Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2022 – 12:47 pm GMT

PDB ID	:	6YFP
Title	:	Virus-like particle of bacteriophage GQ-112
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.10 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 (i) symbol.

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

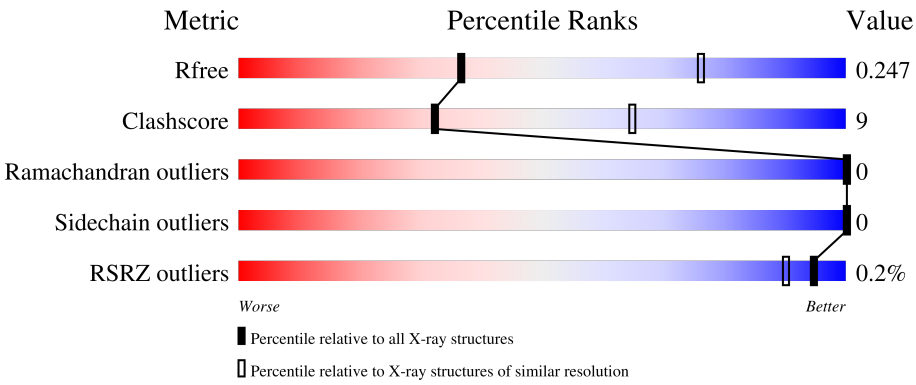
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AA	164	80% 20%
1	AB	164	77% 23%
1	AC	164	% 84% 16%
1	AD	164	79% 21%
1	AE	164	75% 25%

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Mol	Chain	Length	Quality of chain
1	AF	164	82% 18%
1	AG	164	80% 20%
1	AH	164	76% 24%
1	AI	164	% 84% 16%
1	AJ	164	80% 20%
1	AK	164	76% 24%
1	AL	164	% 82% 18%
1	AM	164	79% 21%
1	AN	164	% 79% 21%
1	AO	164	% 82% 18%
1	AP	164	81% 19%
1	AQ	164	78% 22%
1	AR	164	80% 20%
1	AS	164	80% 20%
1	AT	164	76% 24%
1	AU	164	82% 18%
1	AV	164	79% 21%
1	AW	164	76% 24%
1	AX	164	84% 16%
1	AY	164	81% 19%
1	AZ	164	79% 21%
1	BA	164	% 82% 18%
1	BB	164	80% 20%
1	BC	164	76% 24%
1	BD	164	% 83% 17%

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Mol	Chain	Length	Quality of chain
1	BE	164	80% 20%
1	BF	164	77% 23%
1	BG	164	% 80% 20%
1	BH	164	79% 21%
1	BI	164	79% 21%
1	BJ	164	80% 20%
1	BK	164	81% 19%
1	BL	164	77% 23%
1	BM	164	% 84% 16%
1	BN	164	80% 20%
1	BO	164	79% 21%
1	BP	164	84% 16%
1	BQ	164	80% 20%
1	BR	164	79% 21%
1	BS	164	% 90% 10%
1	BT	164	80% 20%
1	BU	164	77% 23%
1	BV	164	% 82% 18%
1	BW	164	80% 20%
1	BX	164	79% 21%
1	BY	164	% 84% 16%
1	BZ	164	80% 20%
1	CA	164	77% 23%
1	CB	164	83% 17%
1	CC	164	80% 20%

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Mol	Chain	Length	Quality of chain
1	CD	164	77% 23%
1	CE	164	82% 18%
1	CF	164	80% 20%
1	CG	164	78% 22%
1	CH	164	.% 90% 10%
1	CI	164	80% 20%
1	CJ	164	79% 21%
1	CK	164	2% 78% 22%
1	CL	164	80% 20%
1	CM	164	77% 23%
1	CN	164	82% 18%
1	CO	164	82% 18%
1	CP	164	78% 22%
1	CQ	164	.% 90% 10%
1	CR	164	80% 20%
1	CS	164	79% 21%
1	CT	164	81% 19%
1	CU	164	80% 20%
1	CV	164	77% 23%
1	CW	164	83% 17%
1	CX	164	80% 20%
1	CY	164	78% 22%
1	CZ	164	.% 83% 17%
1	DA	164	80% 20%
1	DB	164	78% 22%

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Mol	Chain	Length	Quality of chain
1	DC	164	%, 82%, 18%
1	DD	164	81%, 19%
1	DE	164	79%, 21%
1	DF	164	80%, 20%
1	DG	164	80%, 20%
1	DH	164	76%, 24%
1	DI	164	%, 84%, 16%
1	DJ	164	80%, 20%
1	DK	164	78%, 22%
1	DL	164	91%, 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 116370 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 coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	164	1293	811	223	256	3	0	0	0
1	AB	164	1293	811	223	256	3	0	0	0
1	AC	164	1293	811	223	256	3	0	0	0
1	AD	164	1293	811	223	256	3	0	0	0
1	AE	164	1293	811	223	256	3	0	0	0
1	AF	164	1293	811	223	256	3	0	0	0
1	AG	164	1293	811	223	256	3	0	0	0
1	AH	164	1293	811	223	256	3	0	0	0
1	AI	164	1293	811	223	256	3	0	0	0
1	AJ	164	1293	811	223	256	3	0	0	0
1	AK	164	1293	811	223	256	3	0	0	0
1	AL	164	1293	811	223	256	3	0	0	0
1	AM	164	1293	811	223	256	3	0	0	0
1	AN	164	1293	811	223	256	3	0	0	0
1	AO	164	1293	811	223	256	3	0	0	0
1	AP	164	1293	811	223	256	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AR	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AS	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AT	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AU	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AV	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AW	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AX	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AY	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	AZ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BA	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BB	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BC	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BD	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BE	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BF	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BG	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BH	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BI	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BJ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BK	164	1293	811	223	256	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BL	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BM	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BN	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BO	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BP	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BQ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BR	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BS	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BT	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BU	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BV	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BW	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BX	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BY	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	BZ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CA	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CB	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CC	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CD	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CE	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CF	164	1293	811	223	256	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CG	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CH	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CI	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CJ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CK	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CL	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CM	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CN	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CO	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CP	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CQ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CR	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CS	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CT	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CU	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CV	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CW	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CX	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CY	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	CZ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DA	164	1293	811	223	256	3	0	0	0

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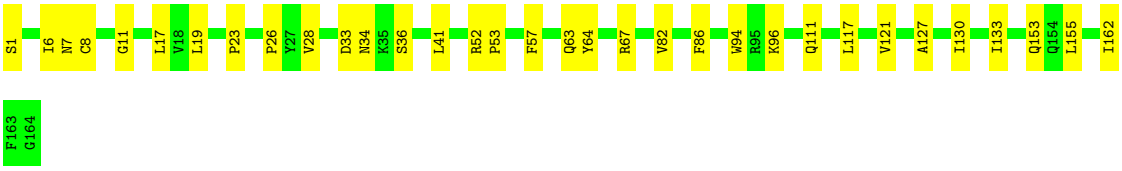
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	DB	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DC	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DD	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DE	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DF	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DG	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DH	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DI	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DJ	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DK	164	1293	811	223	256	3	0	0	0
			Total	C	N	O	S			
1	DL	164	1293	811	223	256	3	0	0	0

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 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.

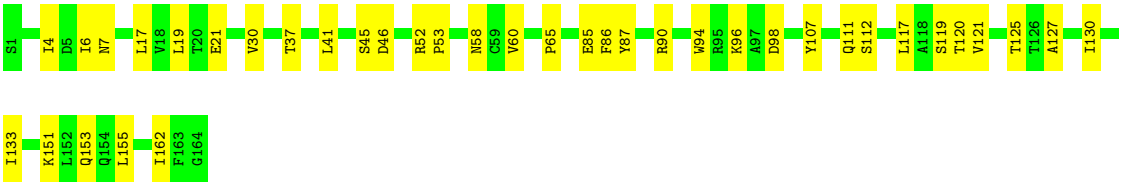
• Molecule 1: coat protein

Chain AA:



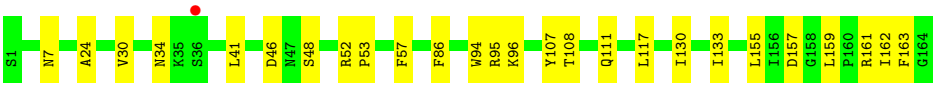
• Molecule 1: coat protein

Chain AB:



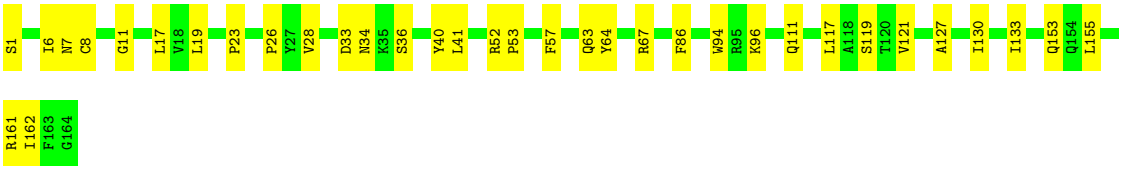
• Molecule 1: coat protein

Chain AC:



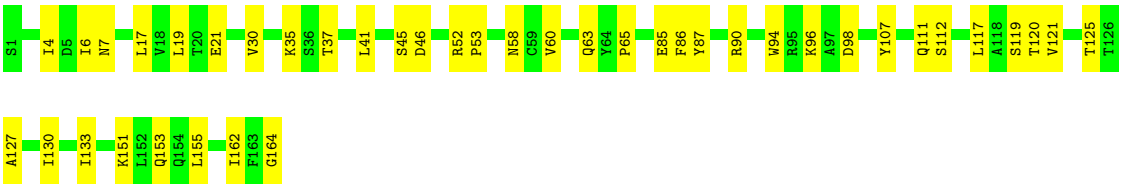
• Molecule 1: coat protein

Chain AD:



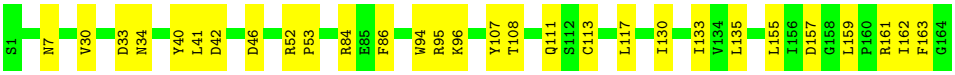
• Molecule 1: coat protein

Chain AE: 75% 25%



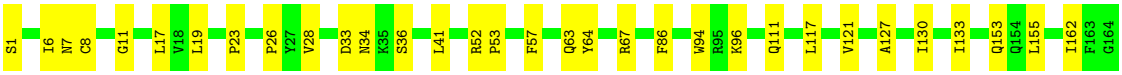
- Molecule 1: coat protein

Chain AF: 82% 18%



- Molecule 1: coat protein

Chain AG: 80% 20%

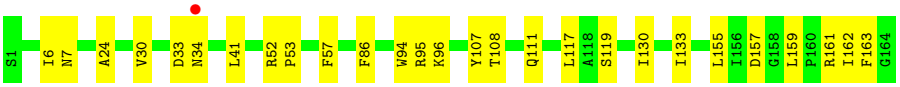


- Molecule 1: coat protein

Chain AH: 76% 24%

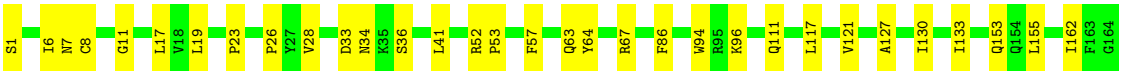
- Molecule 1: coat protein

Chain AI: % 84% 16%



- Molecule 1: coat protein

Chain AJ: 80% 20%

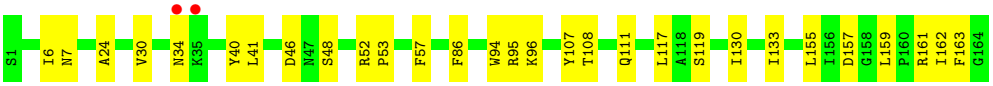


- Molecule 1: coat protein

Chain AK: 76% 24%

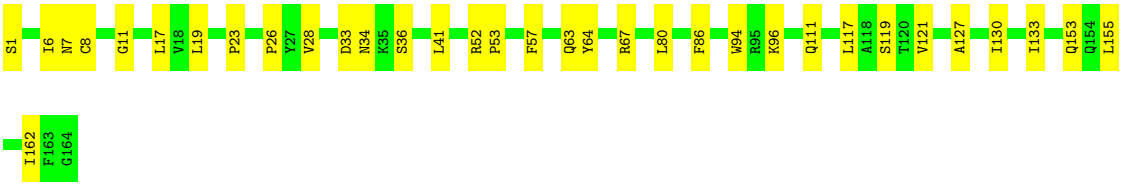
• Molecule 1: coat protein

Chain AL:



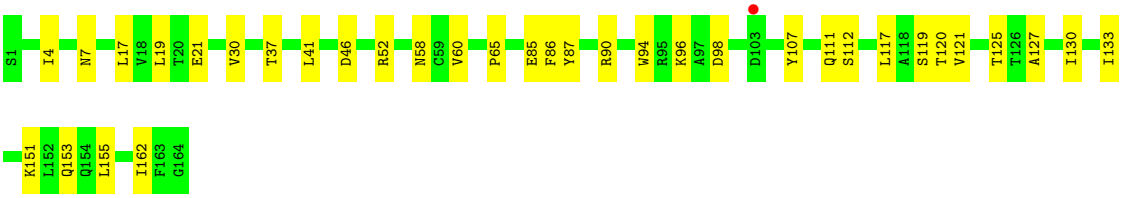
• Molecule 1: coat protein

Chain AM:



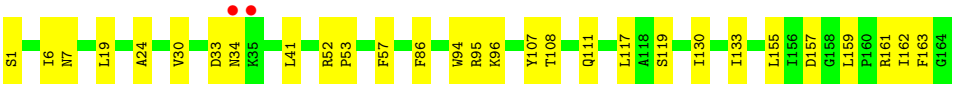
• Molecule 1: coat protein

Chain AN:



• Molecule 1: coat protein

Chain AO:

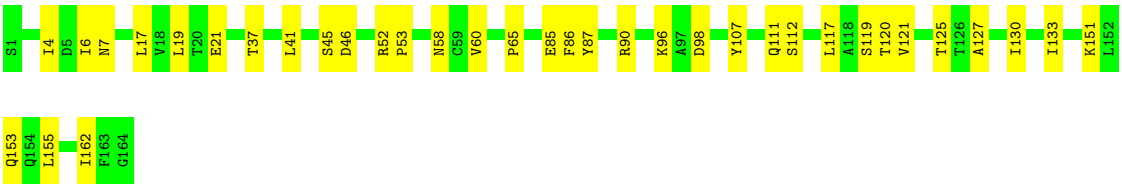


• Molecule 1: coat protein

Chain AP:

