH2	1:H:265:VAL:HG12	2.36	0.40
1:I:117:HIS:HE1	1:I:174:ASN:O	2.03	0.40
1:I:185:LEU:HD13	1:I:190:GLU:HB3	2.04	0.40
1:J:206:ARG:NH1	1:J:242:SER:O	31.86	0.40
1:Q:307:PRO:HG2	1:Q:310:TYR:HB2	4.01	0.40
1:S:214:TYR:HD1	1:S:233:VAL:HG11	1.86	0.40
1:C:324:PRO:HB2	1:S:325:GLU:CG	38.36	0.40
1:T:293:ILE:HG23	1:T:318:ILE:HG23	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLU:OE2	1:B:176:ARG:NH2	3.05	0.40
1:C:252:VAL:HG22	1:C:256:LEU:HD21	6.07	0.40
1:D:285:ILE:HD12	1:D:293:ILE:HD11	2.03	0.40
1:G:150:LYS:O	1:G:154:ARG:HB2	2.21	0.40
1:H:117:HIS:HE1	1:H:174:ASN:O	2.05	0.40
1:N:269:ILE:HD11	1:N:312:PHE:CD2	2.57	0.40
1:N:330:LEU:O	1:N:334:ILE:HG12	2.22	0.40
1:P:165:THR:HB	1:P:193:HIS:CE1	3.06	0.40
1:S:163:ASP:HA	1:S:164:PRO:HD2	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	29 66
1	B	219/230 (95%)	209 (95%)	10 (5%)	0	100 100
1	C	219/230 (95%)	210 (96%)	8 (4%)	1 (0%)	29 66
1	D	219/230 (95%)	209 (95%)	10 (5%)	0	100 100
1	E	219/230 (95%)	208 (95%)	11 (5%)	0	100 100
1	F	219/230 (95%)	209 (95%)	10 (5%)	0	100 100
1	G	219/230 (95%)	206 (94%)	13 (6%)	0	100 100
1	H	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	29 66
1	I	219/230 (95%)	212 (97%)	7 (3%)	0	100 100
1	J	219/230 (95%)	208 (95%)	9 (4%)	2 (1%)	17 54
1	K	219/230 (95%)	210 (96%)	8 (4%)	1 (0%)	29 66
1	L	219/230 (95%)	208 (95%)	11 (5%)	0	100 100
1	M	219/230 (95%)	205 (94%)	14 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	29	66
1	O	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	29	66
1	P	219/230 (95%)	212 (97%)	7 (3%)	0	100	100
1	Q	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	R	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
1	S	219/230 (95%)	206 (94%)	12 (6%)	1 (0%)	29	66
1	T	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	a	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	b	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	c	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	d	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	e	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	f	219/230 (95%)	205 (94%)	13 (6%)	1 (0%)	29	66
1	g	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	29	66
1	h	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	i	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	j	219/230 (95%)	206 (94%)	12 (6%)	1 (0%)	29	66
1	k	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	29	66
1	l	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
1	m	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	n	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	o	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	29	66
1	p	219/230 (95%)	208 (95%)	11 (5%)	0	100	100
1	q	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	r	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	s	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	29	66
1	t	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	29	66
All	All	8760/9200 (95%)	8337 (95%)	407 (5%)	16 (0%)	47	78

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	k	135	ARG

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Mol	Chain	Res	Type
1	o	135	ARG
1	s	135	ARG
1	O	215	GLU
1	A	244	ASP
1	H	215	GLU
1	J	215	GLU
1	N	135	ARG
1	C	135	ARG
1	f	172	LYS
1	j	135	ARG
1	S	135	ARG
1	t	299	GLY
1	J	299	GLY
1	g	299	GLY
1	K	299	GLY

