Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 12:26 pm GMT

PDB ID	:	9HQC
EMDB ID	:	EMD-52341
Title	:	Partial (54mer) encapsulin shell assembly from Mycobacterium tuberculosis
Authors	:	Lewis, C.J.; Berger, C.; Ravelli, R.B.G.
Deposited on	:	2024-12-16
Resolution	:	4.57 Å(reported)
Based on initial model	:	7P1T

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

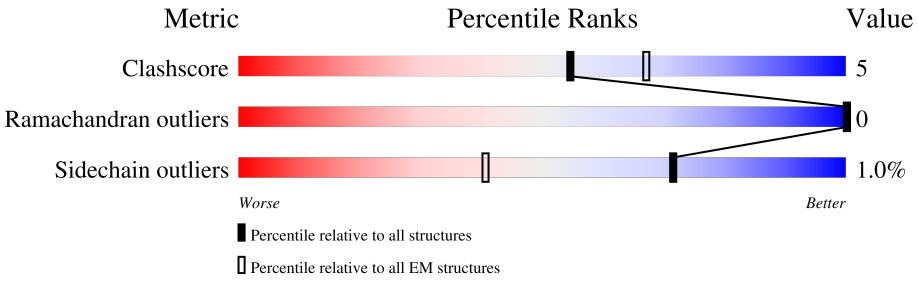
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.57 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	265	94% 6%
1	AB	265	92% 8%
1	BA	265	95% 5%
1	BB	265	94% 6%
1	C	265	91% 8%
1	CA	265	92% 8%
1	D	265	94% 6%
1	DA	265	91% 9%
1	DB	265	93% 7%

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Mol	Chain	Length	Quality of chain
1	E	265	92% 8%
1	EA	265	92% 8%
1	F	265	92% 8%
1	FA	265	92% 8%
1	FB	265	88% 12%
1	G	265	94% 6%
1	GA	265	92% 8%
1	GB	265	93% 7%
1	H	265	91% 8%
1	HA	265	94% 6%
1	HB	265	92% 8%
1	I	265	94% 6%
1	IA	265	92% 8%
1	JA	265	90% 10%
1	K	265	95% 5%
1	KA	265	94% 6%
1	L	265	92% 8%
1	LA	265	94% 6%
1	M	265	94% 6%
1	MA	265	95%
1	N	265	91% 9%
1	NA	265	92% 8%
1	O	265	91% 9%
1	OA	265	94% 6%
1	P	265	94% 6%

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Mol	Chain	Length	Quality of chain
1	PA	265	93% 7%
1	Q	265	92% 8%
1	QA	265	92% 8%
1	R	265	94% 6%
1	RA	265	89% 10%
1	S	265	93% 7%
1	SA	265	92% 8%
1	T	265	90% 9%
1	TA	265	92% 8%
1	U	265	91% 9%
1	UA	265	91% 9%
1	V	265	91% 9%
1	VA	265	94% 6%
1	W	265	93% 7%
1	WA	265	91% 8%
1	X	265	96%
1	XA	265	94% 5%
1	YA	265	89% 10%
1	Z	265	94% 5%
1	ZA	265	94% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 109836 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Type 1 encapsulin shell protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	C	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	D	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	E	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	F	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	G	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	H	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	I	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	K	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	L	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	M	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	N	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	O	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	P	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	Q	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	R	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	S	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	U	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	V	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	W	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	X	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	Z	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	BA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	CA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	DA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	EA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	FA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	GA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	HA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	IA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	JA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	KA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	LA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	MA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	NA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	OA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	PA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		

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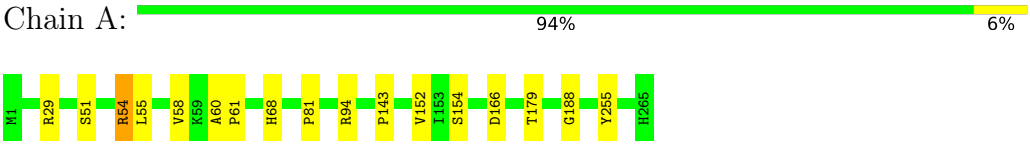
Mol	Chain	Residues	Atoms					AltConf	Trace
1	QA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	RA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	SA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	TA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	UA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	VA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	WA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	XA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	YA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	ZA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	BB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	DB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	FB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	GB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	HB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

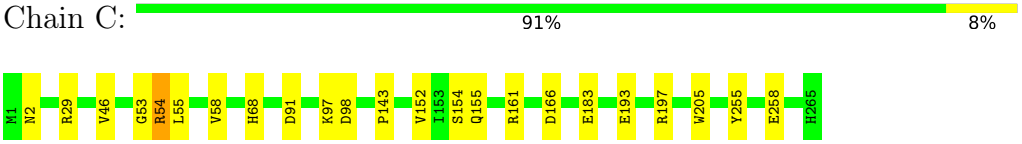
• Molecule 1: Type 1 encapsulin shell protein

Chain A:



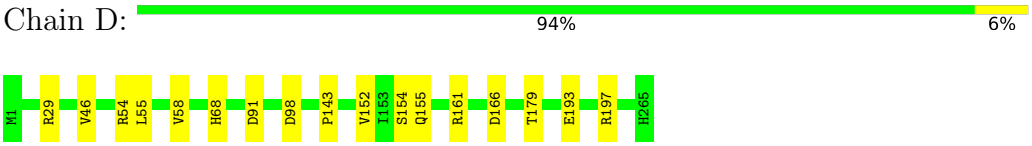
• Molecule 1: Type 1 encapsulin shell protein

Chain C:



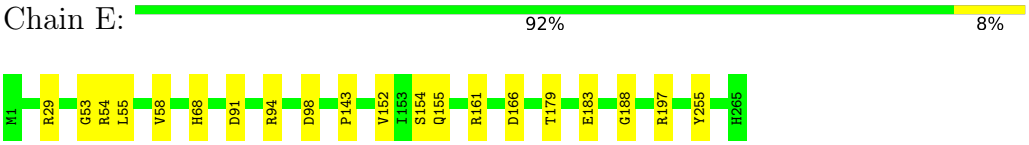
• Molecule 1: Type 1 encapsulin shell protein

Chain D:



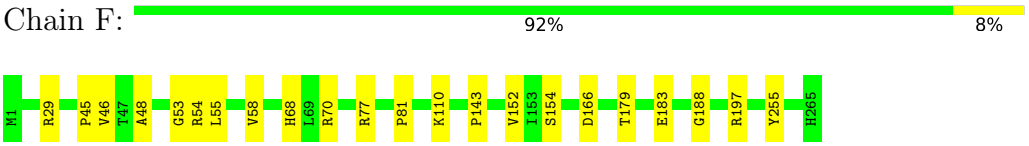
• Molecule 1: Type 1 encapsulin shell protein

Chain E:



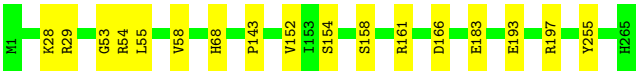
• Molecule 1: Type 1 encapsulin shell protein

Chain F:



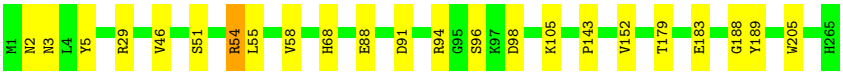
• Molecule 1: Type 1 encapsulin shell protein

Chain G:



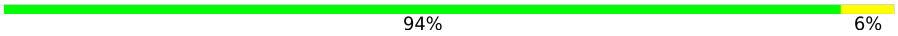
• Molecule 1: Type 1 encapsulin shell protein

Chain H:



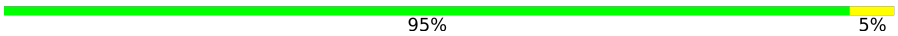
• Molecule 1: Type 1 encapsulin shell protein

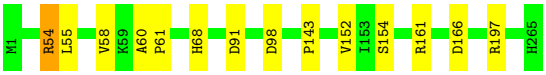
Chain I:



• Molecule 1: Type 1 encapsulin shell protein

Chain K:



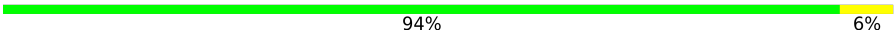


• Molecule 1: Type 1 encapsulin shell protein

Chain L:

• Molecule 1: Type 1 encapsulin shell protein

Chain M:



• Molecule 1: Type 1 encapsulin shell protein

Chain N:

• Molecule 1: Type 1 encapsulin shell protein

Chain O:

• Molecule 1: Type 1 encapsulin shell protein

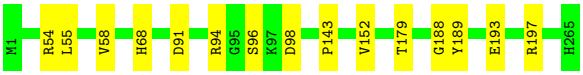
Chain P:

• Molecule 1: Type 1 encapsulin shell protein

Chain Q:

• Molecule 1: Type 1 encapsulin shell protein

Chain R:

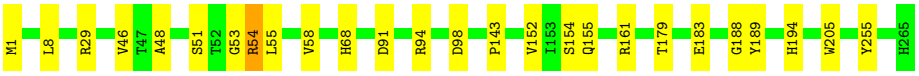


• Molecule 1: Type 1 encapsulin shell protein

Chain S:

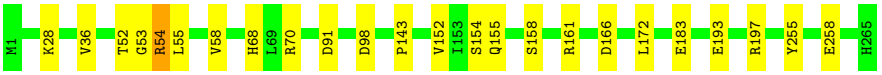
• Molecule 1: Type 1 encapsulin shell protein

Chain T:



• Molecule 1: Type 1 encapsulin shell protein

Chain U:

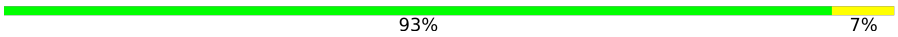


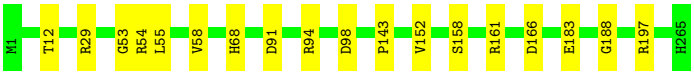
• Molecule 1: Type 1 encapsulin shell protein

Chain V:

• Molecule 1: Type 1 encapsulin shell protein

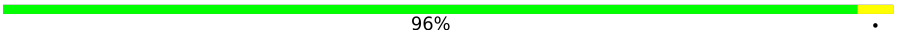
Chain W:





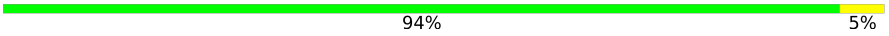
• Molecule 1: Type 1 encapsulin shell protein

Chain X:



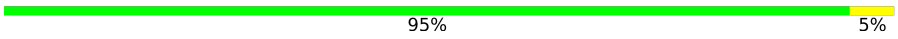
• Molecule 1: Type 1 encapsulin shell protein

Chain Z:



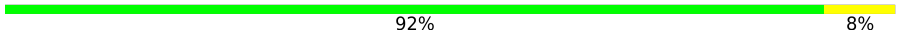
• Molecule 1: Type 1 encapsulin shell protein

Chain BA:



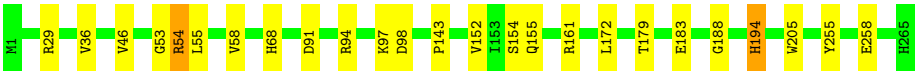
• Molecule 1: Type 1 encapsulin shell protein

Chain CA:



• Molecule 1: Type 1 encapsulin shell protein

Chain DA:

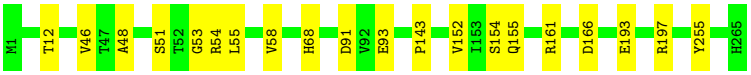


• Molecule 1: Type 1 encapsulin shell protein

Chain EA:

• Molecule 1: Type 1 encapsulin shell protein

Chain FA:

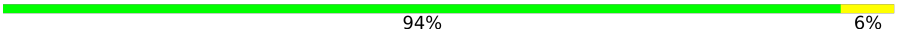


• Molecule 1: Type 1 encapsulin shell protein

Chain GA:

• Molecule 1: Type 1 encapsulin shell protein

Chain HA:

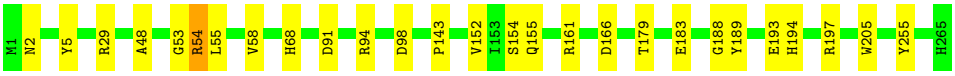


• Molecule 1: Type 1 encapsulin shell protein

Chain IA:

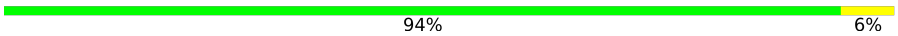
• Molecule 1: Type 1 encapsulin shell protein

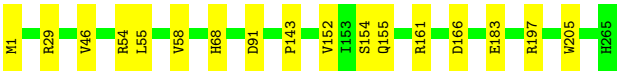
Chain JA:



• Molecule 1: Type 1 encapsulin shell protein

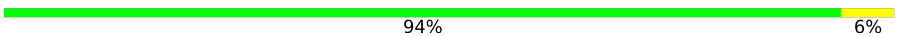
Chain KA:





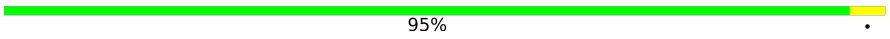
• Molecule 1: Type 1 encapsulin shell protein

Chain LA:



• Molecule 1: Type 1 encapsulin shell protein

Chain MA:

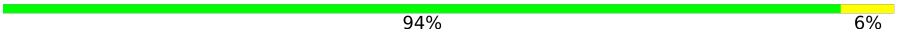


• Molecule 1: Type 1 encapsulin shell protein

Chain NA:

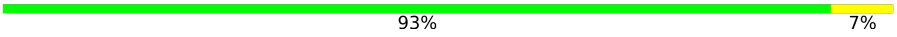
• Molecule 1: Type 1 encapsulin shell protein

Chain OA:



• Molecule 1: Type 1 encapsulin shell protein

Chain PA:

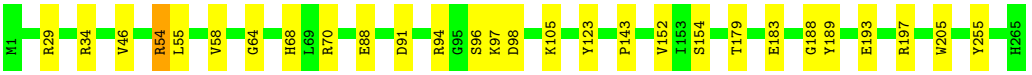


• Molecule 1: Type 1 encapsulin shell protein

Chain QA:

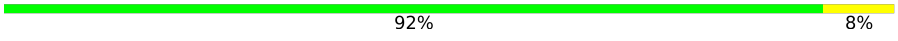
• Molecule 1: Type 1 encapsulin shell protein

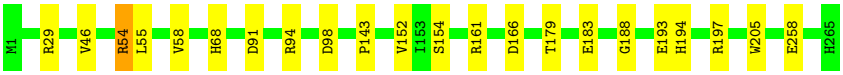
Chain RA:



• Molecule 1: Type 1 encapsulin shell protein

Chain SA:





• Molecule 1: Type 1 encapsulin shell protein

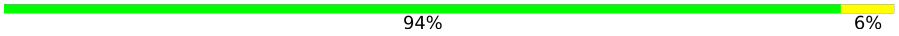
Chain TA:

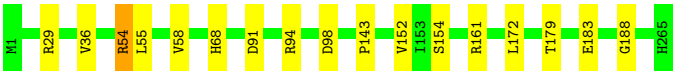
• Molecule 1: Type 1 encapsulin shell protein

Chain UA:

• Molecule 1: Type 1 encapsulin shell protein

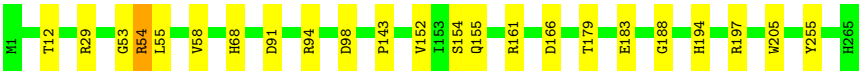
Chain VA:





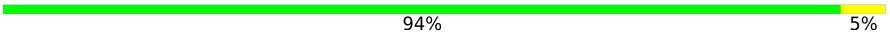
• Molecule 1: Type 1 encapsulin shell protein

Chain WA:



• Molecule 1: Type 1 encapsulin shell protein

Chain XA:

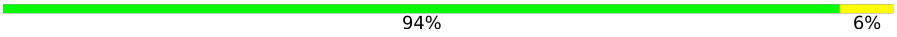


• Molecule 1: Type 1 encapsulin shell protein

Chain YA:

• Molecule 1: Type 1 encapsulin shell protein

Chain ZA:

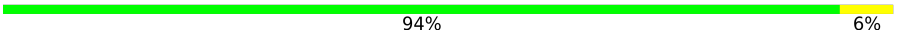


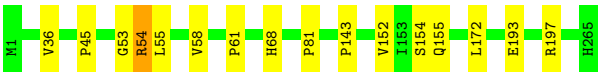
• Molecule 1: Type 1 encapsulin shell protein

Chain AB:

• Molecule 1: Type 1 encapsulin shell protein

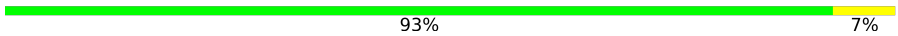
Chain BB:

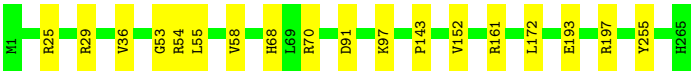




• Molecule 1: Type 1 encapsulin shell protein

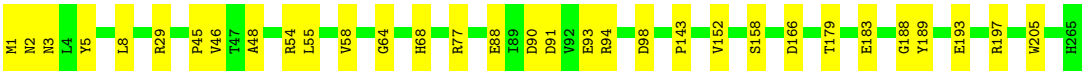
Chain DB:





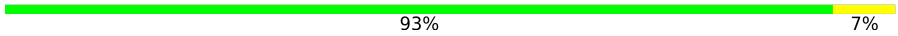
• Molecule 1: Type 1 encapsulin shell protein

Chain FB:



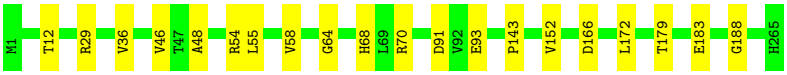
• Molecule 1: Type 1 encapsulin shell protein

Chain GB:



• Molecule 1: Type 1 encapsulin shell protein

Chain HB:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6294	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	163000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

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	0.37	0/2074	0.57	0/2828
1	AB	0.37	0/2074	0.57	0/2828
1	BA	0.37	0/2074	0.57	0/2828
1	BB	0.37	0/2074	0.57	0/2828
1	C	0.37	0/2074	0.57	0/2828
1	CA	0.37	0/2074	0.57	0/2828
1	D	0.37	0/2074	0.57	0/2828
1	DA	0.37	0/2074	0.57	0/2828
1	DB	0.37	0/2074	0.57	0/2828
1	E	0.37	0/2074	0.57	0/2828
1	EA	0.37	0/2074	0.57	0/2828
1	F	0.37	0/2074	0.57	0/2828
1	FA	0.37	0/2074	0.57	0/2828
1	FB	0.37	0/2074	0.57	0/2828
1	G	0.37	0/2074	0.57	0/2828
1	GA	0.37	0/2074	0.56	0/2828
1	GB	0.37	0/2074	0.57	0/2828
1	H	0.37	0/2074	0.57	0/2828
1	HA	0.37	0/2074	0.57	0/2828
1	HB	0.37	0/2074	0.57	0/2828
1	I	0.37	0/2074	0.57	0/2828
1	IA	0.37	0/2074	0.57	0/2828
1	JA	0.37	0/2074	0.57	0/2828
1	K	0.37	0/2074	0.57	0/2828
1	KA	0.37	0/2074	0.57	0/2828
1	L	0.37	0/2074	0.57	0/2828
1	LA	0.37	0/2074	0.57	0/2828
1	M	0.37	0/2074	0.57	0/2828
1	MA	0.37	0/2074	0.57	0/2828
1	N	0.37	0/2074	0.56	0/2828
1	NA	0.37	0/2074	0.57	0/2828
1	O	0.37	0/2074	0.57	0/2828
1	OA	0.37	0/2074	0.57	0/2828
1	P	0.37	0/2074	0.57	0/2828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	PA	0.37	0/2074	0.57	0/2828
1	Q	0.37	0/2074	0.57	0/2828
1	QA	0.37	0/2074	0.57	0/2828
1	R	0.37	0/2074	0.57	0/2828
1	RA	0.37	0/2074	0.57	0/2828
1	S	0.37	0/2074	0.57	0/2828
1	SA	0.37	0/2074	0.57	0/2828
1	T	0.37	0/2074	0.57	0/2828
1	TA	0.37	0/2074	0.57	0/2828
1	U	0.37	0/2074	0.57	0/2828
1	UA	0.37	0/2074	0.56	0/2828
1	V	0.37	0/2074	0.57	0/2828
1	VA	0.37	0/2074	0.56	0/2828
1	W	0.37	0/2074	0.57	0/2828
1	WA	0.37	0/2074	0.57	0/2828
1	X	0.37	0/2074	0.57	0/2828
1	XA	0.37	0/2074	0.57	0/2828
1	YA	0.37	0/2074	0.57	0/2828
1	Z	0.37	0/2074	0.57	0/2828
1	ZA	0.37	0/2074	0.57	0/2828
All	All	0.37	0/111996	0.57	0/152712

There are no bond length outliers.

There are no bond angle outliers.

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	2034	0	2011	45	0
1	AB	2034	0	2013	56	0
1	BA	2034	0	2013	20	0
1	BB	2034	0	2013	12	0
1	C	2034	0	2013	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	2034	0	2013	31	0
1	D	2034	0	2013	31	0
1	DA	2034	0	2013	43	0
1	DB	2034	0	2012	47	0
1	E	2034	0	2013	40	0
1	EA	2034	0	2013	31	0
1	F	2034	0	2011	64	0
1	FA	2034	0	2013	21	0
1	FB	2034	0	2013	72	0
1	G	2034	0	2013	19	0
1	GA	2034	0	2012	57	0
1	GB	2034	0	2013	25	0
1	H	2034	0	2012	60	0
1	HA	2034	0	2013	34	0
1	HB	2034	0	2013	37	0
1	I	2034	0	2013	26	0
1	IA	2034	0	2013	23	0
1	JA	2034	0	2013	65	0
1	K	2034	0	2013	21	0
1	KA	2034	0	2013	20	0
1	L	2034	0	2013	41	0
1	LA	2034	0	2013	20	0
1	M	2034	0	2013	22	0
1	MA	2034	0	2013	9	0
1	N	2034	0	2013	47	0
1	NA	2034	0	2012	39	0
1	O	2034	0	2013	48	0
1	OA	2034	0	2013	37	0
1	P	2034	0	2013	20	0
1	PA	2034	0	2013	23	0
1	Q	2034	0	2013	24	0
1	QA	2034	0	2013	49	0
1	R	2034	0	2013	32	0
1	RA	2034	0	2013	46	0
1	S	2034	0	2012	31	0
1	SA	2034	0	2013	42	0
1	T	2034	0	2013	48	0
1	TA	2034	0	2013	42	0
1	U	2034	0	2013	52	0
1	UA	2034	0	2013	41	0
1	V	2034	0	2013	43	0
1	VA	2034	0	2013	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	2034	0	2012	48	0
1	WA	2034	0	2013	55	0
1	X	2034	0	2012	35	0
1	XA	2034	0	2013	15	0
1	YA	2034	0	2012	75	0
1	Z	2034	0	2013	30	0
1	ZA	2034	0	2013	31	0
All	All	109836	0	108690	1080	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 5.