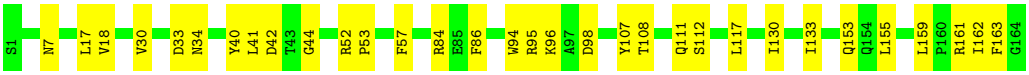
• Molecule 1: coat protein

Chain AQ: 78% 22%



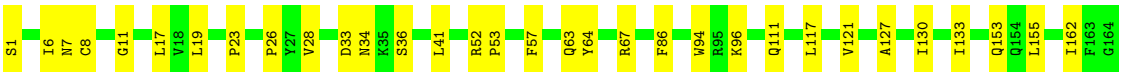
• Molecule 1: coat protein

Chain AR: 80% 20%



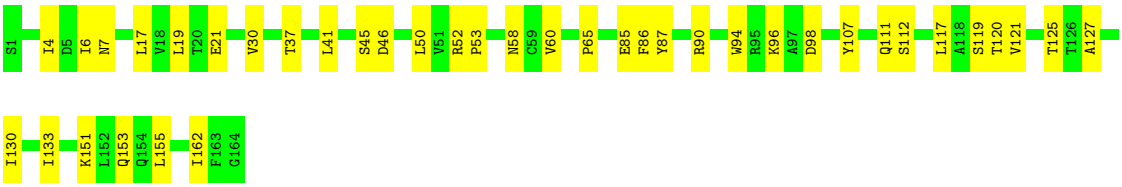
• Molecule 1: coat protein

Chain AS: 80% 20%



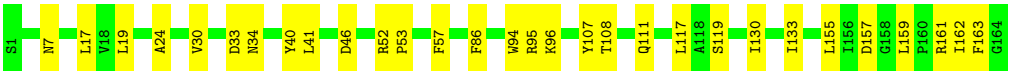
• Molecule 1: coat protein

Chain AT: 76% 24%



• Molecule 1: coat protein

Chain AU: 82% 18%



• Molecule 1: coat protein

Chain AV: 79% 21%

• Molecule 1: coat protein

Chain AW: 76% 24%

S1 I4 D5 I6 N7 L17 V18 L19 T20 E21 V30 T37 L41 S45 D46 R52 P53 N58 C59 V60 P65 E85 F86 Y87 R90 W94 R95 K96 A97 D98 Y107 Q111 S112 L117 A118 S119 T120 V121 T125 T126 A127 I130

I133 K151 L152 Q153 Q154 L155 I162 F163 G164

• Molecule 1: coat protein

Chain AX: 84% 16%

S1 N7 N16 L17 V18 A24 V30 D33 L41 R52 P53 F57 F86 W94 R95 K96 A97 D98 Y107 T108 Q111 L117 A127 I130 I133 Q153 Q154 L155 L159 I162 F163 G164

• Molecule 1: coat protein

Chain AY: 81% 19%

S1 I6 N7 C8 G11 L17 V18 L19 P23 P26 Y27 V28 D33 S36 L41 R52 P53 F57 Q63 Y64 R67 F86 W94 R95 K96 Q111 L117 V121 A127 I130 I133 Q153 Q154 L155 I162 F163 G164

• Molecule 1: coat protein

Chain AZ: 79% 21%

S1 I4 D5 I6 N7 L17 V18 L19 T20 E21 T37 L41 S45 D46 R52 P53 N58 P65 F86 Y87 R90 K96 A97 D98 Y107 Q111 S112 L117 A118 S119 T120 V121 T125 T126 A127 I130 I133 K151 L152 Q153 Q154 L155

I162 F163 G164

• Molecule 1: coat protein

Chain BA: % 82% 18%

S1 N7 A24 V30 D33 N34 Y40 L41 D46 R52 P53 R84 E85 F86 W94 R95 K96 Y107 T108 Q111 L117 I130 I133 W149 L155 I156 D157 G158 L159 P160 R161 I162 F163 G164

• Molecule 1: coat protein

Chain BB: 80% 20%

S1 I6 N7 C8 G11 L17 V18 L19 P23 P26 Y27 V28 D33 S36 Y40 L41 R52 P53 F57 Q63 Y64 R67 L80 F86 W94 R95 K96 Q111 L117 V121 A127 I130 I133 Q153 Q154 L155 I162

F163 G164

• Molecule 1: coat protein

Chain BC: 76% 24%

S1 I4 D5 I6 N7 L17 V18 L19 T20 E21 V30 T37 L41 S45 D46 L50 V51 R52 P53 N58 C59 V60 P65 E85 F86 Y87 R90 K96 A97 D98 Y107 Q111 S112 L117 A118 S119 T120 V121 T125 T126 A127 I130

I133 K151 L152 Q153 Q154 L155 I162 F163 G164

• Molecule 1: coat protein

Chain BD: % 83% 17%

S1 N7 A24 V30 D33 N34 Y40 L41 D46 R52 P53 F57 F86 W94 R95 K96 Y107 T108 Q111 L117 A118 S119 I130 I133 L155 T156 D157 G158 L159 P160 R161 I162 F163 G164

• Molecule 1: coat protein

Chain BE: 80% 20%

S1 I6 N7 C8 G11 L17 V18 L19 P23 P26 Y27 V28 D33 N34 K35 S36 L41 R52 P53 F57 Q63 Y64 R67 F86 W94 R95 K96 Q111 L117 V121 A127 I130 I133 Q153 Q154 L155 T156 D157 I162

F163 G164

• Molecule 1: coat protein

Chain BF: 77% 23%

S1 I4 D5 I6 N7 L17 V18 L19 T20 E21 V30 T37 L41 S45 D46 L50 V51 R52 P53 N58 C59 V60 P65 E85 F86 Y87 R90 K96 A97 D98 Y107 Q111 S112 L117 A118 S119 T120 V121 T125 T126 A127 I130

I133 K151 L152 Q153 Q154 L155 I162 F163 G164

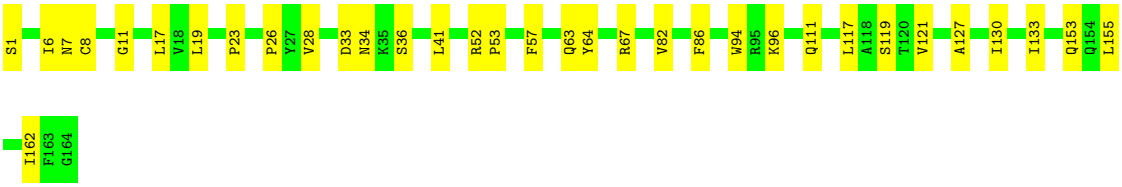
• Molecule 1: coat protein

Chain BG: % 80% 20%

S1 Y2 N7 L19 A24 E25 V30 D33 N34 K35 I38 E39 Y40 L41 L50 V51 R52 P53 F57 D78 F86 W94 R95 K96 Y107 T108 Q111 L117 A118 S119 I130 I133 L155 I156 D157 R161 I162 F163 G164

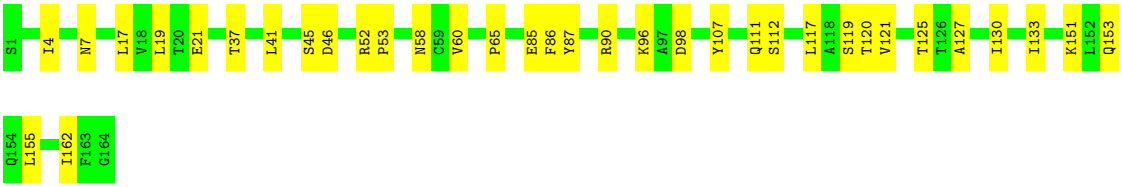
• Molecule 1: coat protein

Chain BH: 79% 21%



• Molecule 1: coat protein

Chain BI: 79% 21%

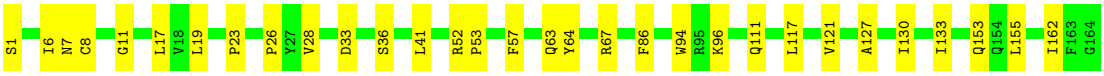


• Molecule 1: coat protein

Chain BJ: 80% 20%

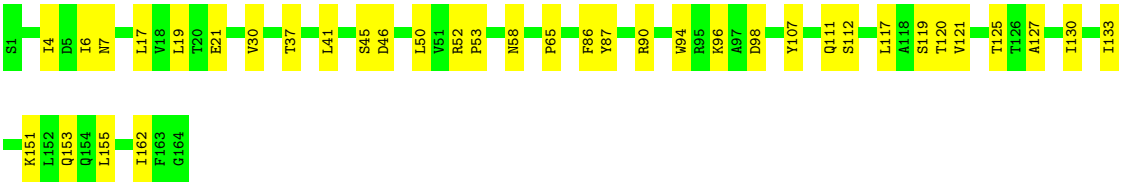
• Molecule 1: coat protein

Chain BK: 81% 19%



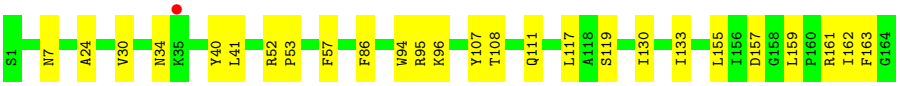
• Molecule 1: coat protein

Chain BL: 77% 23%



• Molecule 1: coat protein

Chain BM: % 84% 16%



• Molecule 1: coat protein

Chain BN: 80% 20%

S1 I6 N7 C8 G11 L17 V18 L19 P23 P26 Y27 V28 D33 N34 K35 S36 L41 R52 P53 F57 Q63 Y64 R67 F86 W94 R95 K96 Q111 L117 V121 A127 I130 I133 Q153 Q154 L155 I162 F163 G164

• Molecule 1: coat protein

Chain BO: 79% 21%

S1 I4 N7 L17 V18 L19 T20 E21 V30 T37 L41 S45 D46 R52 P53 N58 P65 F86 Y87 R90 K96 A97 D98 Y107 Q111 S112 L117 A118 S119 T120 V121 T125 T126 A127 I130 I133 K151 L152 Q153 Q154

L155 I162 F163 G164

• Molecule 1: coat protein

Chain BP: 84% 16%

S1 N7 A24 V30 D33 N34 L41 D46 N47 S48 R52 P53 F57 F86 W94 R95 K96 Y107 T108 Q111 L117 I130 I133 L155 I156 D157 G158 L159 P160 R161 I162 F163 G164

• Molecule 1: coat protein

Chain BQ: 80% 20%

S1 I6 N7 C8 G11 D12 L17 V18 L19 P23 P26 D33 N34 K35 S36 L41 R52 P53 F57 Q63 Y64 R67 V82 F86 W94 R95 K96 Q111 L117 V121 A127 I130 I133 Q153 Q154 L155 I162 F163

G164

• Molecule 1: coat protein

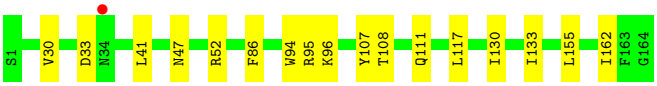
Chain BR: 79% 21%

S1 I4 N7 L17 V18 L19 T20 E21 T37 L41 S45 D46 L50 W51 R52 P53 N58 P65 F86 Y87 R90 W94 R95 K96 A97 D98 Y107 Q111 S112 L117 A118 S119 T120 V121 T125 T126 A127 I130 I133 K151 L152

Q153 Q154 L155 I162 F163 G164

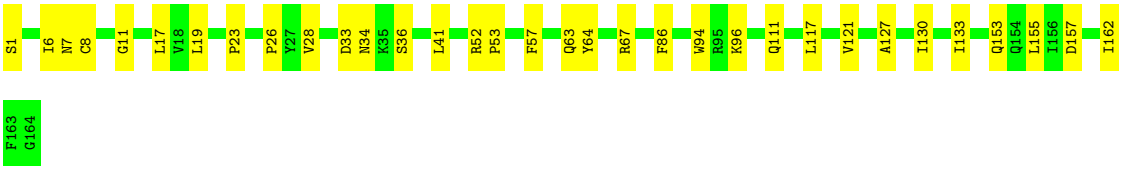
• Molecule 1: coat protein

Chain BS: % 90% 10%



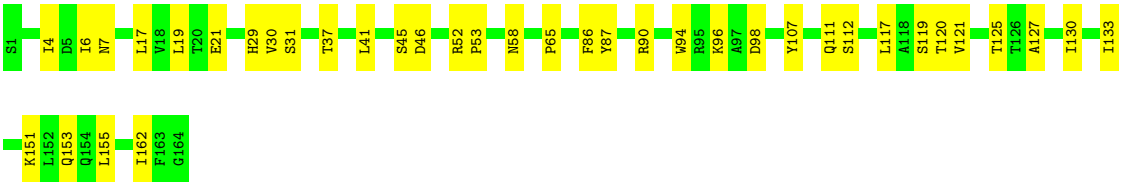
• Molecule 1: coat protein

Chain BT:



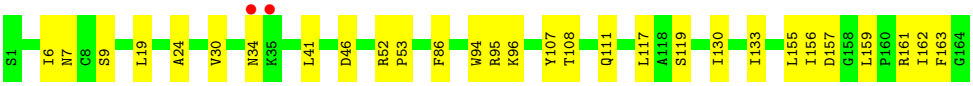
• Molecule 1: coat protein

Chain BU:



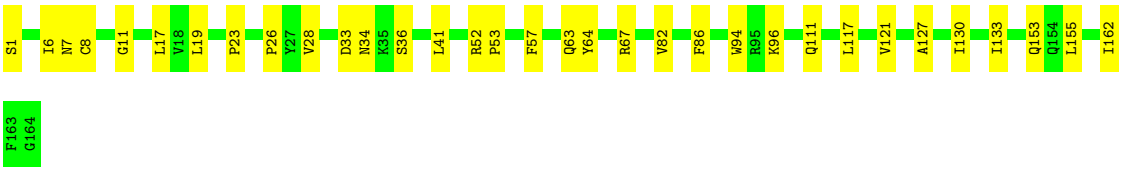
• Molecule 1: coat protein

Chain BV:



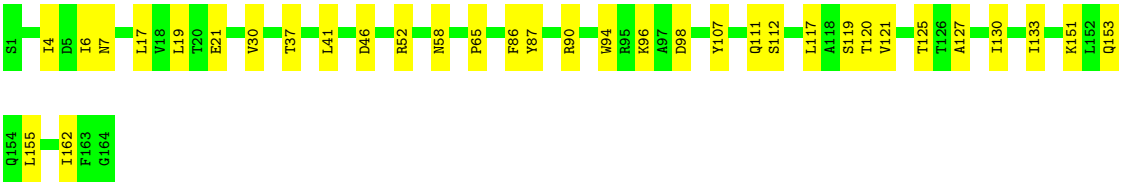
• Molecule 1: coat protein

Chain BW:



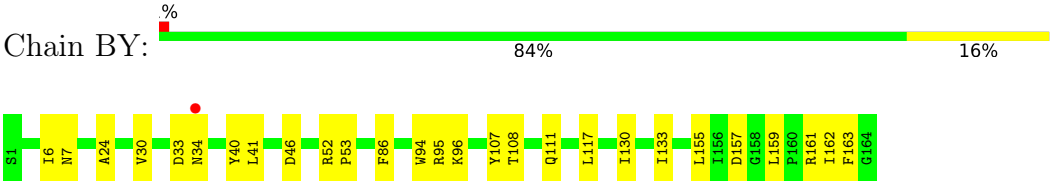
• Molecule 1: coat protein

Chain BX:



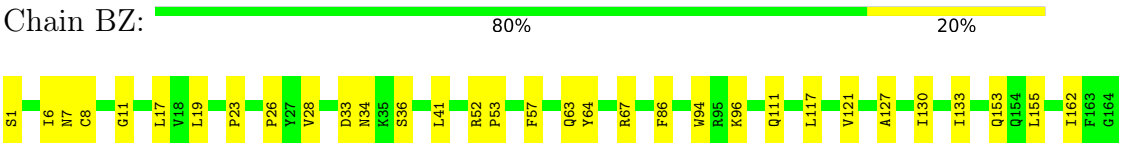
• Molecule 1: coat protein

Chain BY:



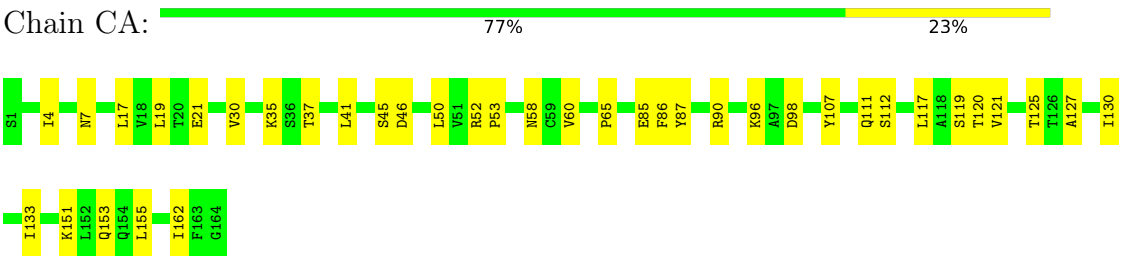
• Molecule 1: coat protein

Chain BZ:



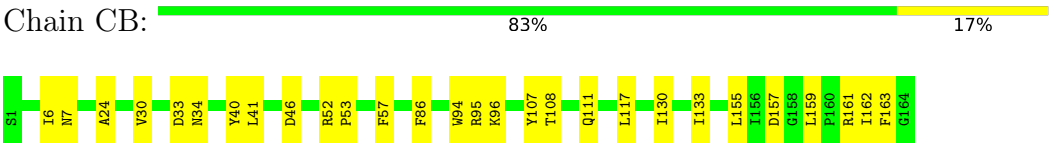
• Molecule 1: coat protein

Chain CA:



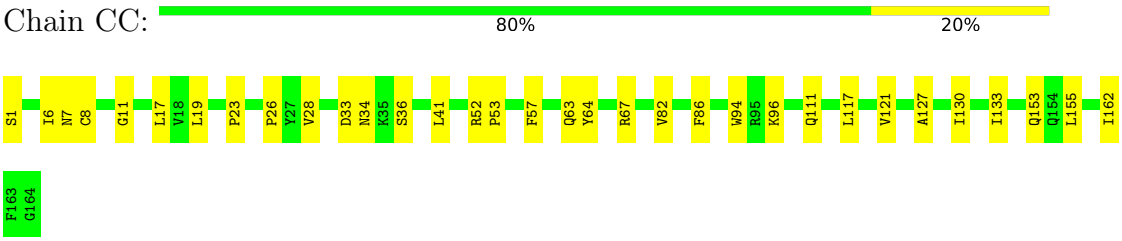
• Molecule 1: coat protein

Chain CB:



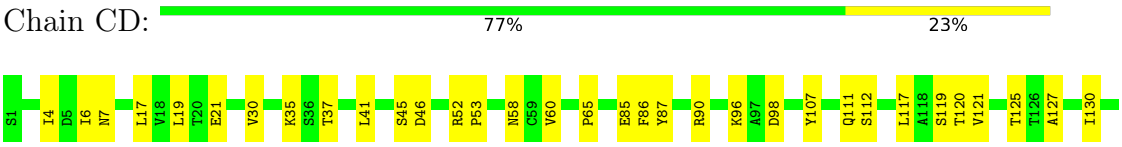
• Molecule 1: coat protein

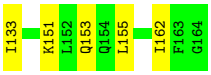
Chain CC:



• Molecule 1: coat protein

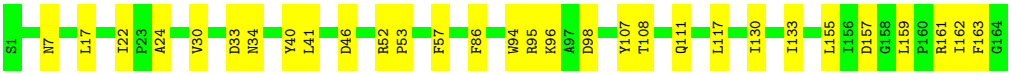
Chain CD:





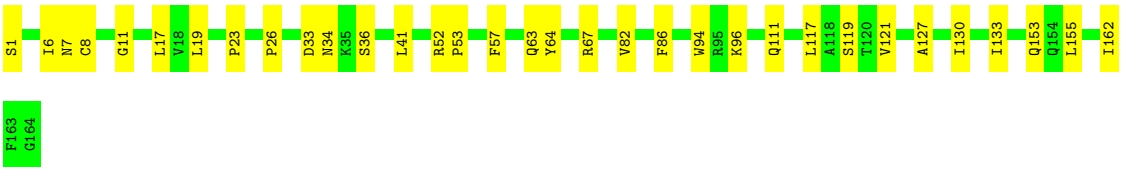
• Molecule 1: coat protein

Chain CE:



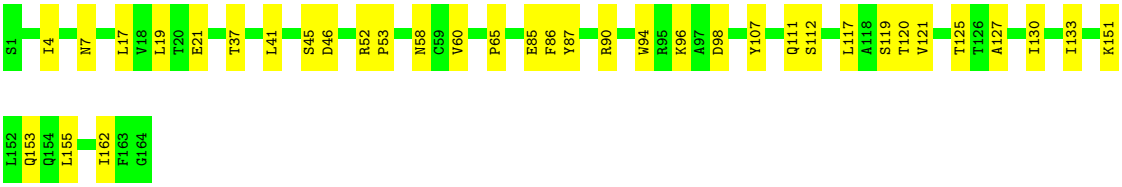
• Molecule 1: coat protein

Chain CF:



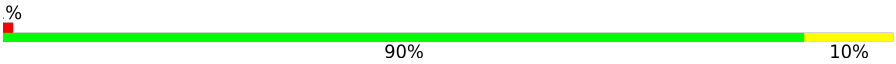
• Molecule 1: coat protein

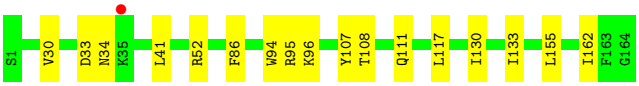
Chain CG:



• Molecule 1: coat protein

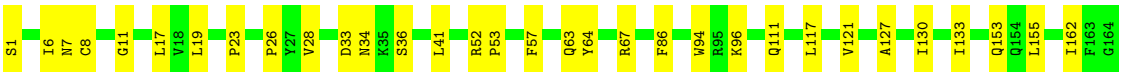
Chain CH:





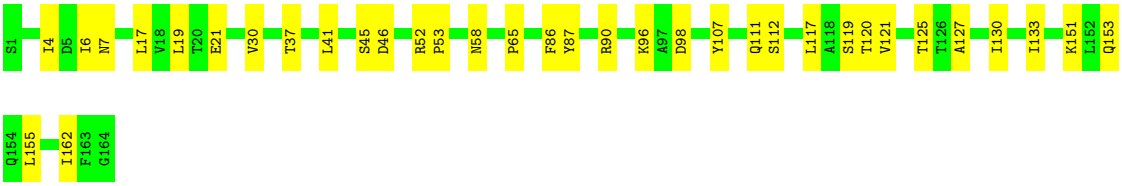
• Molecule 1: coat protein

Chain CI:



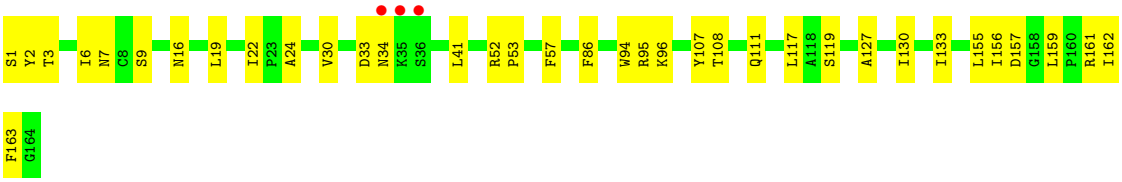
• Molecule 1: coat protein

Chain CJ:



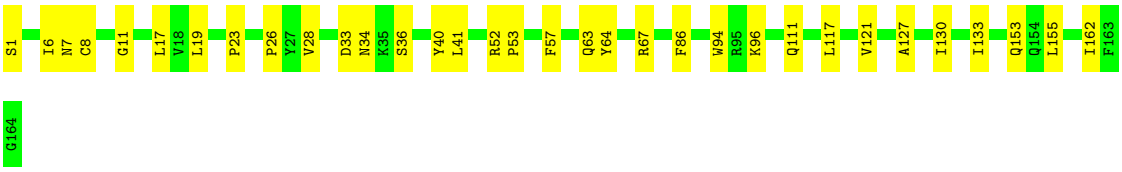
• Molecule 1: coat protein

Chain CK:



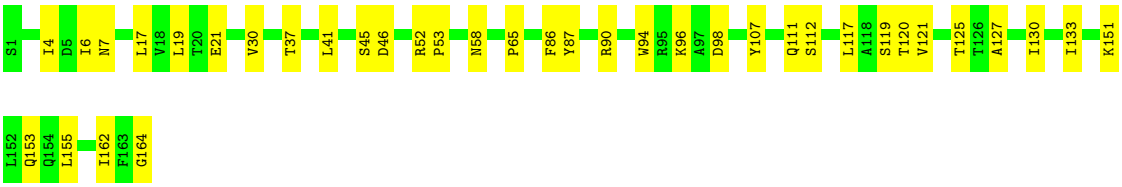
• Molecule 1: coat protein

Chain CL:



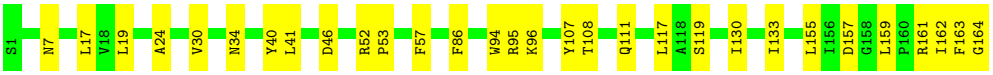
• Molecule 1: coat protein

Chain CM:



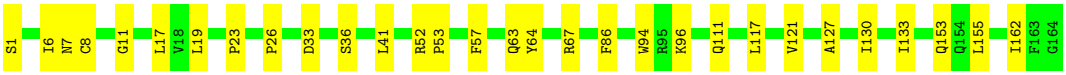
• Molecule 1: coat protein

Chain CN:



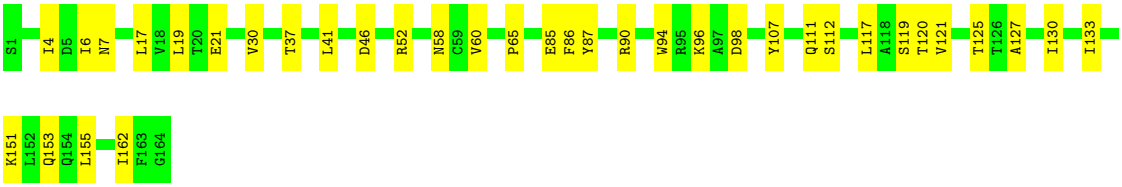
• Molecule 1: coat protein

Chain CO:



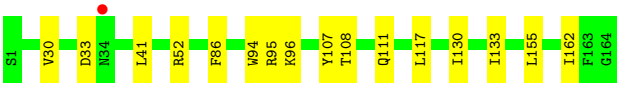
• Molecule 1: coat protein

Chain CP: 78% 22%



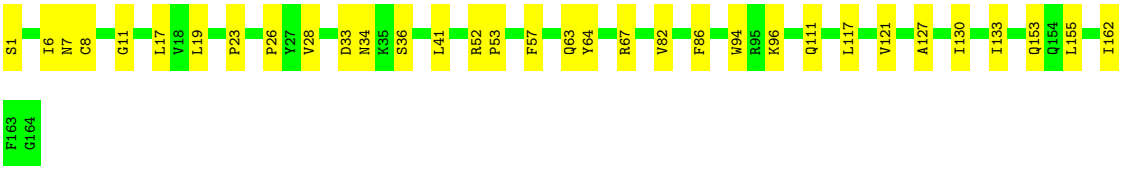
• Molecule 1: coat protein

Chain CQ: % 90% 10%



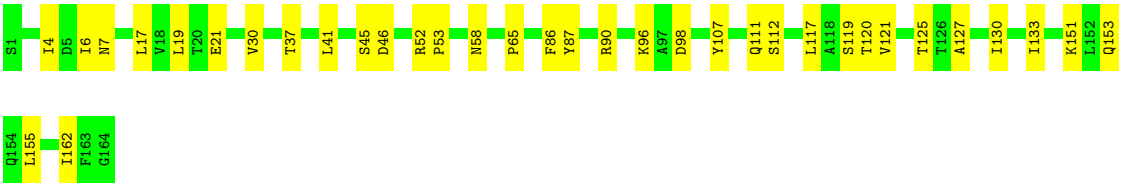
• Molecule 1: coat protein

Chain CR: 80% 20%



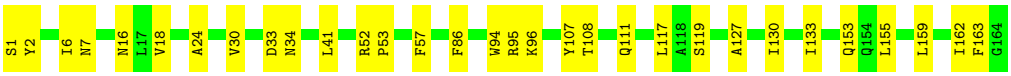
• Molecule 1: coat protein

Chain CS: 79% 21%



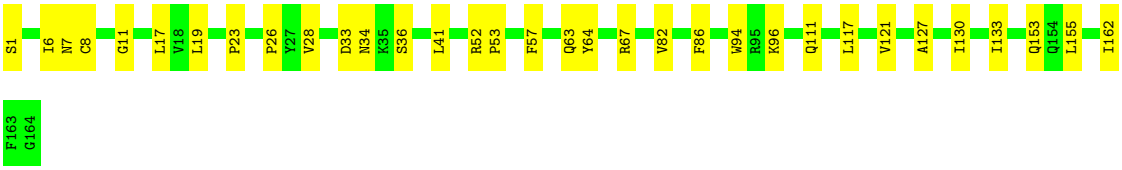
• Molecule 1: coat protein

Chain CT: 81% 19%



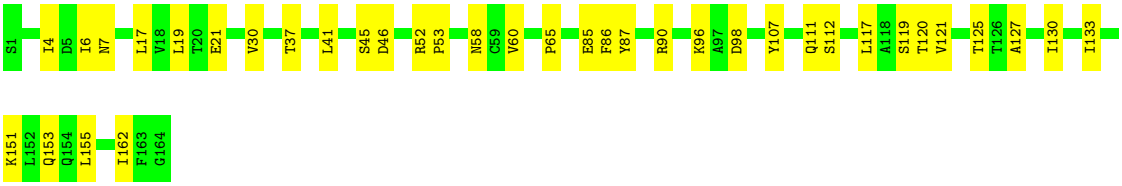
• Molecule 1: coat protein

Chain CU: 80% 20%



• Molecule 1: coat protein

Chain CV: 77% 23%

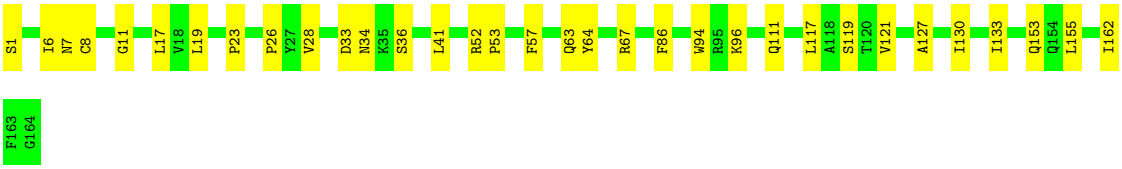


• Molecule 1: coat protein

Chain CW: 83% 17%

• Molecule 1: coat protein

Chain CX: 80% 20%

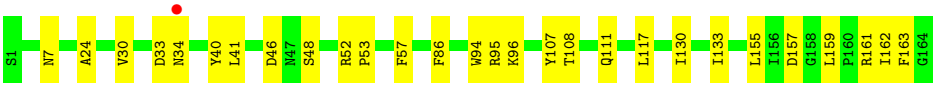


• Molecule 1: coat protein

Chain CY: 78% 22%

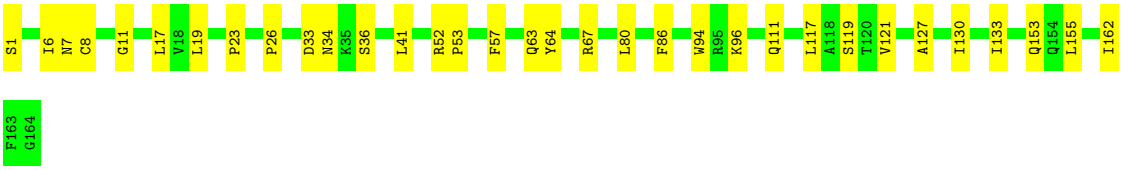
• Molecule 1: coat protein

Chain CZ: % 83% 17%



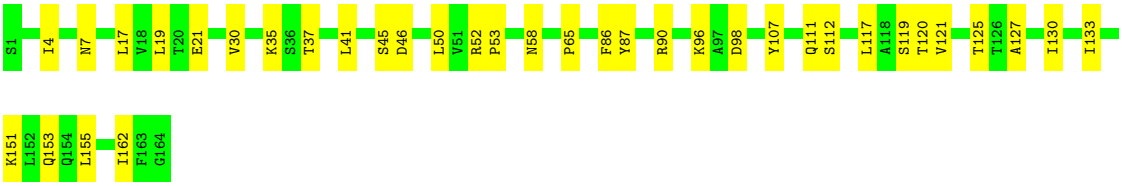
• Molecule 1: coat protein

Chain DA: 80% 20%



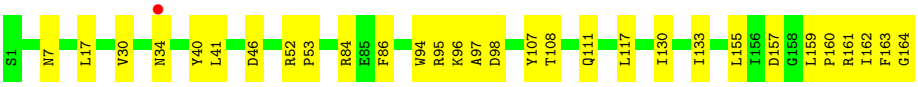
• Molecule 1: coat protein

Chain DB: 78% 22%



• Molecule 1: coat protein

Chain DC: % 82% 18%

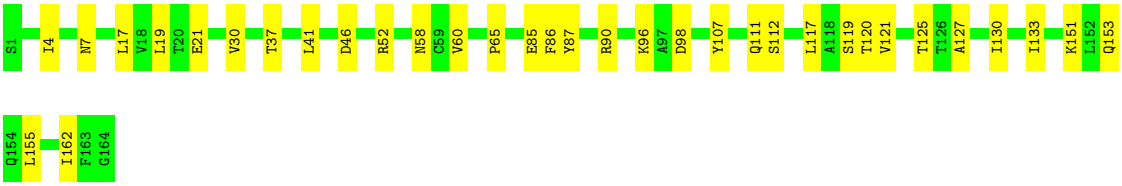


• Molecule 1: coat protein

Chain DD: 81% 19%

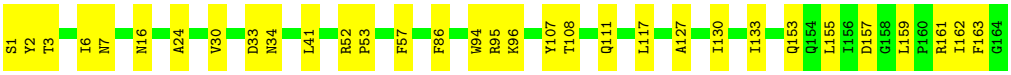
• Molecule 1: coat protein

Chain DE: 79% 21%



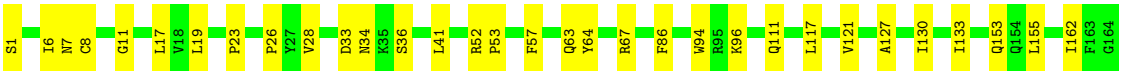
• Molecule 1: coat protein

Chain DF: 80% 20%



• Molecule 1: coat protein

Chain DG:

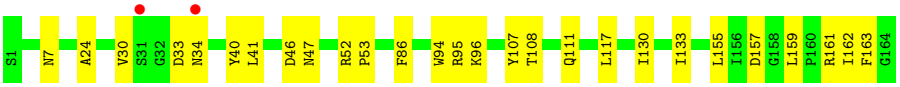


• Molecule 1: coat protein

Chain DH:

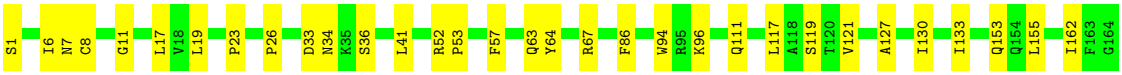
• Molecule 1: coat protein

Chain DI:



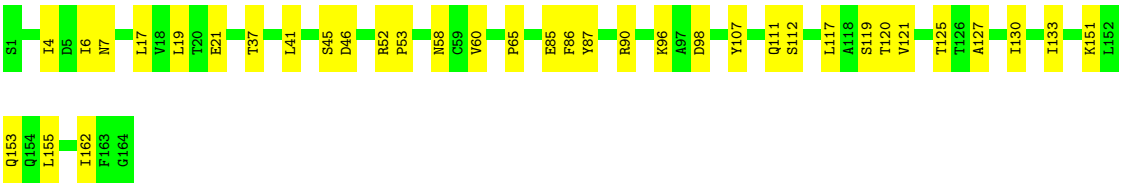
• Molecule 1: coat protein

Chain DJ:



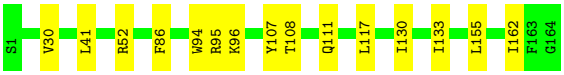
• Molecule 1: coat protein

Chain DK:



• Molecule 1: coat protein

Chain DL:


S1
V30
L41
R52
F86
W94
R95
K96
Y107
T108
Q111
L117
I130
I133
L155
I162
F163
G164

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	469.43Å 332.41Å 293.53Å 90.00° 127.87° 90.00°	Depositor
Resolution (Å)	57.20 – 3.10 57.20 – 3.10	Depositor EDS
% Data completeness (in resolution range)	78.5 (57.20-3.10) 79.1 (57.20-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.31	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.250 , 0.254 0.243 , 0.247	Depositor DCC
R_{free} test set	9935 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	116370	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	AA	0.35	0/1321	0.58	0/1802
1	AB	0.35	0/1321	0.59	0/1802
1	AC	0.35	0/1321	0.56	0/1802
1	AD	0.35	0/1321	0.58	0/1802
1	AE	0.36	0/1321	0.59	0/1802
1	AF	0.35	0/1321	0.56	0/1802
1	AG	0.35	0/1321	0.58	0/1802
1	AH	0.35	0/1321	0.59	0/1802
1	AI	0.35	0/1321	0.56	0/1802
1	AJ	0.35	0/1321	0.58	0/1802
1	AK	0.36	0/1321	0.59	0/1802
1	AL	0.35	0/1321	0.56	0/1802
1	AM	0.35	0/1321	0.58	0/1802
1	AN	0.36	0/1321	0.59	0/1802
1	AO	0.35	0/1321	0.56	0/1802
1	AP	0.35	0/1321	0.58	0/1802
1	AQ	0.36	0/1321	0.59	0/1802
1	AR	0.35	0/1321	0.56	0/1802
1	AS	0.35	0/1321	0.58	0/1802
1	AT	0.36	0/1321	0.59	0/1802
1	AU	0.35	0/1321	0.56	0/1802
1	AV	0.35	0/1321	0.58	0/1802
1	AW	0.36	0/1321	0.59	0/1802
1	AX	0.35	0/1321	0.56	0/1802
1	AY	0.35	0/1321	0.58	0/1802
1	AZ	0.36	0/1321	0.59	0/1802
1	BA	0.35	0/1321	0.56	0/1802
1	BB	0.35	0/1321	0.58	0/1802
1	BC	0.36	0/1321	0.59	0/1802
1	BD	0.35	0/1321	0.56	0/1802
1	BE	0.35	0/1321	0.58	0/1802
1	BF	0.36	0/1321	0.59	0/1802
1	BG	0.35	0/1321	0.56	0/1802
1	BH	0.35	0/1321	0.58	0/1802

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	BI	0.36	0/1321	0.59	0/1802
1	BJ	0.35	0/1321	0.56	0/1802
1	BK	0.35	0/1321	0.58	0/1802
1	BL	0.36	0/1321	0.58	0/1802
1	BM	0.35	0/1321	0.56	0/1802
1	BN	0.35	0/1321	0.58	0/1802
1	BO	0.36	0/1321	0.59	0/1802
1	BP	0.35	0/1321	0.56	0/1802
1	BQ	0.35	0/1321	0.58	0/1802
1	BR	0.36	0/1321	0.59	0/1802
1	BS	0.35	0/1321	0.56	0/1802
1	BT	0.35	0/1321	0.58	0/1802
1	BU	0.36	0/1321	0.59	0/1802
1	BV	0.35	0/1321	0.56	0/1802
1	BW	0.35	0/1321	0.58	0/1802
1	BX	0.36	0/1321	0.59	0/1802
1	BY	0.35	0/1321	0.56	0/1802
1	BZ	0.35	0/1321	0.58	0/1802
1	CA	0.36	0/1321	0.59	0/1802
1	CB	0.35	0/1321	0.56	0/1802
1	CC	0.35	0/1321	0.58	0/1802
1	CD	0.36	0/1321	0.59	0/1802
1	CE	0.35	0/1321	0.56	0/1802
1	CF	0.35	0/1321	0.58	0/1802
1	CG	0.36	0/1321	0.59	0/1802
1	CH	0.35	0/1321	0.56	0/1802
1	CI	0.35	0/1321	0.58	0/1802
1	CJ	0.36	0/1321	0.58	0/1802
1	CK	0.35	0/1321	0.56	0/1802
1	CL	0.35	0/1321	0.58	0/1802
1	CM	0.36	0/1321	0.59	0/1802
1	CN	0.35	0/1321	0.56	0/1802
1	CO	0.35	0/1321	0.58	0/1802
1	CP	0.36	0/1321	0.58	0/1802
1	CQ	0.35	0/1321	0.56	0/1802
1	CR	0.35	0/1321	0.58	0/1802
1	CS	0.36	0/1321	0.59	0/1802
1	CT	0.35	0/1321	0.56	0/1802
1	CU	0.35	0/1321	0.58	0/1802
1	CV	0.36	0/1321	0.58	0/1802
1	CW	0.35	0/1321	0.56	0/1802
1	CX	0.35	0/1321	0.58	0/1802
1	CY	0.36	0/1321	0.59	0/1802

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	CZ	0.35	0/1321	0.56	0/1802
1	DA	0.35	0/1321	0.58	0/1802
1	DB	0.36	0/1321	0.59	0/1802
1	DC	0.35	0/1321	0.56	0/1802
1	DD	0.35	0/1321	0.58	0/1802
1	DE	0.36	0/1321	0.59	0/1802
1	DF	0.35	0/1321	0.56	0/1802
1	DG	0.35	0/1321	0.58	0/1802
1	DH	0.36	0/1321	0.59	0/1802
1	DI	0.35	0/1321	0.56	0/1802
1	DJ	0.35	0/1321	0.58	0/1802
1	DK	0.36	0/1321	0.59	0/1802
1	DL	0.35	0/1321	0.56	0/1802
All	All	0.35	0/118890	0.58	0/162180

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	AA	1293	0	1269	36	0
1	AB	1293	0	1269	35	0
1	AC	1293	0	1269	26	0
1	AD	1293	0	1269	38	0
1	AE	1293	0	1269	41	0
1	AF	1293	0	1269	30	0
1	AG	1293	0	1269	36	0
1	AH	1293	0	1269	37	0
1	AI	1293	0	1269	26	0
1	AJ	1293	0	1269	35	0
1	AK	1293	0	1269	37	0
1	AL	1293	0	1269	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	1293	0	1269	35	0
1	AN	1293	0	1269	33	0
1	AO	1293	0	1269	29	0
1	AP	1293	0	1269	33	0
1	AQ	1293	0	1269	32	0
1	AR	1293	0	1269	43	0
1	AS	1293	0	1269	35	0
1	AT	1293	0	1269	36	0
1	AU	1293	0	1269	32	0
1	AV	1293	0	1269	35	0
1	AW	1293	0	1269	35	0
1	AX	1293	0	1269	28	0
1	AY	1293	0	1269	33	0
1	AZ	1293	0	1269	31	0
1	BA	1293	0	1269	28	1
1	BB	1293	0	1269	35	0
1	BC	1293	0	1269	36	0
1	BD	1293	0	1269	28	0
1	BE	1293	0	1269	36	0
1	BF	1293	0	1269	36	0
1	BG	1293	0	1269	42	0
1	BH	1293	0	1269	37	0
1	BI	1293	0	1269	33	0
1	BJ	1293	0	1269	33	0
1	BK	1293	0	1269	33	0
1	BL	1293	0	1269	36	0
1	BM	1293	0	1269	25	0
1	BN	1293	0	1269	34	0
1	BO	1293	0	1269	32	0
1	BP	1293	0	1269	26	0
1	BQ	1293	0	1269	35	1
1	BR	1293	0	1269	32	0
1	BS	1293	0	1269	11	0
1	BT	1293	0	1269	35	0
1	BU	1293	0	1269	36	0
1	BV	1293	0	1269	28	0
1	BW	1293	0	1269	36	0
1	BX	1293	0	1269	34	0
1	BY	1293	0	1269	26	0
1	BZ	1293	0	1269	33	0
1	CA	1293	0	1269	36	0
1	CB	1293	0	1269	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CC	1293	0	1269	36	0
1	CD	1293	0	1269	34	0
1	CE	1293	0	1269	30	0
1	CF	1293	0	1269	35	0
1	CG	1293	0	1269	34	0
1	CH	1293	0	1269	11	0
1	CI	1293	0	1269	33	0
1	CJ	1293	0	1269	33	0
1	CK	1293	0	1269	45	0
1	CL	1293	0	1269	36	0
1	CM	1293	0	1269	34	0
1	CN	1293	0	1269	31	0
1	CO	1293	0	1269	31	0
1	CP	1293	0	1269	34	0
1	CQ	1293	0	1269	10	0
1	CR	1293	0	1269	34	0
1	CS	1293	0	1269	34	0
1	CT	1293	0	1269	30	0
1	CU	1293	0	1269	36	0
1	CV	1293	0	1269	34	0
1	CW	1293	0	1269	29	0
1	CX	1293	0	1269	34	0
1	CY	1293	0	1269	36	0
1	CZ	1293	0	1269	29	0
1	DA	1293	0	1269	35	0
1	DB	1293	0	1269	35	0
1	DC	1293	0	1269	34	0
1	DD	1293	0	1269	32	0
1	DE	1293	0	1269	32	0
1	DF	1293	0	1269	33	0
1	DG	1293	0	1269	37	0
1	DH	1293	0	1269	35	0
1	DI	1293	0	1269	27	0
1	DJ	1293	0	1269	34	0
1	DK	1293	0	1269	34	0
1	DL	1293	0	1269	10	0
All	All	116370	0	114210	2037	1

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 9.