5.3.2 Protein sidechains (i)

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	189/196 (96%)	178 (94%)	11 (6%)	20 53
1	B	189/196 (96%)	181 (96%)	8 (4%)	30 63
1	C	189/196 (96%)	173 (92%)	16 (8%)	10 36
1	D	189/196 (96%)	179 (95%)	10 (5%)	22 56
1	E	189/196 (96%)	170 (90%)	19 (10%)	7 27
1	F	189/196 (96%)	174 (92%)	15 (8%)	12 40
1	G	189/196 (96%)	177 (94%)	12 (6%)	18 50
1	H	189/196 (96%)	176 (93%)	13 (7%)	15 46
1	I	189/196 (96%)	182 (96%)	7 (4%)	34 67
1	J	189/196 (96%)	171 (90%)	18 (10%)	8 30
1	K	189/196 (96%)	176 (93%)	13 (7%)	15 46
1	L	189/196 (96%)	177 (94%)	12 (6%)	18 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	189/196 (96%)	179 (95%)	10 (5%)	22	56
1	N	188/196 (96%)	174 (93%)	14 (7%)	13	43
1	O	189/196 (96%)	173 (92%)	16 (8%)	10	36
1	P	189/196 (96%)	181 (96%)	8 (4%)	30	63
1	Q	189/196 (96%)	178 (94%)	11 (6%)	20	53
1	R	189/196 (96%)	179 (95%)	10 (5%)	22	56
1	S	189/196 (96%)	177 (94%)	12 (6%)	18	50
1	T	189/196 (96%)	175 (93%)	14 (7%)	13	43
1	a	189/196 (96%)	177 (94%)	12 (6%)	18	50
1	b	189/196 (96%)	180 (95%)	9 (5%)	25	60
1	c	189/196 (96%)	176 (93%)	13 (7%)	15	46
1	d	189/196 (96%)	178 (94%)	11 (6%)	20	53
1	e	189/196 (96%)	177 (94%)	12 (6%)	18	50
1	f	189/196 (96%)	178 (94%)	11 (6%)	20	53
1	g	189/196 (96%)	178 (94%)	11 (6%)	20	53
1	h	189/196 (96%)	178 (94%)	11 (6%)	20	53
1	i	189/196 (96%)	181 (96%)	8 (4%)	30	63
1	j	189/196 (96%)	180 (95%)	9 (5%)	25	60
1	k	189/196 (96%)	177 (94%)	12 (6%)	18	50
1	l	189/196 (96%)	175 (93%)	14 (7%)	13	43
1	m	189/196 (96%)	182 (96%)	7 (4%)	34	67
1	n	189/196 (96%)	176 (93%)	13 (7%)	15	46
1	o	189/196 (96%)	173 (92%)	16 (8%)	10	36
1	p	189/196 (96%)	175 (93%)	14 (7%)	13	43
1	q	189/196 (96%)	183 (97%)	6 (3%)	39	70
1	r	188/196 (96%)	173 (92%)	15 (8%)	12	40
1	s	189/196 (96%)	176 (93%)	13 (7%)	15	46
1	t	189/196 (96%)	178 (94%)	11 (6%)	20	53
All	All	7558/7840 (96%)	7081 (94%)	477 (6%)	18	50

All (477) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	172	LYS
1	A	200	LYS
1	A	215	GLU
1	A	238	LEU
1	A	245	ASP
1	A	260	SER
1	A	271	GLU
1	A	301	GLU
1	A	325	GLU
1	A	330	LEU
1	a	116	ARG
1	a	132	ARG
1	a	134	LEU
1	a	166	ARG
1	a	215	GLU
1	a	237	ARG
1	a	245	ASP
1	a	289	THR
1	a	293	ILE
1	a	311	SER
1	a	325	GLU
1	a	332	ASN
1	B	166	ARG
1	B	172	LYS
1	B	206	ARG
1	B	215	GLU
1	B	245	ASP
1	B	256	LEU
1	B	293	ILE
1	B	330	LEU
1	b	116	ARG
1	b	150	LYS
1	b	166	ARG
1	b	241	ARG
1	b	265	VAL
1	b	273	SER
1	b	293	ILE
1	b	308	ARG
1	b	330	LEU
1	C	116	ARG
1	C	132	ARG
1	C	166	ARG

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Mol	Chain	Res	Type
1	C	218	GLU
1	C	241	ARG
1	C	245	ASP
1	C	264	MET
1	C	265	VAL
1	C	273	SER
1	C	279	SER
1	C	289	THR
1	C	293	ILE
1	C	298	ARG
1	C	311	SER
1	C	325	GLU
1	C	330	LEU
1	c	116	ARG
1	c	134	LEU
1	c	172	LYS
1	c	200	LYS
1	c	215	GLU
1	c	241	ARG
1	c	255	VAL
1	c	256	LEU
1	c	273	SER
1	c	300	ASP
1	c	301	GLU
1	c	311	SER
1	c	330	LEU
1	D	116	ARG
1	D	175	VAL
1	D	176	ARG
1	D	238	LEU
1	D	241	ARG
1	D	245	ASP
1	D	265	VAL
1	D	298	ARG
1	D	325	GLU
1	D	330	LEU
1	d	116	ARG
1	d	128	LEU
1	d	176	ARG
1	d	237	ARG
1	d	238	LEU
1	d	245	ASP