All (1080) 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:F:255:TYR:CD1	1:W:98:ASP:HB3	1.37	1.59
1:F:255:TYR:CD1	1:W:98:ASP:CB	1.88	1.56
1:F:255:TYR:CG	1:W:98:ASP:HB3	1.03	1.54
1:R:188:GLY:CA	1:DB:197:ARG:HH11	1.22	1.51
1:U:166:ASP:HB3	1:AB:29:ARG:CD	1.41	1.48
1:F:255:TYR:CG	1:W:98:ASP:CB	1.95	1.41
1:S:29:ARG:CD	1:NA:166:ASP:HB3	1.46	1.41
1:H:29:ARG:CD	1:YA:166:ASP:HB3	1.51	1.37
1:F:255:TYR:CD1	1:W:98:ASP:CG	1.95	1.36
1:H:188:GLY:O	1:YA:197:ARG:CD	1.75	1.35
1:ZA:197:ARG:CD	1:HB:188:GLY:O	1.77	1.32
1:R:188:GLY:HA3	1:DB:197:ARG:NH1	0.99	1.31
1:F:77:ARG:NH1	1:QA:55:LEU:HD11	1.45	1.31
1:R:188:GLY:CA	1:DB:197:ARG:NH1	1.81	1.30
1:F:46:VAL:O	1:QA:51:SER:HB2	1.23	1.30
1:N:197:ARG:HD2	1:TA:188:GLY:O	1.28	1.28
1:Z:94:ARG:O	1:RA:46:VAL:HG12	1.15	1.28
1:E:161:ARG:NH2	1:WA:179:THR:OG1	1.65	1.28
1:S:188:GLY:HA3	1:NA:197:ARG:NH1	1.46	1.28
1:N:197:ARG:CD	1:TA:188:GLY:O	1.80	1.27
1:F:29:ARG:CD	1:HA:166:ASP:HB3	1.64	1.27
1:F:255:TYR:CD1	1:W:98:ASP:OD2	1.87	1.26
1:V:166:ASP:HB3	1:DA:29:ARG:CD	1.63	1.26
1:D:197:ARG:CD	1:OA:188:GLY:O	1.83	1.25
1:ZA:161:ARG:NH2	1:HB:179:THR:OG1	1.67	1.25
1:A:188:GLY:O	1:X:197:ARG:HD3	1.28	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ARG:NH2	1:QA:55:LEU:HD13	1.53	1.24
1:I:46:VAL:HG12	1:YA:94:ARG:O	1.35	1.23
1:E:197:ARG:CD	1:WA:188:GLY:O	1.87	1.22
1:H:188:GLY:O	1:YA:197:ARG:HD2	1.06	1.22
1:GA:94:ARG:O	1:FB:46:VAL:HG12	1.07	1.21
1:R:179:THR:HG23	1:DB:161:ARG:NH2	1.53	1.21
1:N:161:ARG:NH2	1:TA:179:THR:OG1	1.72	1.20
1:ZA:166:ASP:HB3	1:HB:29:ARG:CD	1.73	1.19
1:L:161:ARG:NH2	1:T:179:THR:OG1	1.72	1.19
1:O:166:ASP:HB3	1:RA:29:ARG:CD	1.73	1.18
1:L:166:ASP:HB3	1:T:29:ARG:CD	1.74	1.18
1:F:46:VAL:O	1:QA:51:SER:CB	1.92	1.17
1:X:123:TYR:OH	1:HA:61:PRO:HG3	1.43	1.17
1:A:166:ASP:CB	1:GA:29:ARG:HD3	1.75	1.17
1:E:197:ARG:NH1	1:WA:188:GLY:HA3	1.60	1.17
1:S:188:GLY:C	1:NA:197:ARG:HH11	1.48	1.17
1:ZA:197:ARG:HD2	1:HB:188:GLY:O	1.31	1.17
1:D:197:ARG:NH1	1:OA:188:GLY:HA3	1.61	1.16
1:F:77:ARG:CZ	1:QA:55:LEU:CD1	2.23	1.16
1:GA:94:ARG:O	1:FB:46:VAL:CG1	1.94	1.16
1:U:70:ARG:CZ	1:AB:94:ARG:HD2	1.77	1.15
1:F:255:TYR:CB	1:W:98:ASP:CB	2.25	1.15
1:F:166:ASP:HB3	1:W:29:ARG:CD	1.75	1.15
1:R:179:THR:CG2	1:DB:161:ARG:NH2	2.09	1.14
1:D:197:ARG:HD2	1:OA:188:GLY:O	1.40	1.14
1:D:161:ARG:NH2	1:OA:179:THR:OG1	1.79	1.14
1:F:77:ARG:CZ	1:QA:55:LEU:HD11	1.77	1.13
1:F:255:TYR:HD1	1:W:98:ASP:OD2	1.26	1.13
1:ZA:197:ARG:NH1	1:HB:188:GLY:HA3	1.63	1.13
1:F:29:ARG:HD3	1:HA:166:ASP:HB3	1.29	1.12
1:N:197:ARG:NH1	1:TA:188:GLY:HA3	1.63	1.12
1:A:154:SER:HB2	1:GA:183:GLU:HG2	1.13	1.12
1:S:188:GLY:CA	1:NA:197:ARG:HH11	1.62	1.12
1:S:188:GLY:CA	1:NA:197:ARG:NH1	2.11	1.11
1:X:123:TYR:OH	1:HA:61:PRO:CG	1.98	1.11
1:W:166:ASP:HB3	1:PA:29:ARG:CD	1.80	1.11
1:Z:255:TYR:HB3	1:QA:98:ASP:HB3	1.20	1.11
1:X:123:TYR:CZ	1:HA:61:PRO:HB3	1.84	1.10
1:F:255:TYR:CB	1:W:98:ASP:HB3	1.81	1.10
1:R:179:THR:OG1	1:DB:161:ARG:NE	1.82	1.10
1:F:183:GLU:OE2	1:HA:158:SER:OG	1.70	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:PRO:O	1:QA:70:ARG:NH2	1.83	1.10
1:V:161:ARG:NH2	1:DA:179:THR:OG1	1.84	1.10
1:U:166:ASP:CB	1:AB:29:ARG:CD	2.27	1.09
1:LA:166:ASP:HB3	1:UA:29:ARG:CD	1.80	1.09
1:A:255:TYR:CG	1:GA:98:ASP:HB3	1.88	1.09
1:E:197:ARG:HD2	1:WA:188:GLY:O	1.50	1.09
1:H:188:GLY:HA3	1:YA:197:ARG:NH1	1.67	1.09
1:O:166:ASP:HB3	1:RA:29:ARG:HD2	1.29	1.09
1:GA:10:PRO:HB3	1:FB:8:LEU:CD1	1.81	1.09
1:S:29:ARG:HD3	1:NA:166:ASP:HB3	1.08	1.08
1:T:46:VAL:HG12	1:NA:94:ARG:O	1.53	1.08
1:R:179:THR:OG1	1:DB:161:ARG:CZ	2.01	1.08
1:F:166:ASP:CB	1:W:29:ARG:HD3	1.83	1.07
1:SA:179:THR:OG1	1:UA:161:ARG:NH2	1.87	1.07
1:A:166:ASP:HB3	1:GA:29:ARG:CD	1.85	1.07
1:V:166:ASP:HB3	1:DA:29:ARG:HD3	1.19	1.07
1:Z:255:TYR:CB	1:QA:98:ASP:HB3	1.85	1.07
1:A:188:GLY:O	1:X:197:ARG:CD	2.04	1.06
1:U:166:ASP:HB3	1:AB:29:ARG:HD3	1.35	1.06
1:F:255:TYR:HB3	1:W:98:ASP:CB	1.87	1.05
1:L:166:ASP:HB3	1:T:29:ARG:HD3	1.36	1.05
1:S:29:ARG:HD2	1:NA:166:ASP:HB3	1.32	1.04
1:U:166:ASP:CB	1:AB:29:ARG:HD2	1.88	1.04
1:N:166:ASP:HB3	1:TA:29:ARG:CD	1.87	1.03
1:S:29:ARG:HD3	1:NA:166:ASP:CB	1.87	1.03
1:JA:255:TYR:CD1	1:FB:98:ASP:HB3	1.92	1.03
1:O:53:GLY:O	1:RA:91:ASP:OD1	1.77	1.03
1:U:91:ASP:OD2	1:RA:54:ARG:NH1	1.91	1.03
1:EA:161:ARG:NH2	1:VA:179:THR:OG1	1.90	1.02
1:H:183:GLU:HG2	1:YA:154:SER:OG	1.59	1.02
1:JA:183:GLU:HG2	1:WA:154:SER:OG	1.58	1.02
1:ZA:197:ARG:HD3	1:HB:188:GLY:O	1.58	1.02
1:E:154:SER:OG	1:WA:183:GLU:HG2	1.59	1.01
1:Z:255:TYR:HB3	1:QA:98:ASP:CB	1.91	1.01
1:H:29:ARG:HD2	1:YA:166:ASP:HB3	1.04	1.01
1:SA:183:GLU:HG2	1:UA:154:SER:OG	1.60	1.01
1:LA:161:ARG:NH2	1:UA:179:THR:OG1	1.94	1.00
1:LA:166:ASP:HB3	1:UA:29:ARG:HD3	1.43	1.00
1:PA:166:ASP:HB3	1:XA:29:ARG:HD3	1.39	1.00
1:GA:12:THR:HB	1:FB:1:MET:O	1.61	0.99
1:H:29:ARG:CD	1:YA:166:ASP:CB	2.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:179:THR:CG2	1:DB:161:ARG:HH21	1.72	0.99
1:Z:94:ARG:O	1:RA:46:VAL:CG1	2.10	0.99
1:V:166:ASP:CB	1:DA:29:ARG:HD3	1.92	0.99
1:C:46:VAL:HG12	1:QA:94:ARG:O	1.61	0.99
1:EA:166:ASP:HB3	1:VA:29:ARG:CD	1.92	0.99
1:H:183:GLU:OE2	1:YA:155:GLN:HA	1.63	0.99
1:R:179:THR:HG23	1:DB:161:ARG:HH22	1.26	0.98
1:W:166:ASP:HB3	1:PA:29:ARG:HD3	1.45	0.98
1:L:154:SER:OG	1:T:183:GLU:HG2	1.62	0.98
1:N:166:ASP:HB3	1:TA:29:ARG:HD2	1.45	0.98
1:X:61:PRO:HB3	1:HA:123:TYR:CZ	1.98	0.98
1:F:77:ARG:NH2	1:QA:55:LEU:CD1	2.26	0.98
1:E:166:ASP:HB3	1:WA:29:ARG:CD	1.94	0.98
1:S:29:ARG:CD	1:NA:166:ASP:CB	2.40	0.98
1:JA:155:GLN:HA	1:FB:183:GLU:OE2	1.63	0.98
1:ZA:166:ASP:HB3	1:HB:29:ARG:HD2	1.45	0.98
1:V:166:ASP:HB3	1:DA:29:ARG:HD2	1.44	0.98
1:PA:166:ASP:HB3	1:XA:29:ARG:CD	1.92	0.98
1:W:166:ASP:HB3	1:PA:29:ARG:HD2	1.47	0.97
1:U:70:ARG:NH1	1:AB:94:ARG:HD2	1.80	0.97
1:F:77:ARG:CZ	1:QA:55:LEU:HD13	1.93	0.97
1:L:197:ARG:HD2	1:T:188:GLY:O	1.62	0.97
1:L:166:ASP:HB3	1:T:29:ARG:HD2	1.45	0.96
1:S:188:GLY:C	1:NA:197:ARG:NH1	2.19	0.96
1:GA:94:ARG:NH1	1:FB:3:ASN:ND2	2.13	0.96
1:F:29:ARG:HD2	1:HA:166:ASP:HB3	1.46	0.96
1:H:29:ARG:HD3	1:YA:166:ASP:HB3	1.46	0.96
1:EA:166:ASP:HB3	1:VA:29:ARG:HD3	1.47	0.96
1:D:197:ARG:HD3	1:OA:188:GLY:O	1.62	0.96
1:K:161:ARG:NH2	1:BA:179:THR:OG1	1.97	0.96
1:E:197:ARG:NH1	1:WA:188:GLY:CA	2.29	0.96
1:JA:154:SER:OG	1:FB:183:GLU:HG2	1.64	0.96
1:A:188:GLY:HA3	1:X:197:ARG:NH1	1.81	0.95
1:ZA:161:ARG:HH21	1:HB:179:THR:HG1	1.07	0.95
1:R:179:THR:OG1	1:DB:161:ARG:NH2	1.98	0.95
1:H:188:GLY:C	1:YA:197:ARG:HH11	1.69	0.95
1:H:46:VAL:HG12	1:FB:94:ARG:O	1.65	0.95
1:U:166:ASP:CB	1:AB:29:ARG:HD3	1.91	0.95
1:LA:166:ASP:HB3	1:UA:29:ARG:HD2	1.48	0.95
1:S:188:GLY:HA3	1:NA:197:ARG:HH12	1.17	0.95
1:I:255:TYR:CE2	1:DB:97:LYS:HD2	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ARG:NH1	1:QA:55:LEU:CD1	2.28	0.94
1:N:197:ARG:HD3	1:TA:188:GLY:O	1.66	0.94
1:E:166:ASP:HB3	1:WA:29:ARG:HD3	1.48	0.94
1:R:188:GLY:C	1:DB:197:ARG:HH11	1.71	0.93
1:F:255:TYR:HB3	1:W:98:ASP:HB2	1.43	0.93
1:A:154:SER:HB2	1:GA:183:GLU:CG	1.99	0.93
1:F:166:ASP:HB3	1:W:29:ARG:HD3	0.93	0.93
1:F:255:TYR:CE1	1:W:98:ASP:CG	2.42	0.93
1:U:54:ARG:NH1	1:AB:88:GLU:OE1	2.02	0.93
1:U:166:ASP:HB3	1:AB:29:ARG:HD2	0.95	0.92
1:GA:64:GLY:O	1:YA:81:PRO:HD2	1.68	0.92
1:A:166:ASP:HB3	1:GA:29:ARG:HD3	0.92	0.92
1:X:123:TYR:CZ	1:HA:61:PRO:CB	2.52	0.92
1:SA:29:ARG:CD	1:UA:166:ASP:HB3	1.98	0.92
1:E:29:ARG:CD	1:G:166:ASP:HB3	2.00	0.92
1:F:255:TYR:CB	1:W:98:ASP:HB2	1.92	0.92
1:H:188:GLY:CA	1:YA:197:ARG:HH11	1.81	0.92
1:O:166:ASP:HB3	1:RA:29:ARG:HD3	1.49	0.92
1:D:197:ARG:HH11	1:OA:188:GLY:CA	1.83	0.92
1:E:197:ARG:HD3	1:WA:188:GLY:O	1.66	0.92
1:N:197:ARG:HH11	1:TA:188:GLY:CA	1.83	0.92
1:E:179:THR:OG1	1:G:161:ARG:NH2	2.02	0.92
1:JA:94:ARG:O	1:GB:46:VAL:HG12	1.70	0.92
1:ZA:166:ASP:HB3	1:HB:29:ARG:HD3	1.47	0.92
1:ZA:197:ARG:HH11	1:HB:188:GLY:CA	1.83	0.91
1:E:197:ARG:HH11	1:WA:188:GLY:CA	1.83	0.91
1:N:183:GLU:HG2	1:DA:154:SER:OG	1.70	0.91
1:F:255:TYR:CD2	1:W:98:ASP:HB3	2.03	0.91
1:JA:161:ARG:HG2	1:FB:205:TRP:CZ2	2.06	0.91
1:E:29:ARG:HD3	1:G:166:ASP:HB3	1.51	0.91
1:D:154:SER:OG	1:OA:183:GLU:HG2	1.71	0.90
1:ZA:197:ARG:HH11	1:HB:188:GLY:HA3	1.28	0.90
1:U:161:ARG:NH2	1:AB:179:THR:OG1	2.03	0.89
1:F:154:SER:OG	1:W:183:GLU:HG2	1.71	0.89
1:C:154:SER:OG	1:V:183:GLU:HG2	1.73	0.88
1:Z:94:ARG:C	1:RA:46:VAL:HG12	1.93	0.88
1:U:255:TYR:CD1	1:AB:98:ASP:HB3	2.09	0.88
1:F:255:TYR:CE1	1:W:98:ASP:OD2	2.26	0.88
1:K:197:ARG:CD	1:BA:188:GLY:O	2.22	0.88
1:E:197:ARG:HH12	1:WA:188:GLY:HA3	1.31	0.88
1:H:91:ASP:OD1	1:YA:53:GLY:O	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ASP:HB3	1:OA:29:ARG:CD	2.04	0.87
1:C:161:ARG:NH2	1:V:179:THR:OG1	2.08	0.87
1:A:188:GLY:HA3	1:X:197:ARG:HH11	1.39	0.87
1:SA:188:GLY:O	1:UA:197:ARG:HD2	1.75	0.87
1:K:197:ARG:HD2	1:BA:188:GLY:O	1.75	0.86
1:F:48:ALA:HB1	1:QA:72:SER:HB3	1.57	0.86
1:N:154:SER:OG	1:TA:183:GLU:HG2	1.75	0.86
1:X:123:TYR:HH	1:HA:61:PRO:HG3	1.40	0.86
1:GA:10:PRO:HB3	1:FB:8:LEU:HD11	1.56	0.86
1:A:154:SER:CB	1:GA:183:GLU:HG2	2.03	0.86
1:R:188:GLY:HA3	1:DB:197:ARG:HH12	1.05	0.86
1:H:188:GLY:HA3	1:YA:197:ARG:HH11	1.38	0.85
1:X:61:PRO:CB	1:HA:123:TYR:OH	2.24	0.85
1:U:255:TYR:HD1	1:AB:98:ASP:HB3	1.41	0.85
1:X:123:TYR:OH	1:HA:61:PRO:CB	2.24	0.85
1:P:29:ARG:CD	1:CA:166:ASP:HB3	2.05	0.85
1:K:166:ASP:HB3	1:BA:29:ARG:CD	2.06	0.85
1:JA:255:TYR:CG	1:FB:98:ASP:HB3	2.11	0.85
1:V:166:ASP:CB	1:DA:29:ARG:CD	2.51	0.85
1:P:179:THR:OG1	1:CA:161:ARG:NH2	2.10	0.84
1:F:48:ALA:CB	1:QA:72:SER:HB3	2.07	0.84
1:W:12:THR:HG22	1:QA:1:MET:O	1.78	0.84
1:F:70:ARG:HH22	1:W:94:ARG:HD2	1.42	0.83
1:U:70:ARG:NH1	1:AB:94:ARG:CD	2.41	0.83
1:R:91:ASP:OD1	1:DB:53:GLY:O	1.95	0.83
1:Z:161:ARG:NH2	1:QA:179:THR:OG1	2.09	0.83
1:D:197:ARG:NH1	1:OA:188:GLY:CA	2.37	0.83
1:N:197:ARG:HH11	1:TA:188:GLY:HA3	1.35	0.83
1:R:179:THR:CB	1:DB:161:ARG:NH2	2.41	0.83
1:V:53:GLY:O	1:DA:91:ASP:OD1	1.96	0.83
1:SA:29:ARG:HD2	1:UA:166:ASP:HB3	1.61	0.83
1:H:29:ARG:HD3	1:YA:166:ASP:CB	2.05	0.83
1:S:183:GLU:HG2	1:NA:154:SER:OG	1.79	0.83
1:H:183:GLU:CG	1:YA:154:SER:OG	2.26	0.83
1:N:197:ARG:NH1	1:TA:188:GLY:CA	2.40	0.83
1:E:161:ARG:HH21	1:WA:179:THR:HG1	1.22	0.83
1:Z:255:TYR:CG	1:QA:98:ASP:HB3	2.13	0.83
1:H:188:GLY:O	1:YA:197:ARG:HD3	1.79	0.82
1:P:29:ARG:HD2	1:CA:166:ASP:HB3	1.61	0.82
1:ZA:158:SER:OG	1:HB:183:GLU:OE2	1.97	0.82
1:U:197:ARG:HD3	1:AB:189:TYR:CE1	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:255:TYR:CZ	1:DB:97:LYS:HD2	2.14	0.81
1:A:255:TYR:HB3	1:GA:98:ASP:CB	2.09	0.81
1:E:197:ARG:HH11	1:WA:188:GLY:C	1.83	0.81
1:F:53:GLY:O	1:W:91:ASP:OD1	1.99	0.81
1:H:179:THR:HG23	1:YA:158:SER:OG	1.81	0.81
1:I:161:ARG:HG3	1:DB:29:ARG:HH21	1.41	0.81
1:K:154:SER:OG	1:BA:183:GLU:HG2	1.80	0.81
1:O:29:ARG:CD	1:Q:166:ASP:HB3	2.11	0.81
1:R:188:GLY:C	1:DB:197:ARG:NH1	2.32	0.81
1:H:29:ARG:HD2	1:YA:166:ASP:CB	2.01	0.81
1:L:166:ASP:CB	1:T:29:ARG:HD3	2.11	0.81
1:V:154:SER:OG	1:DA:183:GLU:HG2	1.79	0.81
1:O:161:ARG:NH2	1:RA:179:THR:OG1	2.10	0.81
1:L:197:ARG:CD	1:T:188:GLY:O	2.28	0.81
1:N:161:ARG:HH21	1:TA:179:THR:HG1	1.24	0.81
1:ZA:161:ARG:HH21	1:HB:179:THR:CB	1.93	0.81
1:O:166:ASP:CB	1:RA:29:ARG:CD	2.58	0.80
1:SA:29:ARG:HD3	1:UA:166:ASP:HB3	1.63	0.80
1:X:123:TYR:CZ	1:HA:61:PRO:HG3	2.16	0.80
1:EA:154:SER:OG	1:VA:183:GLU:HG2	1.82	0.80
1:D:197:ARG:HH12	1:OA:188:GLY:HA3	1.44	0.80
1:H:188:GLY:CA	1:YA:197:ARG:NH1	2.39	0.80
1:N:205:TRP:CZ2	1:DA:161:ARG:HG2	2.17	0.79
1:SA:183:GLU:OE2	1:UA:155:GLN:HA	1.83	0.79
1:A:255:TYR:CD1	1:GA:98:ASP:HB3	2.18	0.79
1:JA:179:THR:OG1	1:WA:161:ARG:NH2	2.15	0.79
1:U:197:ARG:HD3	1:AB:189:TYR:CD1	2.17	0.79
1:U:70:ARG:NH2	1:AB:94:ARG:HB3	1.96	0.79
1:GA:10:PRO:CA	1:FB:8:LEU:HD11	2.14	0.78
1:GA:94:ARG:NH1	1:FB:3:ASN:HD22	1.81	0.78
1:H:88:GLU:OE1	1:YA:54:ARG:NH1	2.15	0.78
1:GA:12:THR:CB	1:FB:1:MET:O	2.32	0.78
1:F:70:ARG:NH2	1:W:94:ARG:HD2	1.97	0.78
1:F:29:ARG:HD3	1:HA:166:ASP:CB	2.11	0.78
1:O:166:ASP:CB	1:RA:29:ARG:HD3	2.14	0.78
1:P:183:GLU:HG2	1:CA:154:SER:OG	1.83	0.78
1:Q:179:THR:OG1	1:AB:161:ARG:NH2	2.16	0.78
1:R:94:ARG:HB3	1:DB:70:ARG:NH2	1.99	0.78
1:GA:10:PRO:CB	1:FB:8:LEU:HD11	2.13	0.78
1:A:255:TYR:CD1	1:GA:98:ASP:OD2	2.36	0.77