All (2037) 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:AR:53:PRO:HG2	1:CK:7:ASN:O	1.68	0.92
1:BJ:53:PRO:HG2	1:DF:7:ASN:O	1.81	0.80
1:AR:34:ASN:HB3	1:CK:161:ARG:HD2	1.65	0.79
1:BG:161:ARG:HD2	1:DC:34:ASN:HB3	1.63	0.79
1:AX:163:PHE:HD2	1:CT:24:ALA:HA	1.49	0.77
1:AF:34:ASN:HB3	1:BV:161:ARG:HD2	1.66	0.77
1:AF:53:PRO:HG2	1:BV:7:ASN:O	1.85	0.75
1:AR:159:LEU:HD13	1:CI:28:VAL:HG11	1.69	0.74
1:AX:159:LEU:HD13	1:CR:28:VAL:HG11	1.70	0.74
1:BG:157:ASP:CG	1:DA:52:ARG:HH22	1.91	0.73
1:AX:153:GLN:OE1	1:CT:127:ALA:HB2	1.89	0.72
1:BF:30:VAL:HA	1:BQ:34:ASN:ND2	2.04	0.72
1:BG:34:ASN:HB3	1:DC:161:ARG:HD2	1.71	0.72
1:BJ:7:ASN:O	1:DF:53:PRO:HG2	1.89	0.71
1:AO:7:ASN:O	1:CE:53:PRO:HG2	1.90	0.71
1:AM:28:VAL:HG11	1:CE:159:LEU:HD13	1.74	0.70
1:AD:52:ARG:HH22	1:BV:157:ASP:CG	1.94	0.69
1:AL:7:ASN:O	1:CB:53:PRO:HG2	1.93	0.69
1:BD:41:LEU:HD11	1:BD:52:ARG:HB2	1.75	0.69
1:CZ:41:LEU:HD11	1:CZ:52:ARG:HB2	1.75	0.69
1:AC:41:LEU:HD11	1:AC:52:ARG:HB2	1.75	0.69
1:AL:41:LEU:HD11	1:AL:52:ARG:HB2	1.75	0.69
1:DI:41:LEU:HD11	1:DI:52:ARG:HB2	1.74	0.69
1:AI:41:LEU:HD11	1:AI:52:ARG:HB2	1.75	0.69
1:CT:41:LEU:HD11	1:CT:52:ARG:HB2	1.75	0.69
1:AR:41:LEU:HD11	1:AR:52:ARG:HB2	1.75	0.69
1:AR:98:ASP:HB3	1:CK:1:SER:C	2.13	0.69
1:CN:41:LEU:HD11	1:CN:52:ARG:HB2	1.75	0.69
1:CB:41:LEU:HD11	1:CB:52:ARG:HB2	1.75	0.69
1:CH:41:LEU:HD11	1:CH:52:ARG:HB2	1.75	0.69
1:DC:41:LEU:HD11	1:DC:52:ARG:HB2	1.75	0.69
1:AO:41:LEU:HD11	1:AO:52:ARG:HB2	1.75	0.69
1:BA:41:LEU:HD11	1:BA:52:ARG:HB2	1.75	0.69
1:BP:41:LEU:HD11	1:BP:52:ARG:HB2	1.75	0.69
1:BS:41:LEU:HD11	1:BS:52:ARG:HB2	1.75	0.69
1:AF:41:LEU:HD11	1:AF:52:ARG:HB2	1.75	0.69
1:BV:41:LEU:HD11	1:BV:52:ARG:HB2	1.75	0.69
1:CQ:41:LEU:HD11	1:CQ:52:ARG:HB2	1.75	0.69
1:BJ:41:LEU:HD11	1:BJ:52:ARG:HB2	1.75	0.68
1:DF:41:LEU:HD11	1:DF:52:ARG:HB2	1.74	0.68
1:DL:41:LEU:HD11	1:DL:52:ARG:HB2	1.75	0.68
1:AR:94:TRP:NE1	1:CK:6:ILE:HG22	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BM:41:LEU:HD11	1:BM:52:ARG:HB2	1.75	0.68
1:AI:7:ASN:O	1:BY:53:PRO:HG2	1.93	0.68
1:BY:41:LEU:HD11	1:BY:52:ARG:HB2	1.75	0.68
1:CW:41:LEU:HD11	1:CW:52:ARG:HB2	1.75	0.68
1:AU:41:LEU:HD11	1:AU:52:ARG:HB2	1.75	0.67
1:BG:7:ASN:O	1:DC:53:PRO:HG2	1.94	0.67
1:CE:41:LEU:HD11	1:CE:52:ARG:HB2	1.75	0.67
1:BG:41:LEU:HD11	1:BG:52:ARG:HB2	1.75	0.67
1:BM:7:ASN:O	1:DI:53:PRO:HG2	1.95	0.67
1:CK:41:LEU:HD11	1:CK:52:ARG:HB2	1.75	0.67
1:AX:24:ALA:HA	1:CT:163:PHE:HD2	1.59	0.67
1:AR:40:TYR:CE1	1:CK:163:PHE:HB2	2.30	0.67
1:AX:41:LEU:HD11	1:AX:52:ARG:HB2	1.75	0.67
1:AF:159:LEU:HD13	1:BT:28:VAL:HG11	1.75	0.66
1:AV:28:VAL:HG11	1:CT:159:LEU:HD13	1.77	0.66
1:AX:127:ALA:HB2	1:CT:153:GLN:OE1	1.96	0.66
1:BH:34:ASN:ND2	1:BL:30:VAL:HA	2.10	0.66
1:AR:163:PHE:HD2	1:CK:24:ALA:HA	1.60	0.65
1:AF:163:PHE:HD2	1:BV:24:ALA:HA	1.62	0.65
1:AX:163:PHE:CD2	1:CT:24:ALA:HA	2.32	0.65
1:BK:28:VAL:HG11	1:DI:159:LEU:HD13	1.79	0.64
1:AL:53:PRO:HG2	1:CB:7:ASN:O	1.97	0.64
1:BD:7:ASN:O	1:CZ:53:PRO:HG2	1.97	0.64
1:BA:53:PRO:HG2	1:CW:7:ASN:O	1.98	0.64
1:BA:34:ASN:HB3	1:CW:161:ARG:HD2	1.77	0.64
1:BA:161:ARG:HD2	1:CW:34:ASN:HB3	1.79	0.63
1:BD:53:PRO:HG2	1:CZ:7:ASN:O	1.99	0.63
1:AO:24:ALA:HA	1:CE:163:PHE:HD2	1.62	0.63
1:AU:34:ASN:HB3	1:CN:161:ARG:HD2	1.80	0.63
1:AY:52:ARG:HH22	1:CW:157:ASP:CG	2.01	0.63
1:CA:30:VAL:HA	1:CF:34:ASN:ND2	2.13	0.63
1:AI:53:PRO:HG2	1:BY:7:ASN:O	1.99	0.63
1:AP:52:ARG:HH22	1:CK:157:ASP:CG	2.02	0.62
1:AC:7:ASN:O	1:BP:53:PRO:HG2	2.00	0.62
1:AG:7:ASN:HD21	1:AH:46:ASP:H	1.48	0.62
1:AH:30:VAL:HA	1:CC:34:ASN:ND2	2.15	0.62
1:AR:96:LYS:HA	1:CK:3:THR:O	2.00	0.62
1:CL:7:ASN:HD21	1:CM:46:ASP:H	1.48	0.61
1:AJ:7:ASN:HD21	1:AK:46:ASP:H	1.49	0.61
1:BM:157:ASP:CG	1:DG:52:ARG:HH22	2.03	0.61
1:BZ:7:ASN:HD21	1:CA:46:ASP:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:7:ASN:HD21	1:AE:46:ASP:H	1.49	0.61
1:AE:35:LYS:NZ	1:BG:34:ASN:HD21	1.97	0.61
1:AS:7:ASN:HD21	1:AT:46:ASP:H	1.48	0.61
1:CC:7:ASN:HD21	1:CD:46:ASP:H	1.48	0.61
1:CO:7:ASN:HD21	1:CP:46:ASP:H	1.48	0.61
1:AP:7:ASN:HD21	1:AQ:46:ASP:H	1.49	0.61
1:BE:28:VAL:HG11	1:DC:159:LEU:HD13	1.82	0.61
1:BG:7:ASN:HD21	1:DC:46:ASP:H	1.48	0.61
1:AK:65:PRO:HB2	1:AK:120:THR:HG22	1.83	0.61
1:AY:7:ASN:HD21	1:AZ:46:ASP:H	1.49	0.61
1:BJ:159:LEU:HD13	1:DD:28:VAL:HG11	1.83	0.61
1:CM:65:PRO:HB2	1:CM:120:THR:HG22	1.83	0.61
1:DJ:7:ASN:HD21	1:DK:46:ASP:H	1.49	0.61
1:CA:65:PRO:HB2	1:CA:120:THR:HG22	1.83	0.61
1:CX:7:ASN:HD21	1:CY:46:ASP:H	1.49	0.61
1:AA:7:ASN:HD21	1:AB:46:ASP:H	1.49	0.61
1:AB:65:PRO:HB2	1:AB:120:THR:HG22	1.83	0.61
1:AE:65:PRO:HB2	1:AE:120:THR:HG22	1.83	0.61
1:AM:7:ASN:HD21	1:AN:46:ASP:H	1.48	0.61
1:AQ:65:PRO:HB2	1:AQ:120:THR:HG22	1.83	0.61
1:AU:53:PRO:HG2	1:CN:7:ASN:O	2.01	0.61
1:BH:7:ASN:HD21	1:BI:46:ASP:H	1.49	0.61
1:DB:65:PRO:HB2	1:DB:120:THR:HG22	1.83	0.61
1:AL:161:ARG:HD2	1:CB:34:ASN:HB3	1.82	0.60
1:DK:65:PRO:HB2	1:DK:120:THR:HG22	1.83	0.60
1:BK:7:ASN:HD21	1:BL:46:ASP:H	1.48	0.60
1:CS:65:PRO:HB2	1:CS:120:THR:HG22	1.83	0.60
1:CU:7:ASN:HD21	1:CV:46:ASP:H	1.49	0.60
1:AN:65:PRO:HB2	1:AN:120:THR:HG22	1.83	0.60
1:BE:7:ASN:HD21	1:BF:46:ASP:H	1.48	0.60
1:CR:7:ASN:HD21	1:CS:46:ASP:H	1.48	0.60
1:DG:130:ILE:O	1:DG:133:ILE:HG22	2.02	0.60
1:BB:7:ASN:HD21	1:BC:46:ASP:H	1.49	0.60
1:BF:65:PRO:HB2	1:BF:120:THR:HG22	1.83	0.60
1:BH:130:ILE:O	1:BH:133:ILE:HG22	2.02	0.60
1:BI:65:PRO:HB2	1:BI:120:THR:HG22	1.83	0.60
1:CF:7:ASN:HD21	1:CG:46:ASP:H	1.48	0.60
1:CL:130:ILE:O	1:CL:133:ILE:HG22	2.02	0.60
1:DH:65:PRO:HB2	1:DH:120:THR:HG22	1.83	0.60
1:AH:65:PRO:HB2	1:AH:120:THR:HG22	1.83	0.60
1:AJ:28:VAL:HG11	1:CB:159:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:130:ILE:O	1:AS:133:ILE:HG22	2.02	0.60
1:BA:159:LEU:HD13	1:CU:28:VAL:HG11	1.84	0.60
1:BM:161:ARG:HD2	1:DI:34:ASN:HB3	1.83	0.60
1:CX:130:ILE:O	1:CX:133:ILE:HG22	2.02	0.60
1:CU:130:ILE:O	1:CU:133:ILE:HG22	2.02	0.60
1:AL:96:LYS:HG2	1:AL:107:TYR:HB2	1.84	0.60
1:BC:65:PRO:HB2	1:BC:120:THR:HG22	1.83	0.60
1:BR:65:PRO:HB2	1:BR:120:THR:HG22	1.83	0.60
1:CY:65:PRO:HB2	1:CY:120:THR:HG22	1.83	0.60
1:AB:41:LEU:HD11	1:AB:52:ARG:HB2	1.84	0.60
1:AD:130:ILE:O	1:AD:133:ILE:HG22	2.02	0.60
1:BA:96:LYS:HG2	1:BA:107:TYR:HB2	1.84	0.60
1:CN:96:LYS:HG2	1:CN:107:TYR:HB2	1.84	0.60
1:CO:130:ILE:O	1:CO:133:ILE:HG22	2.02	0.60
1:DD:7:ASN:HD21	1:DE:46:ASP:H	1.49	0.60
1:DH:41:LEU:HD11	1:DH:52:ARG:HB2	1.84	0.60
1:AE:41:LEU:HD11	1:AE:52:ARG:HB2	1.84	0.60
1:AF:96:LYS:HG2	1:AF:107:TYR:HB2	1.84	0.60
1:AM:33:ASP:H	1:AM:36:SER:HB3	1.67	0.60
1:AW:65:PRO:HB2	1:AW:120:THR:HG22	1.83	0.60
1:BD:96:LYS:HG2	1:BD:107:TYR:HB2	1.84	0.60
1:BW:33:ASP:H	1:BW:36:SER:HB3	1.67	0.60
1:CG:65:PRO:HB2	1:CG:120:THR:HG22	1.83	0.60
1:DI:96:LYS:HG2	1:DI:107:TYR:HB2	1.84	0.60
1:AA:130:ILE:O	1:AA:133:ILE:HG22	2.02	0.60
1:AJ:33:ASP:H	1:AJ:36:SER:HB3	1.67	0.60
1:AJ:130:ILE:O	1:AJ:133:ILE:HG22	2.02	0.60
1:AM:130:ILE:O	1:AM:133:ILE:HG22	2.02	0.60
1:BB:28:VAL:HG11	1:CZ:159:LEU:HD13	1.83	0.60
1:BE:33:ASP:H	1:BE:36:SER:HB3	1.67	0.60
1:BN:33:ASP:H	1:BN:36:SER:HB3	1.67	0.60
1:BO:65:PRO:HB2	1:BO:120:THR:HG22	1.83	0.60
1:CA:41:LEU:HD11	1:CA:52:ARG:HB2	1.84	0.60
1:CU:34:ASN:ND2	1:CY:30:VAL:HA	2.17	0.60
1:DA:7:ASN:HD21	1:DB:46:ASP:H	1.49	0.60