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Mol	Chain	Res	Type
1	d	265	VAL
1	d	273	SER
1	d	298	ARG
1	d	325	GLU
1	d	330	LEU
1	E	116	ARG
1	E	166	ARG
1	E	171	GLU
1	E	172	LYS
1	E	206	ARG
1	E	215	GLU
1	E	218	GLU
1	E	241	ARG
1	E	245	ASP
1	E	263	ARG
1	E	264	MET
1	E	273	SER
1	E	274	LYS
1	E	289	THR
1	E	293	ILE
1	E	298	ARG
1	E	300	ASP
1	E	325	GLU
1	E	330	LEU
1	e	116	ARG
1	e	166	ARG
1	e	206	ARG
1	e	215	GLU
1	e	238	LEU
1	e	243	ILE
1	e	245	ASP
1	e	258	GLU
1	e	293	ILE
1	e	311	SER
1	e	325	GLU
1	e	330	LEU
1	F	116	ARG
1	F	135	ARG
1	F	171	GLU
1	F	175	VAL
1	F	176	ARG
1	F	232	PHE

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Mol	Chain	Res	Type
1	F	238	LEU
1	F	241	ARG
1	F	245	ASP
1	F	262	ARG
1	F	273	SER
1	F	293	ILE
1	F	311	SER
1	F	325	GLU
1	F	330	LEU
1	f	116	ARG
1	f	132	ARG
1	f	166	ARG
1	f	175	VAL
1	f	200	LYS
1	f	222	MET
1	f	238	LEU
1	f	241	ARG
1	f	245	ASP
1	f	325	GLU
1	f	330	LEU
1	G	116	ARG
1	G	135	ARG
1	G	138	GLU
1	G	171	GLU
1	G	241	ARG
1	G	245	ASP
1	G	293	ILE
1	G	298	ARG
1	G	301	GLU
1	G	311	SER
1	G	325	GLU
1	G	330	LEU
1	g	133	GLU
1	g	172	LYS
1	g	241	ARG
1	g	273	SER
1	g	289	THR
1	g	298	ARG
1	g	300	ASP
1	g	301	GLU
1	g	308	ARG
1	g	325	GLU

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Mol	Chain	Res	Type
1	g	332	ASN
1	H	146	GLU
1	H	175	VAL
1	H	183	VAL
1	H	229	ILE
1	H	241	ARG
1	H	262	ARG
1	H	279	SER
1	H	293	ILE
1	H	304	ILE
1	H	309	ASP
1	H	311	SER
1	H	325	GLU
1	H	330	LEU
1	h	116	ARG
1	h	128	LEU
1	h	137	SER
1	h	175	VAL
1	h	256	LEU
1	h	274	LYS
1	h	275	LEU
1	h	293	ILE
1	h	304	ILE
1	h	311	SER
1	h	330	LEU
1	I	116	ARG
1	I	175	VAL
1	I	200	LYS
1	I	238	LEU
1	I	293	ILE
1	I	311	SER
1	I	330	LEU
1	i	116	ARG
1	i	176	ARG
1	i	215	GLU
1	i	238	LEU
1	i	245	ASP
1	i	273	SER
1	i	311	SER
1	i	330	LEU
1	J	138	GLU
1	J	150	LYS

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Mol	Chain	Res	Type
1	J	166	ARG
1	J	172	LYS
1	J	176	ARG
1	J	213	ARG
1	J	241	ARG
1	J	256	LEU
1	J	258	GLU
1	J	273	SER
1	J	276	GLU
1	J	293	ILE
1	J	300	ASP
1	J	309	ASP
1	J	311	SER
1	J	325	GLU
1	J	330	LEU
1	J	334	ILE
1	j	135	ARG
1	j	137	SER
1	j	172	LYS
1	j	176	ARG
1	j	215	GLU
1	j	241	ARG
1	j	273	SER
1	j	293	ILE
1	j	330	LEU
1	K	116	ARG
1	K	151	LYS
1	K	154	ARG
1	K	166	ARG
1	K	172	LYS
1	K	175	VAL
1	K	245	ASP
1	K	293	ILE
1	K	298	ARG
1	K	300	ASP
1	K	325	GLU
1	K	330	LEU
1	K	332	ASN
1	k	116	ARG
1	k	175	VAL
1	k	215	GLU
1	k	245	ASP