1:K:197:ARG:NH1	1:BA:188:GLY:HA3	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:197:ARG:HH11	1:TA:188:GLY:C	1.87	0.77
1:U:197:ARG:CZ	1:AB:189:TYR:CZ	2.68	0.77
1:EA:166:ASP:HB3	1:VA:29:ARG:HD2	1.66	0.77
1:D:29:ARG:CD	1:IA:166:ASP:HB3	2.15	0.76
1:X:61:PRO:CG	1:HA:123:TYR:OH	2.33	0.76
1:ZA:161:ARG:NH2	1:HB:179:THR:CB	2.49	0.76
1:O:29:ARG:HD3	1:Q:166:ASP:HB3	1.67	0.76
1:U:166:ASP:CA	1:AB:29:ARG:HD3	2.14	0.76
1:H:183:GLU:HG2	1:YA:154:SER:CB	2.15	0.76
1:SA:188:GLY:O	1:UA:197:ARG:CD	2.34	0.76
1:N:197:ARG:HH12	1:TA:188:GLY:HA3	1.49	0.76
1:X:61:PRO:HG3	1:HA:123:TYR:OH	1.86	0.76
1:N:166:ASP:HB3	1:TA:29:ARG:HD3	1.66	0.76
1:JA:194:HIS:CE1	1:FB:188:GLY:HA2	2.21	0.76
1:LA:154:SER:OG	1:UA:183:GLU:HG2	1.86	0.76
1:I:3:ASN:ND2	1:YA:94:ARG:NH1	2.34	0.75
1:H:183:GLU:CB	1:YA:154:SER:OG	2.34	0.75
1:K:166:ASP:HB3	1:BA:29:ARG:HD3	1.66	0.75
1:U:70:ARG:HH22	1:AB:94:ARG:HB3	1.50	0.75
1:JA:188:GLY:HA2	1:WA:194:HIS:CE1	2.22	0.75
1:D:166:ASP:HB3	1:OA:29:ARG:HD2	1.67	0.75
1:JA:255:TYR:CB	1:FB:98:ASP:HB3	2.16	0.75
1:GA:10:PRO:HB3	1:FB:8:LEU:HD12	1.68	0.74
1:A:255:TYR:HB3	1:GA:98:ASP:HB2	1.67	0.74
1:E:154:SER:CB	1:WA:183:GLU:HG2	2.18	0.74
1:KA:46:VAL:HG12	1:WA:94:ARG:O	1.86	0.74
1:E:197:ARG:NH1	1:WA:188:GLY:O	2.20	0.74
1:SA:91:ASP:OD1	1:UA:53:GLY:O	2.04	0.74
1:E:154:SER:OG	1:WA:183:GLU:CG	2.36	0.74
1:F:154:SER:CB	1:W:183:GLU:HG2	2.18	0.73
1:T:154:SER:OG	1:GB:183:GLU:HG2	1.88	0.73
1:H:189:TYR:CD1	1:YA:197:ARG:HD3	2.23	0.73
1:O:179:THR:OG1	1:Q:161:ARG:NH2	2.19	0.73
1:PA:161:ARG:NH2	1:XA:179:THR:OG1	2.22	0.73
1:K:91:ASP:OD2	1:MA:54:ARG:NH1	2.21	0.73
1:EA:197:ARG:HD2	1:VA:188:GLY:O	1.88	0.73
1:H:188:GLY:HA3	1:YA:197:ARG:HH12	1.52	0.73
1:LA:166:ASP:CB	1:UA:29:ARG:HD3	2.17	0.73
1:D:91:ASP:OD1	1:IA:53:GLY:O	2.07	0.72
1:A:179:THR:OG1	1:X:161:ARG:NH2	2.21	0.72
1:K:166:ASP:HB3	1:BA:29:ARG:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:70:ARG:CZ	1:RA:94:ARG:HD2	2.18	0.72
1:A:179:THR:CB	1:X:161:ARG:HH21	2.02	0.72
1:Q:183:GLU:HG2	1:AB:154:SER:OG	1.90	0.72
1:V:255:TYR:CD1	1:DA:98:ASP:HB3	2.24	0.72
1:A:255:TYR:CB	1:GA:98:ASP:HB3	2.19	0.72
1:U:166:ASP:N	1:AB:29:ARG:HD3	2.04	0.72
1:EA:29:ARG:CD	1:GB:166:ASP:HB3	2.19	0.71
1:I:255:TYR:CE2	1:DB:97:LYS:CD	2.73	0.71
1:FA:161:ARG:NH2	1:NA:179:THR:OG1	2.22	0.71
1:EA:29:ARG:HD2	1:GB:166:ASP:HB3	1.70	0.71
1:D:29:ARG:HD3	1:IA:166:ASP:HB3	1.72	0.71
1:D:197:ARG:HH11	1:OA:188:GLY:C	1.93	0.71
1:Z:154:SER:OG	1:QA:183:GLU:HG2	1.90	0.71
1:E:166:ASP:HB3	1:WA:29:ARG:HD2	1.71	0.70
1:C:53:GLY:O	1:V:91:ASP:OD1	2.09	0.70
1:GA:10:PRO:HA	1:FB:8:LEU:HD11	1.73	0.70
1:N:91:ASP:OD2	1:DA:54:ARG:NH1	2.23	0.70
1:RA:70:ARG:NH1	1:BB:45:PRO:O	2.17	0.70
1:I:166:ASP:OD1	1:DB:25:ARG:CG	2.39	0.70
1:U:161:ARG:NH2	1:AB:179:THR:HA	2.06	0.70
1:W:158:SER:OG	1:PA:183:GLU:OE2	2.08	0.70
1:EA:197:ARG:CD	1:VA:188:GLY:O	2.40	0.70
1:R:96:SER:HB2	1:DB:53:GLY:HA3	1.74	0.70
1:JA:29:ARG:CD	1:WA:166:ASP:HB3	2.21	0.70
1:LA:197:ARG:HD2	1:UA:188:GLY:O	1.91	0.69
1:C:197:ARG:HD2	1:V:188:GLY:O	1.93	0.69
1:S:255:TYR:HB3	1:YA:98:ASP:HB3	1.74	0.69
1:O:255:TYR:CD1	1:RA:98:ASP:HB3	2.27	0.69
1:JA:205:TRP:CZ2	1:WA:161:ARG:HG2	2.26	0.69
1:ZA:166:ASP:CB	1:HB:29:ARG:HD3	2.22	0.69
1:JA:161:ARG:HD2	1:FB:205:TRP:CE2	2.27	0.69
1:EA:53:GLY:O	1:VA:91:ASP:OD1	2.11	0.69
1:D:166:ASP:HB3	1:OA:29:ARG:HD3	1.74	0.68
1:E:197:ARG:NH1	1:WA:188:GLY:C	2.46	0.68
1:IA:188:GLY:O	1:KA:197:ARG:HD2	1.93	0.68
1:A:154:SER:O	1:GA:183:GLU:OE2	2.11	0.68
1:JA:183:GLU:OE2	1:WA:155:GLN:HA	1.94	0.68
1:U:166:ASP:CA	1:AB:29:ARG:CD	2.70	0.68
1:ZA:197:ARG:HH11	1:HB:188:GLY:C	1.97	0.68
1:JA:53:GLY:O	1:FB:91:ASP:OD1	2.11	0.68
1:F:46:VAL:O	1:QA:51:SER:HB3	1.89	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:158:SER:OG	1:AB:183:GLU:OE2	2.11	0.68
1:C:197:ARG:CD	1:V:188:GLY:O	2.42	0.68
1:O:183:GLU:OE2	1:Q:158:SER:OG	2.06	0.68
1:R:94:ARG:HD2	1:DB:70:ARG:CZ	2.24	0.68
1:R:94:ARG:HD2	1:DB:70:ARG:NH1	2.09	0.67
1:V:166:ASP:CA	1:DA:29:ARG:HD3	2.24	0.67
1:O:197:ARG:CZ	1:RA:189:TYR:CZ	2.78	0.67
1:S:255:TYR:CD1	1:YA:98:ASP:HB3	2.29	0.67
1:W:166:ASP:CB	1:PA:29:ARG:HD3	2.21	0.67
1:C:166:ASP:HB3	1:V:29:ARG:CD	2.23	0.67
1:L:161:ARG:HH21	1:T:179:THR:HG1	1.37	0.67
1:U:197:ARG:NE	1:AB:189:TYR:CE1	2.63	0.67
1:T:46:VAL:HG12	1:NA:94:ARG:C	2.14	0.67
1:V:197:ARG:NH1	1:DA:188:GLY:O	2.22	0.67
1:A:255:TYR:CG	1:GA:98:ASP:CB	2.75	0.67
1:E:29:ARG:HD2	1:G:166:ASP:HB3	1.76	0.67
1:U:54:ARG:HH12	1:AB:88:GLU:CD	1.97	0.67
1:W:12:THR:CG2	1:QA:1:MET:O	2.42	0.67
1:PA:166:ASP:HB3	1:XA:29:ARG:HD2	1.75	0.67
1:SA:98:ASP:HB3	1:UA:255:TYR:CD1	2.29	0.67
1:JA:161:ARG:CG	1:FB:205:TRP:CZ2	2.77	0.66
1:X:123:TYR:CE1	1:HA:61:PRO:HB3	2.30	0.66
1:A:188:GLY:CA	1:X:197:ARG:HH11	2.07	0.66
1:U:197:ARG:CD	1:AB:189:TYR:CE1	2.78	0.66
1:C:98:ASP:HB3	1:TA:255:TYR:CB	2.26	0.66
1:GA:93:GLU:OE1	1:FB:2:ASN:CB	2.44	0.66
1:A:255:TYR:CD1	1:GA:98:ASP:CB	2.79	0.66
1:JA:166:ASP:HB3	1:FB:29:ARG:CD	2.26	0.66
1:L:166:ASP:CB	1:T:29:ARG:CD	2.64	0.66
1:E:183:GLU:HG2	1:G:154:SER:OG	1.96	0.66
1:H:205:TRP:NE1	1:YA:161:ARG:HD2	2.11	0.66
1:O:197:ARG:HD3	1:RA:189:TYR:CD1	2.30	0.66
1:H:188:GLY:C	1:YA:197:ARG:NH1	2.47	0.66
1:L:155:GLN:HA	1:T:183:GLU:OE2	1.96	0.66
1:ZA:197:ARG:HH12	1:HB:188:GLY:HA3	1.56	0.66
1:N:205:TRP:CE2	1:DA:161:ARG:HD2	2.31	0.65
1:JA:154:SER:OG	1:FB:183:GLU:HA	1.96	0.65
1:G:29:ARG:CD	1:FB:166:ASP:HB3	2.26	0.65
1:SA:183:GLU:CG	1:UA:154:SER:OG	2.41	0.65
1:Q:29:ARG:CD	1:AB:166:ASP:HB3	2.26	0.65
1:S:183:GLU:HG2	1:NA:154:SER:CB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:197:ARG:HD2	1:DA:188:GLY:O	1.96	0.65
1:JA:255:TYR:HB3	1:FB:98:ASP:HB3	1.79	0.65
1:P:29:ARG:HD3	1:CA:166:ASP:HB3	1.74	0.65
1:ZA:154:SER:OG	1:HB:183:GLU:HG2	1.96	0.65
1:X:123:TYR:CZ	1:HA:61:PRO:CG	2.74	0.65
1:JA:29:ARG:HD3	1:WA:166:ASP:HB3	1.79	0.65
1:JA:54:ARG:HH12	1:FB:88:GLU:CD	1.99	0.65
1:JA:161:ARG:NH2	1:FB:179:THR:OG1	2.30	0.65
1:C:98:ASP:HB3	1:TA:255:TYR:HB3	1.79	0.65
1:H:96:SER:HB2	1:YA:53:GLY:HA3	1.79	0.65
1:H:183:GLU:HA	1:YA:154:SER:CB	2.27	0.65
1:L:197:ARG:HH11	1:T:188:GLY:C	2.00	0.65
1:U:161:ARG:HH21	1:AB:179:THR:HG1	1.40	0.64
1:R:98:ASP:HB3	1:DB:255:TYR:CD1	2.32	0.64
1:LA:53:GLY:O	1:UA:91:ASP:OD1	2.14	0.64
1:JA:205:TRP:CE2	1:WA:161:ARG:HD2	2.33	0.64
1:A:94:ARG:O	1:HA:46:VAL:HG12	1.98	0.64
1:I:3:ASN:HD21	1:YA:94:ARG:NH1	1.96	0.64
1:L:183:GLU:HG2	1:VA:154:SER:OG	1.98	0.64
1:GA:12:THR:CG2	1:FB:1:MET:O	2.45	0.64
1:S:255:TYR:CB	1:YA:98:ASP:HB3	2.27	0.64
1:FA:166:ASP:HB3	1:NA:29:ARG:CD	2.27	0.64
1:M:205:TRP:CZ2	1:OA:161:ARG:HG2	2.33	0.64
1:N:98:ASP:HB3	1:DA:255:TYR:CB	2.29	0.63
1:O:94:ARG:O	1:SA:46:VAL:HG12	1.98	0.63
1:Q:188:GLY:O	1:AB:197:ARG:HD2	1.97	0.63
1:L:53:GLY:O	1:T:91:ASP:OD1	2.17	0.63
1:FA:53:GLY:O	1:NA:91:ASP:OD1	2.16	0.63
1:D:29:ARG:HD2	1:IA:166:ASP:HB3	1.80	0.63
1:FA:46:VAL:HG12	1:GB:94:ARG:O	1.97	0.63
1:A:255:TYR:HD1	1:GA:98:ASP:OD2	1.77	0.63
1:FA:154:SER:OG	1:NA:183:GLU:HG2	1.98	0.63
1:F:188:GLY:O	1:HA:197:ARG:CD	2.47	0.63
1:EA:255:TYR:CD1	1:VA:98:ASP:HB3	2.33	0.63
1:C:166:ASP:HB3	1:V:29:ARG:HD2	1.80	0.63
1:S:188:GLY:O	1:NA:197:ARG:NH1	2.07	0.63
1:N:94:ARG:O	1:UA:46:VAL:HG12	1.98	0.63
1:CA:189:TYR:CE1	1:SA:197:ARG:HD3	2.34	0.63
1:I:5:TYR:OH	1:YA:90:ASP:OD1	2.12	0.62
1:ZA:161:ARG:NH2	1:HB:179:THR:HA	2.13	0.62
1:P:183:GLU:OE2	1:CA:155:GLN:HA	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:10:PRO:CB	1:FB:8:LEU:CD1	2.67	0.62
1:GA:12:THR:HA	1:FB:1:MET:HG2	1.79	0.62
1:D:155:GLN:HA	1:OA:183:GLU:OE2	1.99	0.62
1:Z:183:GLU:OE2	1:BB:155:GLN:HA	1.98	0.62
1:N:155:GLN:HA	1:TA:183:GLU:OE2	1.98	0.62
1:U:197:ARG:NH2	1:AB:189:TYR:OH	2.33	0.62
1:W:161:ARG:NH2	1:PA:179:THR:OG1	2.27	0.62
1:A:179:THR:HA	1:X:161:ARG:NH2	2.14	0.62
1:F:154:SER:OG	1:W:183:GLU:CG	2.47	0.62
1:M:183:GLU:HG2	1:OA:154:SER:OG	1.99	0.62
1:EA:166:ASP:CB	1:VA:29:ARG:HD3	2.27	0.62
1:C:155:GLN:HA	1:V:183:GLU:OE2	1.99	0.62
1:F:77:ARG:HH12	1:QA:55:LEU:HD11	1.59	0.62
1:O:166:ASP:CA	1:RA:29:ARG:HD3	2.30	0.62
1:JA:54:ARG:NH1	1:FB:88:GLU:OE2	2.32	0.62
1:O:255:TYR:HD1	1:RA:98:ASP:HB3	1.62	0.62
1:R:179:THR:HG1	1:DB:161:ARG:NE	1.98	0.62
1:FA:166:ASP:HB3	1:NA:29:ARG:HD3	1.82	0.62
1:O:197:ARG:HD3	1:RA:189:TYR:CE1	2.33	0.61
1:S:29:ARG:HD2	1:NA:166:ASP:CB	2.20	0.61
1:H:29:ARG:HD3	1:YA:166:ASP:N	2.16	0.61
1:Z:183:GLU:HA	1:BB:154:SER:OG	2.00	0.61
1:EA:183:GLU:HG2	1:GB:154:SER:OG	2.01	0.61
1:A:29:ARG:CD	1:X:166:ASP:HB3	2.30	0.61
1:O:29:ARG:HD2	1:Q:166:ASP:HB3	1.82	0.61
1:Q:188:GLY:O	1:AB:197:ARG:CD	2.48	0.61
1:L:255:TYR:CD1	1:T:98:ASP:HB3	2.35	0.61
1:GA:12:THR:HA	1:FB:1:MET:CG	2.30	0.61
1:D:154:SER:OG	1:OA:183:GLU:CG	2.48	0.61
1:V:54:ARG:NH1	1:DA:91:ASP:OD2	2.34	0.60
1:JA:166:ASP:HB3	1:FB:29:ARG:HD3	1.82	0.60
1:JA:255:TYR:CD1	1:FB:98:ASP:CB	2.77	0.60
1:L:154:SER:OG	1:T:183:GLU:CG	2.43	0.60
1:M:189:TYR:CE1	1:OA:197:ARG:HD3	2.36	0.60
1:K:197:ARG:HD3	1:BA:188:GLY:O	1.98	0.60
1:L:197:ARG:NH1	1:T:188:GLY:HA3	2.17	0.60
1:S:255:TYR:CG	1:YA:98:ASP:HB3	2.37	0.60
1:V:255:TYR:HD1	1:DA:98:ASP:HB3	1.65	0.60
1:A:54:ARG:NH1	1:GA:88:GLU:OE2	2.35	0.60
1:M:188:GLY:HA2	1:OA:194:HIS:CE1	2.36	0.60
1:U:255:TYR:CZ	1:AB:97:LYS:HB2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:GLY:O	1:G:197:ARG:HD2	2.02	0.60
1:U:161:ARG:HH21	1:AB:179:THR:CB	2.12	0.60
1:X:61:PRO:CA	1:HA:123:TYR:OH	2.50	0.60
1:M:91:ASP:OD2	1:OA:54:ARG:NH1	2.35	0.60
1:M:189:TYR:CZ	1:OA:197:ARG:CZ	2.85	0.60
1:P:188:GLY:O	1:CA:197:ARG:HD2	2.01	0.60
1:R:179:THR:HG21	1:DB:161:ARG:HH21	1.62	0.60
1:U:183:GLU:HG2	1:RA:154:SER:OG	2.02	0.60
1:D:197:ARG:HH11	1:OA:188:GLY:HA3	1.37	0.59
1:H:183:GLU:HG2	1:YA:154:SER:C	2.22	0.59
1:H:98:ASP:HB3	1:YA:255:TYR:CD1	2.37	0.59
1:EA:189:TYR:CD1	1:GB:197:ARG:HD3	2.37	0.59
1:GA:94:ARG:NH1	1:FB:3:ASN:HD21	1.94	0.59
1:O:197:ARG:NE	1:RA:189:TYR:CE1	2.71	0.59
1:U:54:ARG:NH1	1:AB:88:GLU:CD	2.56	0.58
1:A:255:TYR:HB3	1:GA:98:ASP:HB3	1.76	0.58
1:FA:255:TYR:CD1	1:NA:98:ASP:HB3	2.37	0.58
1:N:161:ARG:NH2	1:TA:179:THR:CB	2.65	0.58
1:HA:91:ASP:OD2	1:XA:54:ARG:NH1	2.37	0.58
1:G:29:ARG:HD3	1:FB:166:ASP:HB3	1.85	0.58
1:I:255:TYR:HB3	1:DB:97:LYS:O	2.04	0.58
1:JA:29:ARG:HD2	1:WA:166:ASP:HB3	1.83	0.58
1:JA:94:ARG:C	1:GB:46:VAL:HG12	2.24	0.58
1:K:197:ARG:NH1	1:BA:188:GLY:O	2.35	0.58
1:O:166:ASP:CB	1:RA:29:ARG:HD2	2.19	0.58
1:EA:179:THR:OG1	1:GB:161:ARG:NH2	2.31	0.58
1:SA:188:GLY:HA3	1:UA:197:ARG:NH1	2.19	0.58
1:JA:189:TYR:CZ	1:WA:197:ARG:CZ	2.86	0.58
1:Z:91:ASP:OD1	1:BB:53:GLY:O	2.21	0.58
1:SA:205:TRP:CZ2	1:UA:161:ARG:HG2	2.39	0.58
1:Z:255:TYR:HD1	1:QA:98:ASP:OD2	1.87	0.58
1:PA:158:SER:OG	1:XA:183:GLU:OE2	2.09	0.57
1:GA:12:THR:HG22	1:FB:1:MET:HG3	1.85	0.57
1:E:255:TYR:CD1	1:WA:98:ASP:HB3	2.40	0.57
1:I:255:TYR:CD1	1:DB:97:LYS:HB2	2.40	0.57
1:LA:166:ASP:CB	1:UA:29:ARG:CD	2.69	0.57
1:SA:179:THR:HG1	1:UA:161:ARG:HH21	1.45	0.57
1:L:197:ARG:HD3	1:T:189:TYR:CD1	2.40	0.57
1:ZA:155:GLN:HA	1:HB:183:GLU:OE2	2.05	0.57
1:A:255:TYR:CD1	1:GA:98:ASP:CG	2.78	0.57
1:EA:189:TYR:CE1	1:GB:197:ARG:HD3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:29:ARG:HD2	1:KA:166:ASP:HB3	1.85	0.57
1:ZA:197:ARG:NH1	1:HB:188:GLY:CA	2.44	0.57
1:E:166:ASP:CB	1:WA:29:ARG:HD3	2.30	0.57
1:LA:197:ARG:CD	1:UA:188:GLY:O	2.53	0.57
1:L:45:PRO:O	1:HB:70:ARG:NH1	2.37	0.57
1:T:161:ARG:HG2	1:GB:205:TRP:CZ2	2.40	0.57
1:F:255:TYR:HD1	1:W:98:ASP:CB	1.88	0.57
1:H:105:LYS:NZ	1:YA:258:GLU:OE2	2.37	0.56
1:K:197:ARG:HH12	1:BA:188:GLY:HA3	1.70	0.56
1:GA:93:GLU:OE1	1:FB:2:ASN:HB3	2.04	0.56
1:GA:12:THR:HG22	1:FB:1:MET:C	2.26	0.56
1:H:183:GLU:HA	1:YA:154:SER:HB2	1.87	0.56
1:JA:255:TYR:HB3	1:FB:98:ASP:CB	2.35	0.56
1:I:255:TYR:CE1	1:DB:97:LYS:HB2	2.41	0.56
1:T:155:GLN:HA	1:GB:183:GLU:OE2	2.06	0.56
1:PA:166:ASP:CB	1:XA:29:ARG:HD3	2.24	0.56
1:D:154:SER:CB	1:OA:183:GLU:HG2	2.35	0.56
1:E:155:GLN:HA	1:WA:183:GLU:OE2	2.05	0.56
1:P:91:ASP:OD1	1:CA:53:GLY:O	2.22	0.56
1:R:94:ARG:HB3	1:DB:70:ARG:HH22	1.68	0.56
1:JA:189:TYR:CD1	1:WA:197:ARG:HD3	2.40	0.56
1:JA:194:HIS:CE1	1:FB:188:GLY:CA	2.88	0.56
1:F:197:ARG:NH1	1:W:188:GLY:O	2.39	0.56