1:DA:33:ASP:H	1:DA:36:SER:HB3	1.67	0.60
1:AH:41:LEU:HD11	1:AH:52:ARG:HB2	1.84	0.59
1:BO:41:LEU:HD11	1:BO:52:ARG:HB2	1.84	0.59
1:BR:41:LEU:HD11	1:BR:52:ARG:HB2	1.84	0.59
1:CF:33:ASP:H	1:CF:36:SER:HB3	1.67	0.59
1:CG:41:LEU:HD11	1:CG:52:ARG:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:130:ILE:O	1:CI:133:ILE:HG22	2.02	0.59
1:CJ:65:PRO:HB2	1:CJ:120:THR:HG22	1.83	0.59
1:CR:130:ILE:O	1:CR:133:ILE:HG22	2.02	0.59
1:AO:96:LYS:HG2	1:AO:107:TYR:HB2	1.84	0.59
1:BE:130:ILE:O	1:BE:133:ILE:HG22	2.02	0.59
1:BF:41:LEU:HD11	1:BF:52:ARG:HB2	1.84	0.59
1:BJ:94:TRP:NE1	1:DF:6:ILE:HG22	2.17	0.59
1:CB:96:LYS:HG2	1:CB:107:TYR:HB2	1.84	0.59
1:CC:130:ILE:O	1:CC:133:ILE:HG22	2.02	0.59
1:CH:96:LYS:HG2	1:CH:107:TYR:HB2	1.84	0.59
1:CM:41:LEU:HD11	1:CM:52:ARG:HB2	1.84	0.59
1:CT:96:LYS:HG2	1:CT:107:TYR:HB2	1.84	0.59
1:DE:65:PRO:HB2	1:DE:120:THR:HG22	1.83	0.59
1:DG:33:ASP:H	1:DG:36:SER:HB3	1.67	0.59
1:AD:33:ASP:H	1:AD:36:SER:HB3	1.67	0.59
1:AI:96:LYS:HG2	1:AI:107:TYR:HB2	1.84	0.59
1:AQ:41:LEU:HD11	1:AQ:52:ARG:HB2	1.84	0.59
1:BN:7:ASN:HD21	1:BO:46:ASP:H	1.49	0.59
1:CJ:41:LEU:HD11	1:CJ:52:ARG:HB2	1.84	0.59
1:CX:33:ASP:H	1:CX:36:SER:HB3	1.67	0.59
1:AP:130:ILE:O	1:AP:133:ILE:HG22	2.02	0.59
1:BB:130:ILE:O	1:BB:133:ILE:HG22	2.02	0.59
1:BF:30:VAL:HA	1:BQ:34:ASN:HD22	1.65	0.59
1:BI:41:LEU:HD11	1:BI:52:ARG:HB2	1.84	0.59
1:BN:130:ILE:O	1:BN:133:ILE:HG22	2.02	0.59
1:BS:96:LYS:HG2	1:BS:107:TYR:HB2	1.84	0.59
1:BT:7:ASN:HD21	1:BU:46:ASP:H	1.48	0.59
1:BW:130:ILE:O	1:BW:133:ILE:HG22	2.02	0.59
1:CD:65:PRO:HB2	1:CD:120:THR:HG22	1.83	0.59
1:CU:33:ASP:H	1:CU:36:SER:HB3	1.67	0.59
1:CV:41:LEU:HD11	1:CV:52:ARG:HB2	1.84	0.59
1:CV:65:PRO:HB2	1:CV:120:THR:HG22	1.83	0.59
1:DD:33:ASP:H	1:DD:36:SER:HB3	1.67	0.59
1:DJ:130:ILE:O	1:DJ:133:ILE:HG22	2.02	0.59
1:AC:53:PRO:HG2	1:BP:7:ASN:O	2.02	0.59
1:AG:28:VAL:HG11	1:BY:159:LEU:HD13	1.82	0.59
1:AG:130:ILE:O	1:AG:133:ILE:HG22	2.02	0.59
1:AS:33:ASP:H	1:AS:36:SER:HB3	1.67	0.59
1:BM:53:PRO:HG2	1:DI:7:ASN:O	2.01	0.59
1:CF:130:ILE:O	1:CF:133:ILE:HG22	2.02	0.59
1:AP:33:ASP:H	1:AP:36:SER:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:41:LEU:HD11	1:AT:52:ARG:HB2	1.84	0.59
1:AT:65:PRO:HB2	1:AT:120:THR:HG22	1.83	0.59
1:AU:161:ARG:HD2	1:CN:34:ASN:HB3	1.84	0.59
1:AV:130:ILE:O	1:AV:133:ILE:HG22	2.02	0.59
1:BG:163:PHE:HB2	1:DC:40:TYR:CE1	2.37	0.59
1:BL:65:PRO:HB2	1:BL:120:THR:HG22	1.83	0.59
1:BT:33:ASP:H	1:BT:36:SER:HB3	1.67	0.59
1:BT:130:ILE:O	1:BT:133:ILE:HG22	2.02	0.59
1:BZ:130:ILE:O	1:BZ:133:ILE:HG22	2.02	0.59
1:CP:65:PRO:HB2	1:CP:120:THR:HG22	1.83	0.59
1:CS:41:LEU:HD11	1:CS:52:ARG:HB2	1.84	0.59
1:CY:41:LEU:HD11	1:CY:52:ARG:HB2	1.84	0.59
1:DD:130:ILE:O	1:DD:133:ILE:HG22	2.02	0.59
1:DA:130:ILE:O	1:DA:133:ILE:HG22	2.02	0.59
1:DB:41:LEU:HD11	1:DB:52:ARG:HB2	1.84	0.59
1:DF:96:LYS:HG2	1:DF:107:TYR:HB2	1.84	0.59
1:AL:34:ASN:HB3	1:CB:161:ARG:HD2	1.85	0.59
1:AZ:65:PRO:HB2	1:AZ:120:THR:HG22	1.83	0.59
1:BK:130:ILE:O	1:BK:133:ILE:HG22	2.02	0.59
1:BQ:7:ASN:HD21	1:BR:46:ASP:H	1.48	0.59
1:BV:96:LYS:HG2	1:BV:107:TYR:HB2	1.84	0.59
1:CK:96:LYS:HG2	1:CK:107:TYR:HB2	1.84	0.59
1:CR:33:ASP:H	1:CR:36:SER:HB3	1.67	0.59
1:AY:130:ILE:O	1:AY:133:ILE:HG22	2.02	0.59
1:BB:33:ASP:H	1:BB:36:SER:HB3	1.67	0.59
1:BJ:96:LYS:HG2	1:BJ:107:TYR:HB2	1.84	0.59
1:BQ:130:ILE:O	1:BQ:133:ILE:HG22	2.02	0.59
1:BW:7:ASN:HD21	1:BX:46:ASP:H	1.48	0.59
1:AU:159:LEU:HD13	1:CL:28:VAL:HG11	1.83	0.59
1:AV:7:ASN:HD21	1:AW:46:ASP:H	1.49	0.59
1:AX:96:LYS:HG2	1:AX:107:TYR:HB2	1.84	0.59
1:BD:161:ARG:HD2	1:CZ:34:ASN:HB3	1.85	0.59
1:BM:96:LYS:HG2	1:BM:107:TYR:HB2	1.84	0.59
1:BX:65:PRO:HB2	1:BX:120:THR:HG22	1.83	0.59
1:CC:33:ASP:H	1:CC:36:SER:HB3	1.67	0.59
1:DK:41:LEU:HD11	1:DK:52:ARG:HB2	1.84	0.59
1:AC:96:LYS:HG2	1:AC:107:TYR:HB2	1.84	0.58
1:AR:7:ASN:O	1:CK:53:PRO:HG2	2.03	0.58
1:BU:65:PRO:HB2	1:BU:120:THR:HG22	1.83	0.58
1:CO:33:ASP:H	1:CO:36:SER:HB3	1.67	0.58
1:CW:96:LYS:HG2	1:CW:107:TYR:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:53:PRO:HG2	1:CT:7:ASN:O	2.03	0.58
1:BL:41:LEU:HD11	1:BL:52:ARG:HB2	1.84	0.58
1:BU:41:LEU:HD11	1:BU:52:ARG:HB2	1.84	0.58
1:AW:41:LEU:HD11	1:AW:52:ARG:HB2	1.84	0.58
1:CP:41:LEU:HD11	1:CP:52:ARG:HB2	1.84	0.58
1:DL:96:LYS:HG2	1:DL:107:TYR:HB2	1.84	0.58
1:AF:40:TYR:CE1	1:BV:163:PHE:HB2	2.38	0.58
1:AU:96:LYS:HG2	1:AU:107:TYR:HB2	1.84	0.58
1:AY:33:ASP:H	1:AY:36:SER:HB3	1.67	0.58
1:BF:50:LEU:HD11	1:BQ:82:VAL:HG13	1.85	0.58
1:CL:33:ASP:H	1:CL:36:SER:HB3	1.67	0.58
1:AO:161:ARG:HD2	1:CE:34:ASN:HB3	1.85	0.58
1:AR:96:LYS:HG2	1:AR:107:TYR:HB2	1.84	0.58
1:AR:98:ASP:OD2	1:CK:1:SER:OG	2.13	0.58
1:BQ:33:ASP:H	1:BQ:36:SER:HB3	1.67	0.58
1:CQ:96:LYS:HG2	1:CQ:107:TYR:HB2	1.84	0.58
1:DG:7:ASN:HD21	1:DH:46:ASP:H	1.48	0.58
1:DJ:33:ASP:H	1:DJ:36:SER:HB3	1.67	0.58
1:AA:33:ASP:H	1:AA:36:SER:HB3	1.67	0.58
1:AU:163:PHE:HD2	1:CN:24:ALA:HA	1.68	0.58
1:AZ:41:LEU:HD11	1:AZ:52:ARG:HB2	1.84	0.58
1:BC:41:LEU:HD11	1:BC:52:ARG:HB2	1.84	0.58
1:CI:7:ASN:HD21	1:CJ:46:ASP:H	1.49	0.58
1:CZ:96:LYS:HG2	1:CZ:107:TYR:HB2	1.84	0.58
1:AG:33:ASP:H	1:AG:36:SER:HB3	1.67	0.58
1:BA:7:ASN:O	1:CW:53:PRO:HG2	2.04	0.58
1:BK:33:ASP:H	1:BK:36:SER:HB3	1.67	0.58
1:BP:96:LYS:HG2	1:BP:107:TYR:HB2	1.84	0.58
1:AD:34:ASN:ND2	1:DE:30:VAL:HA	2.19	0.58
1:BW:41:LEU:HD11	1:BW:52:ARG:HB2	1.86	0.58
1:BX:41:LEU:HD11	1:BX:52:ARG:HB2	1.84	0.58
1:DD:41:LEU:HD11	1:DD:52:ARG:HB2	1.86	0.58
1:AJ:41:LEU:HD11	1:AJ:52:ARG:HB2	1.86	0.58
1:AN:41:LEU:HD11	1:AN:52:ARG:HB2	1.84	0.58
1:BC:30:VAL:HA	1:BN:34:ASN:ND2	2.18	0.58
1:BG:96:LYS:HG2	1:BG:107:TYR:HB2	1.84	0.58
1:BZ:41:LEU:HD11	1:BZ:52:ARG:HB2	1.86	0.58
1:CD:41:LEU:HD11	1:CD:52:ARG:HB2	1.84	0.58
1:AE:63:GLN:HG3	1:BG:50:LEU:CD2	2.34	0.58
1:BQ:41:LEU:HD11	1:BQ:52:ARG:HB2	1.86	0.58
1:CE:96:LYS:HG2	1:CE:107:TYR:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:7:ASN:O	1:CN:53:PRO:HG2	2.04	0.57
1:AA:34:ASN:ND2	1:DH:30:VAL:HA	2.20	0.57
1:BY:96:LYS:HG2	1:BY:107:TYR:HB2	1.84	0.57
1:DC:96:LYS:HG2	1:DC:107:TYR:HB2	1.84	0.57
1:BM:34:ASN:HB3	1:DI:161:ARG:HD2	1.86	0.57
1:BZ:33:ASP:H	1:BZ:36:SER:HB3	1.67	0.57
1:AD:41:LEU:HD11	1:AD:52:ARG:HB2	1.86	0.57
1:AO:53:PRO:HG2	1:CE:7:ASN:O	2.04	0.57
1:AV:33:ASP:H	1:AV:36:SER:HB3	1.67	0.57
1:AX:18:VAL:HG22	1:CT:16:ASN:OD1	2.04	0.57
1:BX:30:VAL:HA	1:CL:34:ASN:ND2	2.19	0.57
1:DE:41:LEU:HD11	1:DE:52:ARG:HB2	1.84	0.57
1:AP:41:LEU:HD11	1:AP:52:ARG:HB2	1.86	0.57
1:BF:50:LEU:HD21	1:BQ:82:VAL:HG11	1.85	0.57
1:BH:33:ASP:H	1:BH:36:SER:HB3	1.67	0.57
1:CI:33:ASP:H	1:CI:36:SER:HB3	1.67	0.57
1:CU:41:LEU:HD11	1:CU:52:ARG:HB2	1.86	0.57
1:AF:163:PHE:CD2	1:BV:24:ALA:HA	2.40	0.57
1:AK:41:LEU:HD11	1:AK:52:ARG:HB2	1.84	0.57
1:CO:41:LEU:HD11	1:CO:52:ARG:HB2	1.86	0.57
1:CR:34:ASN:ND2	1:DB:30:VAL:HA	2.20	0.57
1:AG:41:LEU:HD11	1:AG:52:ARG:HB2	1.86	0.57
1:AI:161:ARG:HD2	1:BY:34:ASN:HB3	1.87	0.57
1:AM:41:LEU:HD11	1:AM:52:ARG:HB2	1.86	0.57
1:BK:41:LEU:HD11	1:BK:52:ARG:HB2	1.86	0.57
1:CF:41:LEU:HD11	1:CF:52:ARG:HB2	1.86	0.57
1:AI:157:ASP:CG	1:BW:52:ARG:HH22	2.07	0.57
1:BE:41:LEU:HD11	1:BE:52:ARG:HB2	1.86	0.57
1:BG:156:ILE:O	1:DC:84:ARG:HD2	2.05	0.57
1:CR:41:LEU:HD11	1:CR:52:ARG:HB2	1.86	0.57
1:AK:30:VAL:HA	1:BW:34:ASN:ND2	2.19	0.57