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Mol	Chain	Res	Type
1	k	256	LEU
1	k	273	SER
1	k	293	ILE
1	k	298	ARG
1	k	300	ASP
1	k	311	SER
1	k	324	PRO
1	k	330	LEU
1	L	116	ARG
1	L	135	ARG
1	L	172	LYS
1	L	175	VAL
1	L	215	GLU
1	L	238	LEU
1	L	241	ARG
1	L	245	ASP
1	L	289	THR
1	L	293	ILE
1	L	325	GLU
1	L	330	LEU
1	l	116	ARG
1	l	150	LYS
1	l	154	ARG
1	l	175	VAL
1	l	230	SER
1	l	238	LEU
1	l	241	ARG
1	l	245	ASP
1	l	265	VAL
1	l	289	THR
1	l	303	ILE
1	l	311	SER
1	l	325	GLU
1	l	330	LEU
1	M	128	LEU
1	M	166	ARG
1	M	179	ARG
1	M	204	SER
1	M	206	ARG
1	M	215	GLU
1	M	263	ARG
1	M	293	ILE

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Mol	Chain	Res	Type
1	M	325	GLU
1	M	330	LEU
1	m	206	ARG
1	m	215	GLU
1	m	273	SER
1	m	308	ARG
1	m	311	SER
1	m	325	GLU
1	m	330	LEU
1	N	116	ARG
1	N	147	ASN
1	N	163	ASP
1	N	166	ARG
1	N	172	LYS
1	N	204	SER
1	N	213	ARG
1	N	215	GLU
1	N	245	ASP
1	N	281	LEU
1	N	293	ILE
1	N	311	SER
1	N	325	GLU
1	N	330	LEU
1	n	116	ARG
1	n	135	ARG
1	n	172	LYS
1	n	200	LYS
1	n	204	SER
1	n	206	ARG
1	n	215	GLU
1	n	230	SER
1	n	245	ASP
1	n	289	THR
1	n	309	ASP
1	n	311	SER
1	n	330	LEU
1	O	116	ARG
1	O	128	LEU
1	O	131	LEU
1	O	135	ARG
1	O	142	LEU
1	O	175	VAL

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Mol	Chain	Res	Type
1	O	176	ARG
1	O	215	GLU
1	O	230	SER
1	O	232	PHE
1	O	238	LEU
1	O	240	SER
1	O	265	VAL
1	O	273	SER
1	O	325	GLU
1	O	330	LEU
1	o	116	ARG
1	o	132	ARG
1	o	135	ARG
1	o	154	ARG
1	o	175	VAL
1	o	206	ARG
1	o	222	MET
1	o	238	LEU
1	o	241	ARG
1	o	245	ASP
1	o	258	GLU
1	o	269	ILE
1	o	289	THR
1	o	311	SER
1	o	325	GLU
1	o	330	LEU
1	P	206	ARG
1	P	230	SER
1	P	245	ASP
1	P	279	SER
1	P	298	ARG
1	P	300	ASP
1	P	311	SER
1	P	330	LEU
1	p	116	ARG
1	p	132	ARG
1	p	206	ARG
1	p	215	GLU
1	p	238	LEU
1	p	245	ASP
1	p	265	VAL
1	p	279	SER

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Mol	Chain	Res	Type
1	p	289	THR
1	p	293	ILE
1	p	325	GLU
1	p	330	LEU
1	p	332	ASN
1	p	334	ILE
1	Q	135	ARG
1	Q	176	ARG
1	Q	245	ASP
1	Q	273	SER
1	Q	279	SER
1	Q	282	ASP
1	Q	293	ILE
1	Q	298	ARG
1	Q	325	GLU
1	Q	329	ARG
1	Q	330	LEU
1	q	131	LEU
1	q	135	ARG
1	q	172	LYS
1	q	215	GLU
1	q	273	SER
1	q	330	LEU
1	R	163	ASP
1	R	172	LYS
1	R	241	ARG
1	R	260	SER
1	R	262	ARG
1	R	293	ILE
1	R	303	ILE
1	R	311	SER
1	R	325	GLU
1	R	330	LEU
1	r	155	SER
1	r	168	SER
1	r	175	VAL
1	r	200	LYS
1	r	204	SER
1	r	206	ARG
1	r	213	ARG
1	r	215	GLU
1	r	267	VAL