1:H:29:ARG:HD3	1:YA:166:ASP:CA	2.35	0.56
1:H:205:TRP:CZ2	1:YA:161:ARG:HG2	2.40	0.56
1:N:154:SER:OG	1:TA:183:GLU:CG	2.51	0.56
1:P:189:TYR:CD1	1:CA:197:ARG:HD3	2.40	0.56
1:Q:29:ARG:HD2	1:AB:166:ASP:HB3	1.87	0.56
1:E:94:ARG:O	1:XA:46:VAL:HG12	2.05	0.56
1:F:77:ARG:HH22	1:QA:55:LEU:HD13	1.62	0.56
1:W:166:ASP:CB	1:PA:29:ARG:CD	2.71	0.56
1:EA:189:TYR:CZ	1:GB:197:ARG:CZ	2.89	0.56
1:K:197:ARG:NH1	1:BA:188:GLY:CA	2.69	0.56
1:T:46:VAL:CG1	1:NA:94:ARG:O	2.43	0.56
1:IA:8:LEU:CD1	1:XA:10:PRO:HB3	2.36	0.56
1:IA:183:GLU:HG2	1:KA:154:SER:OG	2.06	0.56
1:DA:46:VAL:HG12	1:SA:94:ARG:O	2.06	0.55
1:C:197:ARG:NH1	1:V:188:GLY:HA3	2.21	0.55
1:Q:29:ARG:HD3	1:AB:166:ASP:HB3	1.87	0.55
1:F:188:GLY:O	1:HA:197:ARG:HD2	2.05	0.55
1:N:166:ASP:CB	1:TA:29:ARG:HD3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:VAL:C	1:QA:51:SER:HB2	2.18	0.55
1:K:54:ARG:NH1	1:BA:91:ASP:OD2	2.39	0.55
1:N:91:ASP:OD1	1:DA:53:GLY:O	2.24	0.55
1:O:154:SER:OG	1:RA:183:GLU:HG2	2.05	0.55
1:A:81:PRO:HD2	1:FB:64:GLY:O	2.07	0.55
1:JA:205:TRP:CZ2	1:WA:161:ARG:CG	2.90	0.55
1:F:188:GLY:O	1:HA:197:ARG:HD3	2.07	0.55
1:L:197:ARG:NH1	1:T:188:GLY:O	2.29	0.55
1:ZA:161:ARG:NH2	1:HB:179:THR:CA	2.69	0.55
1:N:98:ASP:HB3	1:DA:255:TYR:CD1	2.42	0.55
1:N:98:ASP:HB3	1:DA:255:TYR:HA	1.89	0.55
1:Z:54:ARG:NH1	1:QA:91:ASP:OD2	2.38	0.55
1:O:94:ARG:C	1:SA:46:VAL:HG12	2.27	0.54
1:P:54:ARG:NH1	1:LA:91:ASP:OD2	2.40	0.54
1:U:52:THR:O	1:AB:96:SER:HB2	2.07	0.54
1:GA:94:ARG:HH11	1:FB:3:ASN:HD22	1.54	0.54
1:JA:154:SER:OG	1:FB:183:GLU:CG	2.47	0.54
1:F:46:VAL:C	1:QA:51:SER:CB	2.73	0.54
1:JA:255:TYR:HD1	1:FB:98:ASP:HB3	1.66	0.54
1:O:188:GLY:O	1:Q:197:ARG:CD	2.55	0.54
1:L:154:SER:CB	1:T:183:GLU:HG2	2.38	0.54
1:N:197:ARG:NH1	1:TA:188:GLY:C	2.60	0.54
1:ZA:158:SER:OG	1:HB:179:THR:HG23	2.07	0.54
1:H:29:ARG:CD	1:YA:166:ASP:CA	2.86	0.54
1:O:166:ASP:N	1:RA:29:ARG:HD3	2.23	0.54
1:V:255:TYR:CZ	1:DA:97:LYS:HB2	2.43	0.54
1:Z:255:TYR:CB	1:QA:98:ASP:CB	2.68	0.54
1:Z:255:TYR:CD1	1:QA:98:ASP:HB3	2.43	0.54
1:JA:166:ASP:HB3	1:FB:29:ARG:HD2	1.89	0.54
1:H:3:ASN:ND2	1:FB:94:ARG:NH1	2.56	0.54
1:CA:29:ARG:HD2	1:SA:166:ASP:HB3	1.89	0.54
1:EA:197:ARG:NH1	1:VA:188:GLY:HA3	2.22	0.54
1:IA:189:TYR:CD1	1:KA:197:ARG:HD3	2.43	0.54
1:L:8:LEU:CD1	1:MA:10:PRO:HB3	2.37	0.54
1:CA:189:TYR:CD1	1:SA:197:ARG:HD3	2.43	0.54
1:S:183:GLU:CG	1:NA:154:SER:OG	2.54	0.54
1:X:123:TYR:OH	1:HA:61:PRO:CA	2.56	0.54
1:Z:154:SER:CB	1:QA:183:GLU:HG2	2.37	0.54
1:EA:29:ARG:HD3	1:GB:166:ASP:HB3	1.90	0.54
1:SA:29:ARG:HD3	1:UA:166:ASP:CB	2.37	0.54
1:E:53:GLY:O	1:WA:91:ASP:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:161:ARG:HG3	1:DB:29:ARG:NH2	2.18	0.53
1:ZA:166:ASP:CB	1:HB:29:ARG:CD	2.66	0.53
1:D:98:ASP:HB3	1:IA:255:TYR:CD1	2.43	0.53
1:N:98:ASP:HB3	1:DA:255:TYR:HB3	1.91	0.53
1:N:205:TRP:CZ2	1:DA:161:ARG:CG	2.89	0.53
1:Z:88:GLU:OE1	1:BB:54:ARG:NH1	2.37	0.53
1:K:197:ARG:HH11	1:BA:188:GLY:CA	2.22	0.53
1:V:197:ARG:CD	1:DA:188:GLY:O	2.56	0.53
1:CA:189:TYR:CZ	1:SA:197:ARG:CZ	2.91	0.53
1:G:29:ARG:HD2	1:FB:166:ASP:HB3	1.90	0.53
1:E:188:GLY:O	1:G:197:ARG:CD	2.57	0.53
1:O:94:ARG:O	1:SA:46:VAL:HA	2.08	0.53
1:IA:29:ARG:CD	1:KA:166:ASP:HB3	2.39	0.53
1:H:98:ASP:HB3	1:YA:255:TYR:HD1	1.71	0.53
1:N:183:GLU:OE2	1:DA:155:GLN:HA	2.08	0.53
1:A:154:SER:CB	1:GA:183:GLU:CG	2.76	0.53
1:JA:183:GLU:CG	1:WA:154:SER:OG	2.47	0.53
1:N:154:SER:CB	1:TA:183:GLU:HG2	2.38	0.52
1:O:197:ARG:NH2	1:RA:189:TYR:OH	2.42	0.52
1:V:70:ARG:CZ	1:DA:94:ARG:HD2	2.39	0.52
1:C:166:ASP:HB3	1:V:29:ARG:HD3	1.90	0.52
1:N:98:ASP:HB3	1:DA:255:TYR:CA	2.40	0.52
1:U:91:ASP:CG	1:RA:54:ARG:HH11	2.12	0.52
1:V:255:TYR:CB	1:DA:98:ASP:HB3	2.39	0.52
1:Z:197:ARG:NH1	1:QA:188:GLY:CA	2.72	0.52
1:JA:189:TYR:CE1	1:WA:197:ARG:NE	2.77	0.52
1:H:205:TRP:CZ2	1:YA:161:ARG:CG	2.93	0.52
1:M:46:VAL:HG12	1:VA:94:ARG:O	2.09	0.52
1:V:166:ASP:CB	1:DA:29:ARG:HD2	2.27	0.52
1:F:154:SER:HB2	1:W:183:GLU:HG2	1.91	0.52
1:A:255:TYR:CB	1:GA:98:ASP:CB	2.77	0.52
1:X:123:TYR:OH	1:HA:61:PRO:CD	2.57	0.52
1:GA:64:GLY:O	1:YA:81:PRO:CD	2.51	0.52
1:A:179:THR:CB	1:X:161:ARG:NH2	2.71	0.52
1:K:197:ARG:HH11	1:BA:188:GLY:C	2.11	0.52
1:R:94:ARG:CD	1:DB:70:ARG:NH1	2.73	0.52
1:C:2:ASN:HA	1:QA:93:GLU:OE1	2.10	0.51
1:I:8:LEU:HD11	1:YA:10:PRO:HB3	1.92	0.51
1:O:70:ARG:NH1	1:RA:94:ARG:HD2	2.24	0.51
1:O:188:GLY:O	1:Q:197:ARG:HD2	2.10	0.51
1:M:154:SER:OG	1:KA:183:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:255:TYR:CZ	1:RA:97:LYS:HB2	2.45	0.51
1:H:205:TRP:CD1	1:YA:161:ARG:HD2	2.46	0.51
1:L:81:PRO:HD2	1:HB:64:GLY:O	2.10	0.51
1:S:29:ARG:HD3	1:NA:166:ASP:CA	2.40	0.51
1:E:98:ASP:HB3	1:G:255:TYR:CD1	2.46	0.51
1:F:81:PRO:HG3	1:QA:66:ILE:HD12	1.93	0.51
1:X:123:TYR:CE2	1:HA:61:PRO:HG3	2.45	0.51
1:A:188:GLY:O	1:X:197:ARG:HD2	2.06	0.51
1:C:255:TYR:CD1	1:V:98:ASP:HB3	2.46	0.51
1:I:8:LEU:CD1	1:YA:10:PRO:HB3	2.40	0.51
1:M:53:GLY:O	1:KA:91:ASP:OD1	2.29	0.51
1:IA:179:THR:OG1	1:KA:161:ARG:NH2	2.33	0.51
1:IA:188:GLY:O	1:KA:197:ARG:CD	2.57	0.51
1:GA:90:ASP:OD1	1:FB:5:TYR:OH	2.19	0.51
1:D:197:ARG:NH1	1:OA:188:GLY:C	2.62	0.51
1:E:161:ARG:NH2	1:WA:179:THR:HG1	1.88	0.51
1:C:29:ARG:CD	1:TA:166:ASP:HB3	2.41	0.51
1:O:197:ARG:CD	1:RA:189:TYR:CE1	2.94	0.51
1:R:179:THR:HG1	1:DB:161:ARG:HE	1.56	0.51
1:U:161:ARG:NH2	1:AB:179:THR:CA	2.74	0.51
1:CA:205:TRP:CZ2	1:SA:161:ARG:HG2	2.46	0.51
1:I:218:ARG:NH1	1:DB:25:ARG:HD2	2.25	0.51
1:X:61:PRO:CB	1:HA:123:TYR:CZ	2.78	0.51
1:LA:255:TYR:CD1	1:UA:98:ASP:HB3	2.46	0.51
1:C:161:ARG:HG2	1:V:205:TRP:CZ2	2.46	0.51
1:V:255:TYR:HA	1:DA:98:ASP:HB3	1.92	0.51
1:CA:183:GLU:HG2	1:SA:154:SER:OG	2.10	0.51
1:FA:155:GLN:HA	1:NA:183:GLU:OE2	2.12	0.50
1:A:51:SER:HB2	1:FB:48:ALA:HB2	1.92	0.50
1:D:197:ARG:NH1	1:OA:188:GLY:O	2.42	0.50
1:JA:98:ASP:HB3	1:WA:255:TYR:CD1	2.46	0.50
1:A:166:ASP:CB	1:GA:29:ARG:CD	2.65	0.50
1:ZA:53:GLY:O	1:HB:91:ASP:OD1	2.29	0.50
1:M:189:TYR:CD1	1:OA:197:ARG:HD3	2.46	0.50
1:H:2:ASN:HA	1:FB:93:GLU:OE1	2.12	0.50
1:P:205:TRP:CZ2	1:CA:161:ARG:HG2	2.46	0.50
1:SA:183:GLU:HG2	1:UA:154:SER:CB	2.41	0.50
1:E:161:ARG:NH2	1:WA:179:THR:CB	2.71	0.50
1:U:53:GLY:HA3	1:AB:96:SER:HB2	1.94	0.50
1:NA:1:MET:HG3	1:HB:12:THR:HA	1.94	0.50
1:R:189:TYR:HA	1:DB:197:ARG:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:197:ARG:NE	1:AB:189:TYR:CZ	2.80	0.49
1:GA:90:ASP:OD1	1:FB:5:TYR:CZ	2.65	0.49
1:JA:161:ARG:CD	1:FB:205:TRP:CE2	2.95	0.49
1:H:189:TYR:CE1	1:YA:197:ARG:NE	2.80	0.49
1:I:46:VAL:CG1	1:YA:94:ARG:O	2.31	0.49
1:I:166:ASP:OD1	1:DB:25:ARG:HG3	2.10	0.49
1:H:183:GLU:CA	1:YA:154:SER:OG	2.60	0.49
1:JA:161:ARG:NH2	1:FB:179:THR:HG1	2.10	0.49
1:H:183:GLU:HA	1:YA:154:SER:OG	2.11	0.49
1:IA:183:GLU:OE2	1:KA:155:GLN:HA	2.12	0.49
1:L:161:ARG:HG2	1:T:205:TRP:CZ2	2.48	0.49
1:T:53:GLY:O	1:GB:91:ASP:OD1	2.31	0.49
1:U:155:GLN:HA	1:AB:183:GLU:OE2	2.12	0.49
1:Z:255:TYR:CD1	1:QA:98:ASP:OD2	2.66	0.49
1:Z:183:GLU:CD	1:BB:155:GLN:HG2	2.32	0.49
1:JA:161:ARG:HD2	1:FB:205:TRP:CD2	2.48	0.49
1:U:197:ARG:CZ	1:AB:189:TYR:OH	2.61	0.48
1:C:29:ARG:HD3	1:TA:166:ASP:HB3	1.93	0.48
1:T:1:MET:O	1:NA:12:THR:HB	2.12	0.48
1:F:255:TYR:HB3	1:W:98:ASP:CA	2.40	0.48
1:H:188:GLY:O	1:YA:197:ARG:NH1	2.37	0.48
1:L:194:HIS:CE1	1:T:188:GLY:HA2	2.48	0.48
1:T:8:LEU:CD1	1:NA:10:PRO:HB3	2.43	0.48
1:W:94:ARG:HG2	1:QA:45:PRO:HB2	1.94	0.48
1:E:29:ARG:HD3	1:G:166:ASP:CB	2.34	0.48
1:I:166:ASP:OD1	1:DB:25:ARG:HG2	2.12	0.48
1:GA:94:ARG:HG2	1:FB:45:PRO:HB2	1.95	0.48
1:SA:98:ASP:HB3	1:UA:255:TYR:HD1	1.78	0.48
1:EA:205:TRP:CZ2	1:GB:161:ARG:HG2	2.49	0.48
1:D:161:ARG:NH2	1:OA:179:THR:CB	2.74	0.48
1:U:166:ASP:HA	1:AB:29:ARG:NE	2.29	0.48
1:E:91:ASP:OD1	1:G:53:GLY:O	2.31	0.48
1:H:183:GLU:HB3	1:YA:154:SER:OG	2.13	0.48
1:L:166:ASP:CA	1:T:29:ARG:HD3	2.44	0.48
1:N:161:ARG:NH2	1:TA:179:THR:HA	2.28	0.48
1:O:91:ASP:OD1	1:Q:53:GLY:O	2.32	0.48
1:O:155:GLN:HA	1:RA:183:GLU:OE2	2.14	0.48
1:L:51:SER:HB2	1:HB:48:ALA:HB2	1.95	0.48
1:L:161:ARG:HD2	1:T:205:TRP:NE1	2.29	0.48
1:R:179:THR:CB	1:DB:161:ARG:HH21	2.11	0.48
1:Z:54:ARG:NH1	1:QA:88:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:61:PRO:HG3	1:S:123:TYR:OH	2.13	0.48
1:L:91:ASP:OD2	1:VA:54:ARG:NH1	2.47	0.48
1:Q:188:GLY:HA3	1:AB:197:ARG:NH1	2.29	0.48
1:EA:143:PRO:HD3	1:EA:152:VAL:HG21	1.96	0.48
1:JA:143:PRO:HD3	1:JA:152:VAL:HG21	1.96	0.48
1:MA:143:PRO:HD3	1:MA:152:VAL:HG21	1.96	0.48
1:UA:143:PRO:HD3	1:UA:152:VAL:HG21	1.96	0.48
1:E:143:PRO:HD3	1:E:152:VAL:HG21	1.96	0.47
1:Q:143:PRO:HD3	1:Q:152:VAL:HG21	1.96	0.47
1:Z:197:ARG:HD3	1:QA:188:GLY:O	2.14	0.47
1:BA:143:PRO:HD3	1:BA:152:VAL:HG21	1.96	0.47
1:PA:143:PRO:HD3	1:PA:152:VAL:HG21	1.96	0.47
1:H:94:ARG:HB3	1:YA:70:ARG:NH2	2.29	0.47
1:K:143:PRO:HD3	1:K:152:VAL:HG21	1.96	0.47
1:T:143:PRO:HD3	1:T:152:VAL:HG21	1.96	0.47
1:W:143:PRO:HD3	1:W:152:VAL:HG21	1.96	0.47
1:W:197:ARG:HD3	1:PA:189:TYR:CD1	2.49	0.47
1:Z:143:PRO:HD3	1:Z:152:VAL:HG21	1.96	0.47
1:LA:143:PRO:HD3	1:LA:152:VAL:HG21	1.96	0.47
1:CA:143:PRO:HD3	1:CA:152:VAL:HG21	1.96	0.47
1:SA:143:PRO:HD3	1:SA:152:VAL:HG21	1.96	0.47
1:BB:143:PRO:HD3	1:BB:152:VAL:HG21	1.96	0.47
1:F:255:TYR:CA	1:W:98:ASP:HB2	2.43	0.47
1:HA:143:PRO:HD3	1:HA:152:VAL:HG21	1.96	0.47
1:JA:197:ARG:CZ	1:FB:189:TYR:CZ	2.98	0.47
1:ZA:143:PRO:HD3	1:ZA:152:VAL:HG21	1.96	0.47
1:FB:143:PRO:HD3	1:FB:152:VAL:HG21	1.96	0.47
1:C:98:ASP:HB3	1:TA:255:TYR:CD1	2.50	0.47
1:R:143:PRO:HD3	1:R:152:VAL:HG21	1.96	0.47
1:GA:143:PRO:HD3	1:GA:152:VAL:HG21	1.96	0.47
1:N:105:LYS:NZ	1:DA:258:GLU:OE2	2.47	0.47
1:T:51:SER:HB2	1:FA:48:ALA:HB2	1.96	0.47
1:RA:143:PRO:HD3	1:RA:152:VAL:HG21	1.96	0.47
1:A:143:PRO:HD3	1:A:152:VAL:HG21	1.96	0.47
1:A:179:THR:HG23	1:X:161:ARG:NH2	2.30	0.47
1:E:183:GLU:OE2	1:G:158:SER:OG	2.20	0.47
1:F:48:ALA:CB	1:QA:72:SER:CB	2.89	0.47
1:N:143:PRO:HD3	1:N:152:VAL:HG21	1.96	0.47
1:O:143:PRO:HD3	1:O:152:VAL:HG21	1.96	0.47
1:O:161:ARG:HG2	1:RA:205:TRP:CZ2	2.50	0.47
1:X:143:PRO:HD3	1:X:152:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:258:GLU:OE2	1:AB:105:LYS:NZ	2.48	0.47
1:EA:189:TYR:CE1	1:GB:197:ARG:NE	2.83	0.47
1:IA:8:LEU:HD11	1:XA:10:PRO:HA	1.97	0.47
1:C:258:GLU:OE2	1:V:105:LYS:NZ	2.48	0.47
1:G:183:GLU:OE2	1:FB:158:SER:OG	2.27	0.47
1:H:51:SER:HB2	1:JA:48:ALA:HB2	1.96	0.47
1:EA:183:GLU:OE2	1:GB:155:GLN:HA	2.14	0.47
1:H:5:TYR:OH	1:FB:90:ASP:OD1	2.24	0.47
1:U:143:PRO:HD3	1:U:152:VAL:HG21	1.96	0.47
1:I:143:PRO:HD3	1:I:152:VAL:HG21	1.96	0.46
1:O:258:GLU:OE2	1:RA:105:LYS:NZ	2.49	0.46
1:S:143:PRO:HD3	1:S:152:VAL:HG21	1.96	0.46
1:BA:197:ARG:HD3	1:ZA:189:TYR:CE1	2.50	0.46
1:TA:143:PRO:HD3	1:TA:152:VAL:HG21	1.96	0.46
1:H:143:PRO:HD3	1:H:152:VAL:HG21	1.96	0.46
1:M:143:PRO:HD3	1:M:152:VAL:HG21	1.96	0.46
1:M:166:ASP:HB3	1:KA:29:ARG:CD	2.45	0.46
1:M:189:TYR:OH	1:OA:197:ARG:NH2	2.48	0.46
1:S:183:GLU:OE2	1:NA:158:SER:OG	2.20	0.46
1:VA:143:PRO:HD3	1:VA:152:VAL:HG21	1.96	0.46
1:WA:143:PRO:HD3	1:WA:152:VAL:HG21	1.96	0.46
1:GB:143:PRO:HD3	1:GB:152:VAL:HG21	1.96	0.46
1:HB:143:PRO:HD3	1:HB:152:VAL:HG21	1.96	0.46
1:A:154:SER:OG	1:GA:183:GLU:CD	2.54	0.46
1:C:143:PRO:HD3	1:C:152:VAL:HG21	1.96	0.46
1:S:255:TYR:HB3	1:YA:98:ASP:CB	2.43	0.46
1:DB:143:PRO:HD3	1:DB:152:VAL:HG21	1.96	0.46
1:L:143:PRO:HD3	1:L:152:VAL:HG21	1.96	0.46
1:DA:143:PRO:HD3	1:DA:152:VAL:HG21	1.96	0.46
1:NA:143:PRO:HD3	1:NA:152:VAL:HG21	1.96	0.46
1:OA:143:PRO:HD3	1:OA:152:VAL:HG21	1.96	0.46
1:D:143:PRO:HD3	1:D:152:VAL:HG21	1.96	0.46
1:F:143:PRO:HD3	1:F:152:VAL:HG21	1.96	0.46
1:G:143:PRO:HD3	1:G:152:VAL:HG21	1.96	0.46
1:N:197:ARG:NH1	1:TA:188:GLY:O	2.44	0.46
1:O:70:ARG:NH2	1:RA:94:ARG:HB3	2.30	0.46
1:V:143:PRO:HD3	1:V:152:VAL:HG21	1.96	0.46
1:Z:54:ARG:HH12	1:QA:88:GLU:CD	2.19	0.46
1:JA:161:ARG:CG	1:FB:205:TRP:CE2	2.98	0.46
1:QA:143:PRO:HD3	1:QA:152:VAL:HG21	1.96	0.46
1:XA:143:PRO:HD3	1:XA:152:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ARG:HD3	1:V:188:GLY:O	2.14	0.46
1:L:161:ARG:NH2	1:T:179:THR:CB	2.74	0.46
1:N:166:ASP:CB	1:TA:29:ARG:CD	2.78	0.46
1:CA:51:SER:HB2	1:MA:48:ALA:HB2	1.98	0.46
1:FA:143:PRO:HD3	1:FA:152:VAL:HG21	1.96	0.46
1:FA:166:ASP:HB3	1:NA:29:ARG:HD2	1.95	0.46
1:IA:143:PRO:HD3	1:IA:152:VAL:HG21	1.96	0.46