1:BB:41:LEU:HD11	1:BB:52:ARG:HB2	1.86	0.57
1:BM:24:ALA:HA	1:DI:163:PHE:HD2	1.69	0.57
1:DJ:41:LEU:HD11	1:DJ:52:ARG:HB2	1.86	0.57
1:AI:24:ALA:HA	1:BY:163:PHE:HD2	1.70	0.56
1:BH:41:LEU:HD11	1:BH:52:ARG:HB2	1.86	0.56
1:CI:41:LEU:HD11	1:CI:52:ARG:HB2	1.86	0.56
1:CT:34:ASN:HD21	1:DB:35:LYS:NZ	2.03	0.56
1:AG:34:ASN:ND2	1:CS:30:VAL:HA	2.20	0.56
1:BG:24:ALA:HA	1:DC:163:PHE:HD2	1.70	0.56
1:AZ:86:PHE:CE1	1:AZ:117:LEU:HD23	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:24:ALA:HA	1:CZ:163:PHE:HD2	1.71	0.56
1:BH:86:PHE:HE2	1:BH:117:LEU:HD23	1.71	0.56
1:CL:41:LEU:HD11	1:CL:52:ARG:HB2	1.86	0.56
1:CM:86:PHE:CE1	1:CM:117:LEU:HD23	2.41	0.56
1:CP:86:PHE:CE1	1:CP:117:LEU:HD23	2.41	0.56
1:AQ:86:PHE:CE1	1:AQ:117:LEU:HD23	2.41	0.56
1:BI:86:PHE:CE1	1:BI:117:LEU:HD23	2.41	0.56
1:BL:86:PHE:CE1	1:BL:117:LEU:HD23	2.41	0.56
1:BT:41:LEU:HD11	1:BT:52:ARG:HB2	1.86	0.56
1:BW:86:PHE:HE2	1:BW:117:LEU:HD23	1.71	0.56
1:CY:86:PHE:CE1	1:CY:117:LEU:HD23	2.41	0.56
1:DG:41:LEU:HD11	1:DG:52:ARG:HB2	1.86	0.56
1:AH:86:PHE:CE1	1:AH:117:LEU:HD23	2.41	0.56
1:AR:42:ASP:OD2	1:CK:9:SER:N	2.38	0.56
1:AS:41:LEU:HD11	1:AS:52:ARG:HB2	1.86	0.56
1:AV:41:LEU:HD11	1:AV:52:ARG:HB2	1.86	0.56
1:CD:86:PHE:CE1	1:CD:117:LEU:HD23	2.41	0.56
1:CX:41:LEU:HD11	1:CX:52:ARG:HB2	1.86	0.56
1:AS:86:PHE:HE2	1:AS:117:LEU:HD23	1.71	0.56
1:AV:86:PHE:HE2	1:AV:117:LEU:HD23	1.71	0.56
1:CJ:86:PHE:CE1	1:CJ:117:LEU:HD23	2.41	0.56
1:CO:86:PHE:HE2	1:CO:117:LEU:HD23	1.71	0.56
1:DH:86:PHE:CE1	1:DH:117:LEU:HD23	2.41	0.56
1:BN:41:LEU:HD11	1:BN:52:ARG:HB2	1.86	0.56
1:AA:28:VAL:HG11	1:BP:159:LEU:HD13	1.86	0.56
1:AY:86:PHE:HE2	1:AY:117:LEU:HD23	1.71	0.56
1:BA:163:PHE:HD2	1:CW:24:ALA:HA	1.71	0.56
1:BB:86:PHE:HE2	1:BB:117:LEU:HD23	1.71	0.56
1:BQ:86:PHE:HE2	1:BQ:117:LEU:HD23	1.71	0.56
1:BX:86:PHE:CE1	1:BX:117:LEU:HD23	2.41	0.56
1:CG:86:PHE:CE1	1:CG:117:LEU:HD23	2.41	0.56
1:DA:41:LEU:HD11	1:DA:52:ARG:HB2	1.86	0.56
1:DE:86:PHE:CE1	1:DE:117:LEU:HD23	2.41	0.56
1:DK:86:PHE:CE1	1:DK:117:LEU:HD23	2.41	0.56
1:AK:86:PHE:CE1	1:AK:117:LEU:HD23	2.41	0.56
1:AW:86:PHE:CE1	1:AW:117:LEU:HD23	2.41	0.56
1:AY:41:LEU:HD11	1:AY:52:ARG:HB2	1.86	0.56
1:DG:86:PHE:HE2	1:DG:117:LEU:HD23	1.71	0.56
1:AA:41:LEU:HD11	1:AA:52:ARG:HB2	1.86	0.56
1:AB:86:PHE:CE1	1:AB:117:LEU:HD23	2.41	0.56
1:BD:34:ASN:HB3	1:CZ:161:ARG:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:86:PHE:CE1	1:CA:117:LEU:HD23	2.41	0.56
1:CF:86:PHE:HE2	1:CF:117:LEU:HD23	1.71	0.56
1:CI:86:PHE:HE2	1:CI:117:LEU:HD23	1.71	0.56
1:AJ:34:ASN:ND2	1:CV:30:VAL:HA	2.22	0.55
1:AN:86:PHE:CE1	1:AN:117:LEU:HD23	2.41	0.55
1:BZ:86:PHE:HE2	1:BZ:117:LEU:HD23	1.71	0.55
1:CC:41:LEU:HD11	1:CC:52:ARG:HB2	1.86	0.55
1:CR:86:PHE:HE2	1:CR:117:LEU:HD23	1.71	0.55
1:DB:86:PHE:CE1	1:DB:117:LEU:HD23	2.41	0.55
1:AT:86:PHE:CE1	1:AT:117:LEU:HD23	2.41	0.55
1:CS:86:PHE:CE1	1:CS:117:LEU:HD23	2.41	0.55
1:CU:86:PHE:HE2	1:CU:117:LEU:HD23	1.71	0.55
1:CV:86:PHE:CE1	1:CV:117:LEU:HD23	2.41	0.55
1:AO:157:ASP:CG	1:CC:52:ARG:HH22	2.10	0.55
1:AT:30:VAL:HA	1:AV:34:ASN:ND2	2.21	0.55
1:DD:86:PHE:HE2	1:DD:117:LEU:HD23	1.71	0.55
1:BC:86:PHE:CE1	1:BC:117:LEU:HD23	2.41	0.55
1:BK:86:PHE:HE2	1:BK:117:LEU:HD23	1.71	0.55
1:BN:86:PHE:HE2	1:BN:117:LEU:HD23	1.71	0.55
1:BU:86:PHE:CE1	1:BU:117:LEU:HD23	2.41	0.55
1:AD:86:PHE:HE2	1:AD:117:LEU:HD23	1.71	0.55
1:BD:159:LEU:HD13	1:CX:28:VAL:HG11	1.88	0.55
1:BO:86:PHE:CE1	1:BO:117:LEU:HD23	2.41	0.55
1:BT:111:GLN:OE1	1:BU:119:SER:HB2	2.07	0.55
1:AE:86:PHE:CE1	1:AE:117:LEU:HD23	2.41	0.55
1:AG:86:PHE:HE2	1:AG:117:LEU:HD23	1.71	0.55
1:AL:24:ALA:HA	1:CB:163:PHE:HD2	1.72	0.55
1:AS:111:GLN:OE1	1:AT:119:SER:HB2	2.07	0.55
1:AY:111:GLN:OE1	1:AZ:119:SER:HB2	2.07	0.55
1:BG:53:PRO:HG2	1:DC:7:ASN:O	2.07	0.55
1:BR:86:PHE:CE1	1:BR:117:LEU:HD23	2.41	0.55
1:CI:111:GLN:OE1	1:CJ:119:SER:HB2	2.07	0.55
1:CO:111:GLN:OE1	1:CP:119:SER:HB2	2.07	0.55
1:DJ:111:GLN:OE1	1:DK:119:SER:HB2	2.07	0.55
1:BG:119:SER:HB2	1:DC:111:GLN:OE1	2.07	0.55
1:CL:86:PHE:HE2	1:CL:117:LEU:HD23	1.71	0.55
1:CX:86:PHE:HE2	1:CX:117:LEU:HD23	1.71	0.55
1:CX:111:GLN:OE1	1:CY:119:SER:HB2	2.07	0.55
1:AG:111:GLN:OE1	1:AH:119:SER:HB2	2.07	0.55
1:AL:157:ASP:CG	1:BZ:52:ARG:HH22	2.10	0.55
1:BE:86:PHE:HE2	1:BE:117:LEU:HD23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:86:PHE:CE1	1:BF:117:LEU:HD23	2.41	0.55
1:BH:8:CYS:SG	1:BI:90:ARG:NH1	2.80	0.55
1:BW:8:CYS:SG	1:BX:90:ARG:NH1	2.80	0.55
1:BW:111:GLN:OE1	1:BX:119:SER:HB2	2.07	0.55
1:DA:111:GLN:OE1	1:DB:119:SER:HB2	2.07	0.55
1:AA:64:TYR:HD2	1:AA:67:ARG:NH2	2.05	0.55
1:AA:111:GLN:OE1	1:AB:119:SER:HB2	2.07	0.55
1:AM:64:TYR:HD2	1:AM:67:ARG:NH2	2.05	0.55
1:BQ:64:TYR:HD2	1:BQ:67:ARG:NH2	2.05	0.55
1:CL:8:CYS:SG	1:CM:90:ARG:NH1	2.80	0.55
1:CL:64:TYR:HD2	1:CL:67:ARG:NH2	2.05	0.55
1:CL:111:GLN:OE1	1:CM:119:SER:HB2	2.07	0.55
1:AC:24:ALA:HA	1:BP:163:PHE:HD2	1.71	0.54
1:AJ:8:CYS:SG	1:AK:90:ARG:NH1	2.80	0.54
1:AM:86:PHE:HE2	1:AM:117:LEU:HD23	1.71	0.54
1:BB:111:GLN:OE1	1:BC:119:SER:HB2	2.07	0.54
1:BE:111:GLN:OE1	1:BF:119:SER:HB2	2.07	0.54
1:BN:64:TYR:HD2	1:BN:67:ARG:NH2	2.05	0.54
1:BT:86:PHE:HE2	1:BT:117:LEU:HD23	1.71	0.54
1:CC:111:GLN:OE1	1:CD:119:SER:HB2	2.07	0.54
1:CR:8:CYS:SG	1:CS:90:ARG:NH1	2.80	0.54
1:CX:64:TYR:HD2	1:CX:67:ARG:NH2	2.05	0.54
1:DD:64:TYR:HD2	1:DD:67:ARG:NH2	2.05	0.54
1:AS:28:VAL:HG11	1:CN:159:LEU:HD13	1.88	0.54
1:BB:64:TYR:HD2	1:BB:67:ARG:NH2	2.05	0.54
1:BD:157:ASP:CG	1:CX:52:ARG:HH22	2.10	0.54
1:BJ:94:TRP:CE2	1:BJ:111:GLN:HG3	2.43	0.54
1:BM:94:TRP:CE2	1:BM:111:GLN:HG3	2.43	0.54
1:BV:94:TRP:CE2	1:BV:111:GLN:HG3	2.43	0.54
1:CC:64:TYR:HD2	1:CC:67:ARG:NH2	2.05	0.54
1:CC:86:PHE:HE2	1:CC:117:LEU:HD23	1.71	0.54
1:CT:94:TRP:CE2	1:CT:111:GLN:HG3	2.43	0.54
1:DF:94:TRP:CE2	1:DF:111:GLN:HG3	2.43	0.54
1:DJ:8:CYS:SG	1:DK:90:ARG:NH1	2.80	0.54
1:AC:94:TRP:CE2	1:AC:111:GLN:HG3	2.43	0.54
1:AE:30:VAL:HA	1:BE:34:ASN:ND2	2.22	0.54
1:AI:94:TRP:CE2	1:AI:111:GLN:HG3	2.43	0.54
1:AJ:64:TYR:HD2	1:AJ:67:ARG:NH2	2.05	0.54
1:BG:94:TRP:CE2	1:BG:111:GLN:HG3	2.43	0.54
1:BO:30:VAL:HA	1:DJ:34:ASN:ND2	2.23	0.54
1:CC:8:CYS:SG	1:CD:90:ARG:NH1	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:94:TRP:CE2	1:CE:111:GLN:HG3	2.43	0.54
1:CF:111:GLN:OE1	1:CG:119:SER:HB2	2.07	0.54
1:CK:94:TRP:CE2	1:CK:111:GLN:HG3	2.43	0.54
1:CN:94:TRP:CE2	1:CN:111:GLN:HG3	2.43	0.54
1:DA:64:TYR:HD2	1:DA:67:ARG:NH2	2.05	0.54
1:DA:86:PHE:HE2	1:DA:117:LEU:HD23	1.71	0.54
1:DC:94:TRP:CE2	1:DC:111:GLN:HG3	2.43	0.54
1:AA:86:PHE:HE2	1:AA:117:LEU:HD23	1.71	0.54
1:AD:8:CYS:SG	1:AE:90:ARG:NH1	2.80	0.54
1:AD:111:GLN:OE1	1:AE:119:SER:HB2	2.07	0.54
1:AJ:86:PHE:HE2	1:AJ:117:LEU:HD23	1.71	0.54
1:AL:94:TRP:CE2	1:AL:111:GLN:HG3	2.43	0.54
1:AM:111:GLN:OE1	1:AN:119:SER:HB2	2.07	0.54
1:AP:8:CYS:SG	1:AQ:90:ARG:NH1	2.80	0.54
1:AP:86:PHE:HE2	1:AP:117:LEU:HD23	1.71	0.54
1:BH:64:TYR:HD2	1:BH:67:ARG:NH2	2.05	0.54
1:BH:111:GLN:OE1	1:BI:119:SER:HB2	2.07	0.54
1:BJ:163:PHE:HD2	1:DF:24:ALA:HA	1.72	0.54
1:CB:94:TRP:CE2	1:CB:111:GLN:HG3	2.43	0.54
1:CQ:94:TRP:CE2	1:CQ:111:GLN:HG3	2.43	0.54
1:CW:94:TRP:CE2	1:CW:111:GLN:HG3	2.43	0.54
1:DD:111:GLN:OE1	1:DE:119:SER:HB2	2.07	0.54
1:DI:94:TRP:CE2	1:DI:111:GLN:HG3	2.43	0.54