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Mol	Chain	Res	Type
1	r	293	ILE
1	r	298	ARG
1	r	309	ASP
1	r	311	SER
1	r	325	GLU
1	r	330	LEU
1	S	116	ARG
1	S	147	ASN
1	S	172	LYS
1	S	175	VAL
1	S	215	GLU
1	S	238	LEU
1	S	265	VAL
1	S	273	SER
1	S	289	THR
1	S	325	GLU
1	S	330	LEU
1	S	331	LYS
1	s	116	ARG
1	s	133	GLU
1	s	153	LEU
1	s	160	VAL
1	s	175	VAL
1	s	238	LEU
1	s	241	ARG
1	s	265	VAL
1	s	270	PRO
1	s	279	SER
1	s	311	SER
1	s	325	GLU
1	s	330	LEU
1	T	149	ARG
1	T	166	ARG
1	T	206	ARG
1	T	213	ARG
1	T	215	GLU
1	T	232	PHE
1	T	241	ARG
1	T	245	ASP
1	T	263	ARG
1	T	298	ARG
1	T	300	ASP

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Mol	Chain	Res	Type
1	T	311	SER
1	T	325	GLU
1	T	330	LEU
1	t	116	ARG
1	t	172	LYS
1	t	182	ILE
1	t	222	MET
1	t	245	ASP
1	t	293	ILE
1	t	298	ARG
1	t	311	SER
1	t	325	GLU
1	t	330	LEU
1	t	334	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	147	ASN
1	A	286	HIS
1	a	253	GLN
1	B	117	HIS
1	b	117	HIS
1	b	253	GLN
1	C	219	GLN
1	C	253	GLN
1	c	117	HIS
1	c	286	HIS
1	E	117	HIS
1	E	147	ASN
1	E	286	HIS
1	e	117	HIS
1	e	147	ASN
1	F	147	ASN
1	F	253	GLN
1	f	117	HIS
1	f	253	GLN
1	G	286	HIS
1	g	253	GLN
1	g	332	ASN
1	H	117	HIS

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Mol	Chain	Res	Type
1	H	161	HIS
1	H	253	GLN
1	h	253	GLN
1	h	286	HIS
1	I	117	HIS
1	I	147	ASN
1	I	286	HIS
1	i	253	GLN
1	J	117	HIS
1	J	216	ASN
1	J	253	GLN
1	J	286	HIS
1	j	253	GLN
1	K	286	HIS
1	k	147	ASN
1	L	117	HIS
1	l	117	HIS
1	M	253	GLN
1	M	286	HIS
1	m	174	ASN
1	m	253	GLN
1	N	147	ASN
1	n	286	HIS
1	O	147	ASN
1	O	253	GLN
1	o	117	HIS
1	o	253	GLN
1	P	117	HIS
1	P	253	GLN
1	p	147	ASN
1	p	253	GLN
1	p	286	HIS
1	Q	147	ASN
1	q	117	HIS
1	q	147	ASN
1	q	253	GLN
1	r	147	ASN
1	r	253	GLN
1	r	286	HIS
1	S	147	ASN
1	T	117	HIS
1	t	286	HIS