1:JA:194:HIS:ND1	1:FB:188:GLY:HA2	2.29	0.46
1:AB:143:PRO:HD3	1:AB:152:VAL:HG21	1.96	0.46
1:F:166:ASP:CB	1:W:29:ARG:CD	2.64	0.46
1:F:179:THR:OG1	1:HA:161:ARG:NH2	2.45	0.46
1:I:3:ASN:ND2	1:YA:94:ARG:HH11	2.12	0.46
1:CA:29:ARG:CD	1:SA:166:ASP:HB3	2.46	0.46
1:EA:188:GLY:HA2	1:GB:194:HIS:CE1	2.50	0.46
1:YA:143:PRO:HD3	1:YA:152:VAL:HG21	1.96	0.46
1:H:94:ARG:HD2	1:YA:70:ARG:CZ	2.45	0.46
1:N:205:TRP:CD2	1:DA:161:ARG:HD2	2.50	0.46
1:P:143:PRO:HD3	1:P:152:VAL:HG21	1.96	0.46
1:KA:143:PRO:HD3	1:KA:152:VAL:HG21	1.97	0.46
1:P:188:GLY:HA2	1:CA:194:HIS:CE1	2.51	0.46
1:FA:12:THR:HG22	1:JA:5:TYR:CE1	2.51	0.46
1:RA:64:GLY:O	1:BB:81:PRO:HD2	2.15	0.46
1:SA:188:GLY:C	1:UA:197:ARG:HH11	2.16	0.46
1:O:194:HIS:CE1	1:RA:188:GLY:HA2	2.51	0.45
1:EA:197:ARG:HD3	1:VA:188:GLY:O	2.16	0.45
1:H:179:THR:CG2	1:YA:158:SER:OG	2.59	0.45
1:CA:91:ASP:OD2	1:SA:54:ARG:NH1	2.48	0.45
1:EA:197:ARG:NH1	1:VA:188:GLY:O	2.44	0.45
1:L:8:LEU:HD11	1:MA:10:PRO:HA	1.98	0.45
1:ZA:154:SER:CB	1:HB:183:GLU:HG2	2.46	0.45
1:F:53:GLY:HA3	1:W:91:ASP:OD1	2.16	0.45
1:K:98:ASP:HB3	1:MA:255:TYR:HA	1.99	0.45
1:T:54:ARG:NH1	1:GB:91:ASP:OD2	2.48	0.45
1:JA:188:GLY:CA	1:WA:194:HIS:CE1	2.96	0.45
1:N:158:SER:OG	1:TA:179:THR:HG23	2.17	0.45
1:L:197:ARG:NE	1:T:189:TYR:CE1	2.85	0.45
1:M:105:LYS:NZ	1:OA:258:GLU:OE2	2.49	0.45
1:S:155:GLN:HA	1:YA:183:GLU:OE2	2.16	0.45
1:CA:105:LYS:NZ	1:SA:258:GLU:OE2	2.48	0.45
1:F:77:ARG:HH22	1:QA:55:LEU:CD1	2.21	0.45
1:L:161:ARG:HD2	1:T:205:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:98:ASP:HB3	1:WA:255:TYR:CB	2.47	0.45
1:M:188:GLY:CA	1:OA:194:HIS:CE1	2.99	0.44
1:O:54:ARG:NH1	1:RA:88:GLU:OE1	2.32	0.44
1:P:189:TYR:CZ	1:CA:197:ARG:CZ	3.00	0.44
1:V:255:TYR:CE2	1:DA:97:LYS:HB2	2.52	0.44
1:N:188:GLY:HA2	1:DA:194:HIS:CD2	2.52	0.44
1:C:98:ASP:HB3	1:TA:255:TYR:CA	2.47	0.44
1:K:166:ASP:CB	1:BA:29:ARG:HD3	2.44	0.44
1:L:161:ARG:CG	1:T:205:TRP:CZ2	3.00	0.44
1:T:46:VAL:HA	1:NA:94:ARG:O	2.18	0.44
1:IA:189:TYR:CE1	1:KA:197:ARG:HD3	2.52	0.44
1:M:161:ARG:HG2	1:KA:205:TRP:CZ2	2.53	0.44
1:M:183:GLU:OE2	1:OA:155:GLN:HA	2.18	0.44
1:M:189:TYR:CE1	1:OA:197:ARG:NE	2.85	0.44
1:JA:161:ARG:HD2	1:FB:205:TRP:NE1	2.32	0.44
1:C:205:TRP:CZ2	1:TA:161:ARG:HG2	2.52	0.44
1:L:205:TRP:CZ2	1:VA:161:ARG:HG2	2.53	0.44
1:Z:197:ARG:NH1	1:QA:188:GLY:HA3	2.33	0.44
1:O:166:ASP:CA	1:RA:29:ARG:CD	2.92	0.44
1:LA:166:ASP:CA	1:UA:29:ARG:HD3	2.47	0.44
1:LA:197:ARG:HD3	1:UA:189:TYR:CD1	2.53	0.44
1:U:161:ARG:NH2	1:AB:179:THR:CB	2.78	0.43
1:O:54:ARG:HH12	1:RA:88:GLU:CD	2.19	0.43
1:W:197:ARG:CZ	1:PA:189:TYR:CZ	3.01	0.43
1:GA:90:ASP:OD1	1:FB:5:TYR:CE2	2.71	0.43
1:U:154:SER:OG	1:AB:183:GLU:HA	2.18	0.43
1:U:158:SER:CB	1:AB:183:GLU:OE2	2.65	0.43
1:SA:205:TRP:CZ2	1:UA:161:ARG:CG	3.00	0.43
1:I:54:ARG:NH1	1:DB:91:ASP:OD2	2.51	0.43
1:M:189:TYR:CE1	1:OA:197:ARG:CD	3.01	0.43
1:Z:154:SER:OG	1:QA:183:GLU:CG	2.64	0.43
1:GA:65:VAL:HA	1:YA:79:ARG:O	2.17	0.43
1:PA:197:ARG:HD2	1:XA:188:GLY:O	2.18	0.43
1:XA:55:LEU:HD22	1:XA:68:HIS:HB3	2.01	0.43
1:M:55:LEU:HD22	1:M:68:HIS:HB3	2.01	0.43
1:M:166:ASP:HB3	1:KA:29:ARG:HD2	2.00	0.43
1:S:189:TYR:CD1	1:NA:197:ARG:HD3	2.53	0.43
1:BA:55:LEU:HD22	1:BA:68:HIS:HB3	2.01	0.43
1:DA:55:LEU:HD22	1:DA:68:HIS:HB3	2.01	0.43
1:EA:91:ASP:OD1	1:GB:53:GLY:O	2.37	0.43
1:IA:51:SER:HB2	1:PA:48:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:55:LEU:HD22	1:UA:68:HIS:HB3	2.01	0.43
1:DB:55:LEU:HD22	1:DB:68:HIS:HB3	2.01	0.43
1:K:55:LEU:HD22	1:K:68:HIS:HB3	2.01	0.43
1:NA:2:ASN:HB2	1:HB:93:GLU:OE1	2.18	0.43
1:HB:55:LEU:HD22	1:HB:68:HIS:HB3	2.01	0.43
1:A:179:THR:CA	1:X:161:ARG:NH2	2.81	0.43
1:H:55:LEU:HD22	1:H:68:HIS:HB3	2.01	0.43
1:N:55:LEU:HD22	1:N:68:HIS:HB3	2.01	0.43
1:R:55:LEU:HD22	1:R:68:HIS:HB3	2.01	0.43
1:T:55:LEU:HD22	1:T:68:HIS:HB3	2.01	0.43
1:V:55:LEU:HD22	1:V:68:HIS:HB3	2.01	0.43
1:V:161:ARG:HD2	1:DA:205:TRP:CE2	2.53	0.43
1:FA:93:GLU:OE1	1:JA:2:ASN:HA	2.19	0.43
1:KA:1:MET:O	1:WA:12:THR:HB	2.18	0.43
1:H:205:TRP:CE2	1:YA:161:ARG:CG	3.02	0.43
1:FA:255:TYR:HB3	1:NA:98:ASP:HB3	2.01	0.43
1:D:46:VAL:HA	1:TA:94:ARG:O	2.19	0.42
1:E:55:LEU:HD22	1:E:68:HIS:HB3	2.01	0.42
1:R:98:ASP:HB3	1:DB:255:TYR:HD1	1.81	0.42
1:U:55:LEU:HD22	1:U:68:HIS:HB3	2.01	0.42
1:MA:55:LEU:HD22	1:MA:68:HIS:HB3	2.01	0.42
1:C:55:LEU:HD22	1:C:68:HIS:HB3	2.01	0.42
1:H:94:ARG:HD2	1:YA:70:ARG:NH1	2.34	0.42
1:Q:55:LEU:HD22	1:Q:68:HIS:HB3	2.01	0.42
1:S:55:LEU:HD22	1:S:68:HIS:HB3	2.01	0.42
1:RA:55:LEU:HD22	1:RA:68:HIS:HB3	2.01	0.42
1:GB:55:LEU:HD22	1:GB:68:HIS:HB3	2.01	0.42
1:Z:55:LEU:HD22	1:Z:68:HIS:HB3	2.01	0.42
1:Z:154:SER:HB2	1:QA:183:GLU:HG2	2.01	0.42
1:LA:55:LEU:HD22	1:LA:68:HIS:HB3	2.01	0.42
1:OA:55:LEU:HD22	1:OA:68:HIS:HB3	2.01	0.42
1:PA:55:LEU:HD22	1:PA:68:HIS:HB3	2.01	0.42
1:ZA:55:LEU:HD22	1:ZA:68:HIS:HB3	2.01	0.42
1:A:29:ARG:HD3	1:X:166:ASP:HB3	2.00	0.42
1:H:189:TYR:CZ	1:YA:197:ARG:NE	2.88	0.42
1:V:255:TYR:CA	1:DA:98:ASP:HB3	2.49	0.42
1:W:53:GLY:O	1:PA:91:ASP:OD1	2.37	0.42
1:EA:155:GLN:HA	1:VA:183:GLU:OE2	2.18	0.42
1:GA:55:LEU:HD22	1:GA:68:HIS:HB3	2.01	0.42
1:FB:55:LEU:HD22	1:FB:68:HIS:HB3	2.01	0.42
1:L:197:ARG:NH1	1:T:188:GLY:C	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:91:ASP:OD2	1:AB:54:ARG:NH1	2.52	0.42
1:CA:55:LEU:HD22	1:CA:68:HIS:HB3	2.01	0.42
1:CA:188:GLY:HA2	1:SA:194:HIS:CE1	2.54	0.42
1:FA:55:LEU:HD22	1:FA:68:HIS:HB3	2.01	0.42
1:KA:55:LEU:HD22	1:KA:68:HIS:HB3	2.01	0.42
1:LA:54:ARG:NH1	1:UA:91:ASP:OD2	2.52	0.42
1:C:205:TRP:CE2	1:TA:161:ARG:HD2	2.55	0.42
1:IA:55:LEU:HD22	1:IA:68:HIS:HB3	2.01	0.42
1:SA:205:TRP:CE2	1:UA:161:ARG:HD2	2.55	0.42
1:WA:55:LEU:HD22	1:WA:68:HIS:HB3	2.01	0.42
1:H:29:ARG:NE	1:YA:166:ASP:HA	2.34	0.42
1:QA:55:LEU:HD22	1:QA:68:HIS:HB3	2.01	0.42
1:D:55:LEU:HD22	1:D:68:HIS:HB3	2.01	0.42
1:E:154:SER:OG	1:WA:183:GLU:CB	2.68	0.42
1:F:29:ARG:CD	1:HA:166:ASP:CB	2.60	0.42
1:W:12:THR:CB	1:QA:1:MET:O	2.67	0.42
1:FA:93:GLU:CD	1:JA:2:ASN:HA	2.40	0.42
1:JA:91:ASP:OD1	1:WA:53:GLY:O	2.37	0.42
1:C:154:SER:OG	1:V:183:GLU:CG	2.57	0.42
1:H:54:ARG:NH1	1:FA:91:ASP:OD2	2.53	0.42
1:H:91:ASP:CG	1:YA:53:GLY:O	2.55	0.42
1:L:197:ARG:HH11	1:T:188:GLY:CA	2.32	0.42
1:EA:55:LEU:HD22	1:EA:68:HIS:HB3	2.01	0.42
1:JA:55:LEU:HD22	1:JA:68:HIS:HB3	2.01	0.42
1:JA:98:ASP:HB3	1:WA:255:TYR:HB3	2.02	0.42
1:LA:45:PRO:O	1:OA:70:ARG:NH1	2.43	0.42
1:VA:55:LEU:HD22	1:VA:68:HIS:HB3	2.01	0.42
1:ZA:158:SER:CB	1:HB:183:GLU:OE2	2.66	0.42
1:BB:55:LEU:HD22	1:BB:68:HIS:HB3	2.01	0.42
1:D:98:ASP:HB3	1:IA:255:TYR:CB	2.50	0.42
1:F:55:LEU:HD22	1:F:68:HIS:HB3	2.01	0.42
1:N:179:THR:OG1	1:DA:161:ARG:NH2	2.50	0.42
1:P:55:LEU:HD22	1:P:68:HIS:HB3	2.01	0.42
1:W:55:LEU:HD22	1:W:68:HIS:HB3	2.01	0.42
1:JA:161:ARG:HD2	1:FB:205:TRP:CD1	2.55	0.42
1:NA:55:LEU:HD22	1:NA:68:HIS:HB3	2.01	0.42
1:P:189:TYR:CE1	1:CA:197:ARG:NE	2.88	0.41
1:HA:55:LEU:HD22	1:HA:68:HIS:HB3	2.01	0.41
1:JA:188:GLY:O	1:WA:197:ARG:HD2	2.20	0.41
1:KA:46:VAL:HA	1:WA:94:ARG:O	2.20	0.41
1:RA:123:TYR:OH	1:BB:61:PRO:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:55:LEU:HD22	1:SA:68:HIS:HB3	2.01	0.41
1:TA:55:LEU:HD22	1:TA:68:HIS:HB3	2.01	0.41
1:E:161:ARG:HG2	1:WA:205:TRP:CZ2	2.55	0.41
1:O:52:THR:O	1:RA:96:SER:HB2	2.20	0.41
1:O:188:GLY:O	1:Q:197:ARG:HD3	2.19	0.41
1:FA:12:THR:HG23	1:JA:5:TYR:OH	2.20	0.41
1:AB:55:LEU:HD22	1:AB:68:HIS:HB3	2.01	0.41
1:F:110:LYS:HD3	1:QA:65:VAL:HG22	2.02	0.41
1:I:55:LEU:HD22	1:I:68:HIS:HB3	2.01	0.41
1:L:55:LEU:HD22	1:L:68:HIS:HB3	2.01	0.41
1:JA:188:GLY:HA2	1:WA:194:HIS:ND1	2.33	0.41
1:YA:55:LEU:HD22	1:YA:68:HIS:HB3	2.01	0.41
1:C:91:ASP:OD1	1:TA:53:GLY:O	2.38	0.41
1:FA:255:TYR:CB	1:NA:98:ASP:HB3	2.50	0.41
1:MA:29:ARG:HD2	1:HB:166:ASP:HB3	2.02	0.41
1:C:255:TYR:HD1	1:V:98:ASP:HB3	1.86	0.41
1:O:55:LEU:HD22	1:O:68:HIS:HB3	2.01	0.41
1:K:60:ALA:HA	1:K:61:PRO:HD3	1.99	0.41
1:L:197:ARG:NH1	1:T:188:GLY:CA	2.82	0.41
1:M:205:TRP:CE2	1:OA:161:ARG:HD2	2.54	0.41
1:T:94:ARG:O	1:HB:46:VAL:HA	2.21	0.41
1:Z:53:GLY:O	1:QA:91:ASP:OD1	2.38	0.41
1:IA:48:ALA:HB2	1:PA:51:SER:HB2	2.01	0.41
1:KA:46:VAL:HG12	1:WA:94:ARG:C	2.38	0.41
1:I:255:TYR:CZ	1:DB:97:LYS:HB2	2.55	0.41
1:N:197:ARG:HD3	1:TA:189:TYR:CD1	2.55	0.41
1:O:161:ARG:NH2	1:RA:179:THR:HA	2.36	0.41
1:X:55:LEU:HD22	1:X:68:HIS:HB3	2.01	0.41
1:CA:189:TYR:CE1	1:SA:197:ARG:NE	2.88	0.41
1:A:55:LEU:HD11	1:FB:77:ARG:CZ	2.50	0.41
1:P:29:ARG:HD3	1:CA:166:ASP:CB	2.46	0.41
1:P:98:ASP:HB3	1:CA:255:TYR:CD1	2.55	0.41
1:CA:189:TYR:CE1	1:SA:197:ARG:CD	3.01	0.41
1:SA:205:TRP:NE1	1:UA:161:ARG:HD2	2.35	0.41
1:A:179:THR:CG2	1:X:161:ARG:HH21	2.33	0.41
1:C:54:ARG:NH1	1:V:91:ASP:OD2	2.50	0.41
1:C:183:GLU:HG2	1:TA:154:SER:OG	2.21	0.41
1:G:55:LEU:HD22	1:G:68:HIS:HB3	2.01	0.41
1:L:197:ARG:CZ	1:T:189:TYR:CZ	3.04	0.41
1:Q:60:ALA:HA	1:Q:61:PRO:HD3	1.99	0.41
1:RA:34:ARG:HH11	1:RA:34:ARG:HD3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:183:GLU:HG2	1:Q:154:SER:OG	2.21	0.41
1:GA:81:PRO:HD2	1:YA:64:GLY:O	2.21	0.41
1:A:55:LEU:HD22	1:A:68:HIS:HB3	2.01	0.40
1:A:60:ALA:HA	1:A:61:PRO:HD3	1.99	0.40
1:C:193:GLU:O	1:C:197:ARG:HG3	2.22	0.40
1:N:193:GLU:O	1:N:197:ARG:HG3	2.22	0.40
1:O:193:GLU:O	1:O:197:ARG:HG3	2.22	0.40
1:P:189:TYR:CE1	1:CA:197:ARG:HD3	2.56	0.40
1:R:193:GLU:O	1:R:197:ARG:HG3	2.22	0.40
1:T:255:TYR:CD1	1:GB:98:ASP:HB3	2.56	0.40
1:U:54:ARG:NH1	1:AB:88:GLU:OE2	2.53	0.40
1:BA:193:GLU:O	1:BA:197:ARG:HG3	2.21	0.40
1:TA:193:GLU:O	1:TA:197:ARG:HG3	2.21	0.40
1:VA:36:VAL:HG11	1:VA:172:LEU:HD11	2.04	0.40
1:YA:193:GLU:O	1:YA:197:ARG:HG3	2.21	0.40
1:BB:193:GLU:O	1:BB:197:ARG:HG3	2.22	0.40
1:HB:36:VAL:HG11	1:HB:172:LEU:HD11	2.04	0.40
1:C:97:LYS:HB2	1:TA:255:TYR:CE2	2.56	0.40
1:Q:36:VAL:HG11	1:Q:172:LEU:HD11	2.04	0.40
1:S:166:ASP:HB3	1:YA:29:ARG:HD3	2.02	0.40
1:T:48:ALA:HB2	1:FA:51:SER:HB2	2.02	0.40
1:U:36:VAL:HG11	1:U:172:LEU:HD11	2.04	0.40
1:DA:36:VAL:HG11	1:DA:172:LEU:HD11	2.04	0.40
1:GA:36:VAL:HG11	1:GA:172:LEU:HD11	2.04	0.40
1:JA:189:TYR:OH	1:WA:197:ARG:NH2	2.54	0.40
1:LA:193:GLU:O	1:LA:197:ARG:HG3	2.22	0.40
1:SA:179:THR:HG23	1:UA:158:SER:OG	2.21	0.40
1:SA:188:GLY:O	1:UA:197:ARG:NH1	2.43	0.40
1:SA:193:GLU:O	1:SA:197:ARG:HG3	2.21	0.40
1:D:179:THR:OG1	1:IA:161:ARG:NH2	2.39	0.40
1:D:193:GLU:O	1:D:197:ARG:HG3	2.21	0.40
1:N:36:VAL:HG11	1:N:172:LEU:HD11	2.04	0.40
1:Q:188:GLY:O	1:AB:197:ARG:HD3	2.20	0.40
1:R:91:ASP:CG	1:DB:53:GLY:O	2.59	0.40
1:S:193:GLU:O	1:S:197:ARG:HG3	2.22	0.40
1:U:98:ASP:CB	1:RA:255:TYR:O	2.70	0.40
1:U:193:GLU:O	1:U:197:ARG:HG3	2.22	0.40
1:EA:193:GLU:O	1:EA:197:ARG:HG3	2.21	0.40
1:JA:91:ASP:OD2	1:WA:54:ARG:NH1	2.53	0.40
1:JA:193:GLU:O	1:JA:197:ARG:HG3	2.21	0.40
1:LA:36:VAL:HG11	1:LA:172:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:193:GLU:O	1:RA:197:ARG:HG3	2.21	0.40
1:AB:193:GLU:O	1:AB:197:ARG:HG3	2.22	0.40
1:BB:36:VAL:HG11	1:BB:172:LEU:HD11	2.04	0.40
1:G:193:GLU:O	1:G:197:ARG:HG3	2.22	0.40
1:S:36:VAL:HG11	1:S:172:LEU:HD11	2.04	0.40
1:U:28:LYS:HB2	1:U:28:LYS:HE2	1.96	0.40
1:EA:189:TYR:CE1	1:GB:197:ARG:CD	3.03	0.40
1:GA:193:GLU:O	1:GA:197:ARG:HG3	2.22	0.40
1:HA:193:GLU:O	1:HA:197:ARG:HG3	2.22	0.40
1:MA:36:VAL:HG11	1:MA:172:LEU:HD11	2.04	0.40
1:PA:193:GLU:O	1:PA:197:ARG:HG3	2.22	0.40
1:TA:36:VAL:HG11	1:TA:172:LEU:HD11	2.04	0.40
1:XA:36:VAL:HG11	1:XA:172:LEU:HD11	2.04	0.40
1:ZA:193:GLU:O	1:ZA:197:ARG:HG3	2.21	0.40
1:DB:36:VAL:HG11	1:DB:172:LEU:HD11	2.04	0.40
1:G:28:LYS:HB2	1:G:28:LYS:HE2	1.96	0.40
1:I:193:GLU:O	1:I:197:ARG:HG3	2.22	0.40
1:P:36:VAL:HG11	1:P:172:LEU:HD11	2.04	0.40
1:V:36:VAL:HG11	1:V:172:LEU:HD11	2.04	0.40
1:W:197:ARG:HD3	1:PA:189:TYR:CE1	2.57	0.40
1:FA:193:GLU:O	1:FA:197:ARG:HG3	2.21	0.40
1:HA:36:VAL:HG11	1:HA:172:LEU:HD11	2.04	0.40
1:IA:36:VAL:HG11	1:IA:172:LEU:HD11	2.04	0.40
1:JA:155:GLN:HG2	1:FB:183:GLU:CD	2.41	0.40
1:UA:193:GLU:O	1:UA:197:ARG:HG3	2.22	0.40
1:XA:84:LEU:HD23	1:XA:84:LEU:HA	1.93	0.40
1:YA:36:VAL:HG11	1:YA:172:LEU:HD11	2.04	0.40
1:DB:193:GLU:O	1:DB:197:ARG:HG3	2.22	0.40
1:FB:193:GLU:O	1:FB:197:ARG:HG3	2.22	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 PDB entries followed by that with respect to all EM entries.