1:DJ:86:PHE:HE2	1:DJ:117:LEU:HD23	1.71	0.54
1:BP:94:TRP:CE2	1:BP:111:GLN:HG3	2.43	0.54
1:BQ:8:CYS:SG	1:BR:90:ARG:NH1	2.80	0.54
1:CI:64:TYR:HD2	1:CI:67:ARG:NH2	2.05	0.54
1:CR:64:TYR:HD2	1:CR:67:ARG:NH2	2.05	0.54
1:CU:64:TYR:HD2	1:CU:67:ARG:NH2	2.05	0.54
1:CU:111:GLN:OE1	1:CV:119:SER:HB2	2.07	0.54
1:DG:111:GLN:OE1	1:DH:119:SER:HB2	2.07	0.54
1:AB:37:THR:HG23	1:AB:58:ASN:HB3	1.90	0.54
1:AH:37:THR:HG23	1:AH:58:ASN:HB3	1.90	0.54
1:AV:8:CYS:SG	1:AW:90:ARG:NH1	2.80	0.54
1:AW:37:THR:HG23	1:AW:58:ASN:HB3	1.90	0.54
1:AX:94:TRP:CE2	1:AX:111:GLN:HG3	2.43	0.54
1:AY:8:CYS:SG	1:AZ:90:ARG:NH1	2.80	0.54
1:BA:94:TRP:CE2	1:BA:111:GLN:HG3	2.43	0.54
1:BB:8:CYS:SG	1:BC:90:ARG:NH1	2.80	0.54
1:BK:8:CYS:SG	1:BL:90:ARG:NH1	2.80	0.54
1:BN:8:CYS:SG	1:BO:90:ARG:NH1	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BN:111:GLN:OE1	1:BO:119:SER:HB2	2.07	0.54
1:BT:64:TYR:HD2	1:BT:67:ARG:NH2	2.05	0.54
1:CF:8:CYS:SG	1:CG:90:ARG:NH1	2.80	0.54
1:DB:37:THR:HG23	1:DB:58:ASN:HB3	1.90	0.54
1:DG:8:CYS:SG	1:DH:90:ARG:NH1	2.80	0.54
1:AD:64:TYR:HD2	1:AD:67:ARG:NH2	2.05	0.54
1:AF:94:TRP:CE2	1:AF:111:GLN:HG3	2.43	0.54
1:AJ:111:GLN:OE1	1:AK:119:SER:HB2	2.07	0.54
1:AS:64:TYR:HD2	1:AS:67:ARG:NH2	2.05	0.54
1:CI:8:CYS:SG	1:CJ:90:ARG:NH1	2.80	0.54
1:DD:8:CYS:SG	1:DE:90:ARG:NH1	2.80	0.54
1:AM:8:CYS:SG	1:AN:90:ARG:NH1	2.80	0.54
1:AT:37:THR:HG23	1:AT:58:ASN:HB3	1.90	0.54
1:AU:94:TRP:CE2	1:AU:111:GLN:HG3	2.43	0.54
1:BE:8:CYS:SG	1:BF:90:ARG:NH1	2.80	0.54
1:BE:64:TYR:HD2	1:BE:67:ARG:NH2	2.05	0.54
1:BY:94:TRP:CE2	1:BY:111:GLN:HG3	2.43	0.54
1:BZ:111:GLN:OE1	1:CA:119:SER:HB2	2.07	0.54
1:CP:37:THR:HG23	1:CP:58:ASN:HB3	1.90	0.54
1:CY:37:THR:HG23	1:CY:58:ASN:HB3	1.90	0.54
1:DA:8:CYS:SG	1:DB:90:ARG:NH1	2.80	0.54
1:DA:19:LEU:HD11	1:DB:17:LEU:HD22	1.90	0.54
1:DL:94:TRP:CE2	1:DL:111:GLN:HG3	2.43	0.54
1:AP:111:GLN:OE1	1:AQ:119:SER:HB2	2.07	0.54
1:AR:94:TRP:CE2	1:AR:111:GLN:HG3	2.43	0.54
1:BA:157:ASP:CG	1:CU:52:ARG:HH22	2.11	0.54
1:BE:19:LEU:HD11	1:BF:17:LEU:HD22	1.90	0.54
1:BK:64:TYR:HD2	1:BK:67:ARG:NH2	2.05	0.54
1:BK:111:GLN:OE1	1:BL:119:SER:HB2	2.07	0.54
1:BN:19:LEU:HD11	1:BO:17:LEU:HD22	1.90	0.54
1:CO:8:CYS:SG	1:CP:90:ARG:NH1	2.80	0.54
1:CO:19:LEU:HD11	1:CP:17:LEU:HD22	1.90	0.54
1:CU:8:CYS:SG	1:CV:90:ARG:NH1	2.80	0.54
1:AN:30:VAL:HA	1:BZ:34:ASN:ND2	2.23	0.54
1:CA:37:THR:HG23	1:CA:58:ASN:HB3	1.90	0.54
1:CD:30:VAL:HA	1:CI:34:ASN:ND2	2.23	0.54
1:CR:111:GLN:OE1	1:CS:119:SER:HB2	2.07	0.54
1:AG:8:CYS:SG	1:AH:90:ARG:NH1	2.80	0.53
1:AG:19:LEU:HD11	1:AH:17:LEU:HD22	1.90	0.53
1:AG:64:TYR:HD2	1:AG:67:ARG:NH2	2.06	0.53
1:AN:37:THR:HG23	1:AN:58:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:94:TRP:CE2	1:AO:111:GLN:HG3	2.43	0.53
1:AR:163:PHE:CD2	1:CK:24:ALA:HA	2.42	0.53
1:AV:111:GLN:OE1	1:AW:119:SER:HB2	2.07	0.53
1:BW:64:TYR:HD2	1:BW:67:ARG:NH2	2.05	0.53
1:CC:19:LEU:HD11	1:CD:17:LEU:HD22	1.90	0.53
1:CX:8:CYS:SG	1:CY:90:ARG:NH1	2.80	0.53
1:CZ:94:TRP:CE2	1:CZ:111:GLN:HG3	2.43	0.53
1:DJ:64:TYR:HD2	1:DJ:67:ARG:NH2	2.05	0.53
1:AY:19:LEU:HD11	1:AZ:17:LEU:HD22	1.90	0.53
1:BZ:19:LEU:HD11	1:CA:17:LEU:HD22	1.90	0.53
1:DG:64:TYR:HD2	1:DG:67:ARG:NH2	2.05	0.53
1:DK:37:THR:HG23	1:DK:58:ASN:HB3	1.90	0.53
1:AA:8:CYS:SG	1:AB:90:ARG:NH1	2.80	0.53
1:AP:64:TYR:HD2	1:AP:67:ARG:NH2	2.05	0.53
1:AS:19:LEU:HD11	1:AT:17:LEU:HD22	1.90	0.53
1:BD:94:TRP:CE2	1:BD:111:GLN:HG3	2.43	0.53
1:BS:94:TRP:CE2	1:BS:111:GLN:HG3	2.43	0.53
1:CI:19:LEU:HD11	1:CJ:17:LEU:HD22	1.90	0.53
1:DE:37:THR:HG23	1:DE:58:ASN:HB3	1.90	0.53
1:AC:163:PHE:HD2	1:BP:24:ALA:HA	1.74	0.53
1:BJ:6:ILE:HG22	1:DF:94:TRP:NE1	2.23	0.53
1:BK:19:LEU:HD11	1:BL:17:LEU:HD22	1.90	0.53
1:BQ:19:LEU:HD11	1:BR:17:LEU:HD22	1.90	0.53
1:BQ:111:GLN:OE1	1:BR:119:SER:HB2	2.07	0.53
1:CF:19:LEU:HD11	1:CG:17:LEU:HD22	1.90	0.53
1:CX:19:LEU:HD11	1:CY:17:LEU:HD22	1.90	0.53
1:AK:37:THR:HG23	1:AK:58:ASN:HB3	1.90	0.53
1:AS:8:CYS:SG	1:AT:90:ARG:NH1	2.80	0.53
1:BF:37:THR:HG23	1:BF:58:ASN:HB3	1.90	0.53
1:BR:37:THR:HG23	1:BR:58:ASN:HB3	1.90	0.53
1:BT:8:CYS:SG	1:BU:90:ARG:NH1	2.80	0.53
1:BZ:8:CYS:SG	1:CA:90:ARG:NH1	2.80	0.53
1:CF:64:TYR:HD2	1:CF:67:ARG:NH2	2.05	0.53
1:CH:94:TRP:CE2	1:CH:111:GLN:HG3	2.43	0.53
1:DK:96:LYS:HG2	1:DK:107:TYR:HB2	1.91	0.53
1:AE:96:LYS:HG2	1:AE:107:TYR:HB2	1.91	0.53
1:AV:64:TYR:HD2	1:AV:67:ARG:NH2	2.05	0.53
1:AZ:96:LYS:HG2	1:AZ:107:TYR:HB2	1.91	0.53
1:BC:37:THR:HG23	1:BC:58:ASN:HB3	1.90	0.53
1:BE:52:ARG:HH22	1:DC:157:ASP:CG	2.12	0.53
1:CG:96:LYS:HG2	1:CG:107:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CO:64:TYR:HD2	1:CO:67:ARG:NH2	2.05	0.53
1:CU:19:LEU:HD11	1:CV:17:LEU:HD22	1.90	0.53
1:DD:19:LEU:HD11	1:DE:17:LEU:HD22	1.90	0.53
1:AU:24:ALA:HA	1:CN:163:PHE:HD2	1.72	0.53
1:BD:163:PHE:HD2	1:CZ:24:ALA:HA	1.74	0.53
1:BZ:64:TYR:HD2	1:BZ:67:ARG:NH2	2.05	0.53
1:CD:96:LYS:HG2	1:CD:107:TYR:HB2	1.91	0.53
1:AW:30:VAL:HA	1:BT:34:ASN:ND2	2.24	0.53
1:BB:19:LEU:HD11	1:BC:17:LEU:HD22	1.90	0.53
1:CG:37:THR:HG23	1:CG:58:ASN:HB3	1.90	0.53
1:AH:96:LYS:HG2	1:AH:107:TYR:HB2	1.91	0.53
1:AQ:37:THR:HG23	1:AQ:58:ASN:HB3	1.90	0.53
1:BA:46:ASP:H	1:CW:7:ASN:HD21	1.56	0.53
1:BO:37:THR:HG23	1:BO:58:ASN:HB3	1.90	0.53
1:CM:96:LYS:HG2	1:CM:107:TYR:HB2	1.91	0.53
1:CV:96:LYS:HG2	1:CV:107:TYR:HB2	1.91	0.53
1:DG:19:LEU:HD11	1:DH:17:LEU:HD22	1.90	0.53
1:BH:82:VAL:HG13	1:BL:50:LEU:HD11	1.91	0.53
1:BI:37:THR:HG23	1:BI:58:ASN:HB3	1.90	0.53
1:BL:96:LYS:HG2	1:BL:107:TYR:HB2	1.91	0.53
1:CD:37:THR:HG23	1:CD:58:ASN:HB3	1.90	0.53
1:CS:37:THR:HG23	1:CS:58:ASN:HB3	1.90	0.53
1:AQ:96:LYS:HG2	1:AQ:107:TYR:HB2	1.91	0.52
1:BI:96:LYS:HG2	1:BI:107:TYR:HB2	1.91	0.52
1:BW:19:LEU:HD11	1:BX:17:LEU:HD22	1.90	0.52
1:CJ:96:LYS:HG2	1:CJ:107:TYR:HB2	1.91	0.52
1:CR:19:LEU:HD11	1:CS:17:LEU:HD22	1.90	0.52
1:AA:19:LEU:HD11	1:AB:17:LEU:HD22	1.90	0.52
1:AE:37:THR:HG23	1:AE:58:ASN:HB3	1.90	0.52
1:AI:34:ASN:HB3	1:BY:161:ARG:HD2	1.90	0.52
1:AX:24:ALA:HA	1:CT:163:PHE:CD2	2.43	0.52
1:AZ:37:THR:HG23	1:AZ:58:ASN:HB3	1.90	0.52
1:BH:19:LEU:HD11	1:BI:17:LEU:HD22	1.90	0.52
1:BX:96:LYS:HG2	1:BX:107:TYR:HB2	1.91	0.52
1:BG:40:TYR:CE1	1:DC:163:PHE:HB2	2.44	0.52
1:BR:96:LYS:HG2	1:BR:107:TYR:HB2	1.91	0.52
1:CM:37:THR:HG23	1:CM:58:ASN:HB3	1.90	0.52
1:DE:96:LYS:HG2	1:DE:107:TYR:HB2	1.91	0.52
1:AJ:19:LEU:HD11	1:AK:17:LEU:HD22	1.90	0.52
1:AO:159:LEU:HD13	1:CC:28:VAL:HG11	1.91	0.52
1:AR:86:PHE:CD2	1:CK:155:LEU:HD13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AY:64:TYR:HD2	1:AY:67:ARG:NH2	2.05	0.52
1:BX:37:THR:HG23	1:BX:58:ASN:HB3	1.90	0.52
1:CJ:37:THR:HG23	1:CJ:58:ASN:HB3	1.90	0.52
1:AD:19:LEU:HD11	1:AE:17:LEU:HD22	1.90	0.52
1:AF:7:ASN:HD21	1:BV:46:ASP:H	1.58	0.52
1:AV:19:LEU:HD11	1:AW:17:LEU:HD22	1.91	0.52
1:AW:96:LYS:HG2	1:AW:107:TYR:HB2	1.91	0.52
1:BT:19:LEU:HD11	1:BU:17:LEU:HD22	1.90	0.52
1:CY:96:LYS:HG2	1:CY:107:TYR:HB2	1.91	0.52
1:DD:17:LEU:HD22	1:DE:19:LEU:HD11	1.92	0.52
1:AG:17:LEU:HD22	1:AH:19:LEU:HD11	1.92	0.52
1:AS:52:ARG:HH22	1:CN:157:ASP:CG	2.13	0.52
1:AY:17:LEU:HD22	1:AZ:19:LEU:HD11	1.92	0.52
1:BE:17:LEU:HD22	1:BF:19:LEU:HD11	1.92	0.52
1:BL:37:THR:HG23	1:BL:58:ASN:HB3	1.90	0.52
1:CR:17:LEU:HD22	1:CS:19:LEU:HD11	1.92	0.52
1:CV:37:THR:HG23	1:CV:58:