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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	221/230 (96%)	-0.01	5 (2%)	60	46	36, 70, 112, 146	0
1	B	221/230 (96%)	-0.02	3 (1%)	75	63	53, 90, 142, 153	0
1	C	221/230 (96%)	-0.09	3 (1%)	75	63	49, 71, 105, 156	0
1	D	221/230 (96%)	-0.19	1 (0%)	91	86	36, 61, 89, 111	0
1	E	221/230 (96%)	0.01	3 (1%)	75	63	38, 68, 110, 128	0
1	F	221/230 (96%)	-0.12	1 (0%)	91	86	34, 61, 93, 125	0
1	G	221/230 (96%)	0.02	3 (1%)	75	63	42, 76, 120, 151	0
1	H	221/230 (96%)	-0.06	3 (1%)	75	63	48, 79, 114, 152	0
1	I	221/230 (96%)	-0.06	0	100	100	44, 76, 122, 144	0
1	J	221/230 (96%)	0.06	1 (0%)	91	86	51, 79, 118, 138	0
1	K	221/230 (96%)	-0.03	3 (1%)	75	63	43, 71, 113, 133	0
1	L	221/230 (96%)	-0.18	1 (0%)	91	86	33, 62, 90, 121	0
1	M	221/230 (96%)	0.04	3 (1%)	75	63	63, 92, 126, 149	0
1	N	221/230 (96%)	0.06	4 (1%)	68	55	53, 76, 113, 138	0
1	O	221/230 (96%)	-0.12	2 (0%)	84	75	39, 59, 89, 133	0
1	P	221/230 (96%)	0.02	6 (2%)	54	39	46, 81, 130, 161	0
1	Q	221/230 (96%)	0.53	22 (9%)	7	4	78, 115, 147, 161	0
1	R	221/230 (96%)	0.24	6 (2%)	54	39	64, 87, 118, 146	0
1	S	221/230 (96%)	-0.16	1 (0%)	91	86	45, 65, 98, 137	0
1	T	221/230 (96%)	-0.03	3 (1%)	75	63	50, 87, 133, 172	0
1	a	221/230 (96%)	-0.05	1 (0%)	91	86	47, 70, 106, 138	0
1	b	221/230 (96%)	0.08	4 (1%)	68	55	56, 92, 127, 147	0
1	c	221/230 (96%)	-0.07	2 (0%)	84	75	36, 72, 114, 130	0
1	d	221/230 (96%)	-0.14	2 (0%)	84	75	33, 57, 85, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	e	221/230 (96%)	-0.04	3 (1%) 75 63	38, 71, 118, 139	0
1	f	221/230 (96%)	-0.24	1 (0%) 91 86	35, 59, 90, 114	0
1	g	221/230 (96%)	0.07	8 (3%) 42 27	47, 71, 102, 138	0
1	h	221/230 (96%)	0.08	8 (3%) 42 27	48, 84, 115, 145	0
1	i	221/230 (96%)	-0.04	4 (1%) 68 55	50, 76, 114, 140	0
1	j	221/230 (96%)	0.03	2 (0%) 84 75	48, 85, 118, 147	0
1	k	221/230 (96%)	-0.11	3 (1%) 75 63	39, 72, 118, 148	0
1	l	221/230 (96%)	-0.16	0 100 100	37, 61, 89, 113	0
1	m	221/230 (96%)	0.21	4 (1%) 68 55	63, 99, 129, 150	0
1	n	221/230 (96%)	-0.05	2 (0%) 84 75	42, 77, 120, 136	0
1	o	221/230 (96%)	-0.21	0 100 100	40, 58, 84, 105	0
1	p	221/230 (96%)	0.07	3 (1%) 75 63	57, 84, 114, 144	0
1	q	221/230 (96%)	0.51	20 (9%) 9 5	71, 117, 152, 170	0
1	r	221/230 (96%)	0.14	6 (2%) 54 39	51, 82, 120, 149	0
1	s	221/230 (96%)	-0.20	1 (0%) 91 86	46, 62, 92, 109	0
1	t	221/230 (96%)	0.18	6 (2%) 54 39	62, 88, 119, 138	0
All	All	8840/9200 (96%)	-0.00	154 (1%) 70 57	33, 76, 124, 172	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	GLY	6.1
1	r	336	ALA	5.3
1	g	312	PHE	4.8
1	r	158	ASN	4.7
1	H	136	GLY	4.2
1	d	136	GLY	4.1
1	E	136	GLY	3.9