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	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	BA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	BB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	C	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	CA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	D	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	DA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	DB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	E	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	EA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	F	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	FA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	FB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	G	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	GA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	GB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	H	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	HA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	HB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	I	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	IA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	JA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	K	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	KA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	L	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	LA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	M	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	MA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	N	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	NA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	O	263/265 (99%)	259 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	P	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	PA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Q	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	QA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	R	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	RA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	S	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	SA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	T	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	TA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	U	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	UA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	V	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	VA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	W	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	WA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	X	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	XA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	YA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Z	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	ZA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
All	All	14202/14310 (99%)	13986 (98%)	216 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	AB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	BA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	BB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	C	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	CA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	D	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	DA	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	DB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	E	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	EA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	F	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	FA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	FB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	G	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	GA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	GB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	H	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	HA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	HB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	I	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	IA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	JA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	K	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	KA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	L	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	LA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	M	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	MA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	N	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	NA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	O	218/218 (100%)	216 (99%)	2 (1%)	75	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	OA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	P	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	PA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	Q	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	QA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	R	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	RA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	S	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	SA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	T	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	TA	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	U	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	UA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	V	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	VA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	W	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	WA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	X	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	XA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	YA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	Z	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	ZA	218/218 (100%)	216 (99%)	2 (1%)	75	83
All	All	11772/11772 (100%)	11660 (99%)	112 (1%)	71	81

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	58	VAL
1	C	54	ARG
1	C	58	VAL
1	D	54	ARG
1	D	58	VAL
1	E	54	ARG

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Mol	Chain	Res	Type
1	E	58	VAL
1	F	54	ARG
1	F	58	VAL
1	G	54	ARG
1	G	58	VAL
1	H	54	ARG
1	H	58	VAL
1	I	54	ARG
1	I	58	VAL
1	K	54	ARG
1	K	58	VAL
1	L	54	ARG
1	L	58	VAL
1	M	54	ARG
1	M	58	VAL
1	N	54	ARG
1	N	58	VAL
1	O	54	ARG
1	O	58	VAL
1	P	54	ARG
1	P	58	VAL
1	Q	54	ARG
1	Q	58	VAL
1	R	54	ARG
1	R	58	VAL
1	S	54	ARG
1	S	58	VAL
1	T	54	ARG
1	T	58	VAL
1	T	194	HIS
1	U	54	ARG
1	U	58	VAL
1	V	54	ARG
1	V	58	VAL
1	V	194	HIS
1	W	54	ARG
1	W	58	VAL
1	X	54	ARG
1	X	58	VAL
1	Z	54	ARG
1	Z	58	VAL
1	BA	54	ARG

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Mol	Chain	Res	Type
1	BA	58	VAL
1	CA	54	ARG
1	CA	58	VAL
1	DA	54	ARG
1	DA	58	VAL
1	DA	194	HIS
1	EA	54	ARG
1	EA	58	VAL
1	FA	54	ARG
1	FA	58	VAL
1	GA	54	ARG
1	GA	58	VAL
1	HA	54	ARG
1	HA	58	VAL
1	IA	54	ARG
1	IA	58	VAL
1	JA	54	ARG
1	JA	58	VAL
1	KA	54	ARG
1	KA	58	VAL
1	LA	54	ARG
1	LA	58	VAL
1	MA	54	ARG
1	MA	58	VAL
1	NA	54	ARG
1	NA	58	VAL
1	OA	54	ARG
1	OA	58	VAL
1	PA	54	ARG
1	PA	58	VAL
1	QA	54	ARG
1	QA	58	VAL
1	RA	54	ARG
1	RA	58	VAL
1	SA	54	ARG
1	SA	58	VAL
1	TA	54	ARG
1	TA	58	VAL
1	TA	194	HIS
1	UA	54	ARG
1	UA	58	VAL
1	VA	54	ARG

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Mol	Chain	Res	Type
1	VA	58	VAL
1	WA	54	ARG
1	WA	58	VAL
1	XA	54	ARG
1	XA	58	VAL
1	YA	54	ARG
1	YA	58	VAL
1	ZA	54	ARG
1	ZA	58	VAL
1	AB	54	ARG
1	AB	58	VAL
1	BB	54	ARG
1	BB	58	VAL
1	DB	54	ARG
1	DB	58	VAL
1	FB	54	ARG
1	FB	58	VAL
1	GB	54	ARG
1	GB	58	VAL
1	HB	54	ARG
1	HB	58	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	ASN
1	I	3	ASN
1	JA	194	HIS
1	OA	194	HIS
1	WA	194	HIS
1	FB	3	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.