1	T	336	ALA	3.9
1	q	312	PHE	3.9
1	a	136	GLY	3.9
1	h	136	GLY	3.9
1	e	314	ALA	3.8
1	R	136	GLY	3.8
1	S	136	GLY	3.8
1	m	136	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	T	243	ILE	3.6
1	p	136	GLY	3.6
1	k	336	ALA	3.6
1	j	271	GLU	3.6
1	E	135	ARG	3.5
1	m	271	GLU	3.5
1	q	314	ALA	3.5
1	Q	180	ALA	3.4
1	Q	118	VAL	3.4
1	g	136	GLY	3.4
1	O	135	ARG	3.4
1	M	314	ALA	3.4
1	N	136	GLY	3.3
1	b	136	GLY	3.3
1	R	122	GLY	3.3
1	r	135	ARG	3.3
1	Q	272	GLY	3.2
1	Q	322	GLY	3.2
1	G	336	ALA	3.1
1	N	135	ARG	3.1
1	m	312	PHE	3.1
1	A	314	ALA	3.1
1	h	226	ASP	3.0
1	q	136	GLY	3.0
1	d	135	ARG	3.0
1	G	314	ALA	3.0
1	H	135	ARG	2.9
1	E	137	SER	2.9
1	F	136	GLY	2.9
1	A	312	PHE	2.9
1	Q	269	ILE	2.9
1	Q	273	SER	2.8
1	g	144	GLU	2.8
1	Q	331	LYS	2.8
1	c	331	LYS	2.8
1	H	137	SER	2.8
1	b	138	GLU	2.7
1	P	136	GLY	2.7
1	q	118	VAL	2.7
1	g	275	LEU	2.7
1	K	271	GLU	2.7
1	Q	271	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	q	138	GLU	2.7
1	P	314	ALA	2.7
1	p	135	ARG	2.6
1	q	313	ARG	2.6
1	k	244	ASP	2.6
1	Q	333	TYR	2.6
1	J	135	ARG	2.6
1	N	137	SER	2.6
1	i	275	LEU	2.6
1	Q	270	PRO	2.6
1	e	318	ILE	2.6
1	q	271	GLU	2.6
1	t	135	ARG	2.6
1	b	158	ASN	2.6
1	Q	157	ALA	2.5
1	Q	138	GLU	2.5
1	t	136	GLY	2.5
1	R	135	ARG	2.5
1	B	136	GLY	2.5
1	g	278	VAL	2.5
1	L	136	GLY	2.5
1	t	138	GLU	2.5
1	Q	274	LYS	2.5
1	i	176	ARG	2.4
1	O	136	GLY	2.4
1	Q	335	SER	2.4
1	B	272	GLY	2.4
1	p	272	GLY	2.4
1	C	135	ARG	2.4
1	c	312	PHE	2.3
1	Q	300	ASP	2.3
1	A	318	ILE	2.3
1	K	136	GLY	2.3
1	t	175	VAL	2.3
1	q	307	PRO	2.3
1	j	136	GLY	2.3
1	q	300	ASP	2.3
1	Q	275	LEU	2.3
1	G	136	GLY	2.3
1	M	136	GLY	2.3
1	T	271	GLU	2.3
1	Q	268	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	271	GLU	2.3
1	R	277	GLY	2.3
1	e	336	ALA	2.3
1	q	306	PRO	2.3
1	A	275	LEU	2.3
1	q	137	SER	2.3
1	b	272	GLY	2.3
1	i	136	GLY	2.3
1	t	158	ASN	2.3
1	h	135	ARG	2.3
1	q	270	PRO	2.3
1	q	269	ILE	2.2
1	A	288	VAL	2.2
1	M	271	GLU	2.2
1	q	332	ASN	2.2
1	q	299	GLY	2.2
1	Q	291	VAL	2.2
1	C	138	GLU	2.2
1	R	225	ALA	2.2
1	r	269	ILE	2.2
1	f	135	ARG	2.2
1	h	303	ILE	2.2
1	q	280	VAL	2.2
1	h	134	LEU	2.1
1	g	311	SER	2.1
1	P	276	GLU	2.1
1	q	288	VAL	2.1
1	r	118	VAL	2.1
1	Q	321	ILE	2.1
1	g	272	GLY	2.1
1	Q	136	GLY	2.1
1	q	268	PRO	2.1
1	r	243	ILE	2.1
1	t	227	GLN	2.1
1	B	312	PHE	2.1
1	D	271	GLU	2.1
1	n	139	VAL	2.1
1	h	137	SER	2.1
1	n	333	TYR	2.1
1	s	137	SER	2.1
1	R	207	ILE	2.1
1	Q	314	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	h	158	ASN	2.1
1	N	270	PRO	2.1
1	Q	181	VAL	2.1
1	P	135	ARG	2.1
1	P	336	ALA	2.1
1	g	162	GLY	2.1
1	h	271	GLU	2.0
1	i	171	GLU	2.0
1	m	278	VAL	2.0
1	k	136	GLY	2.0
1	K	245	ASP	2.0
1	q	309	ASP	2.0
1	q	336	ALA	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.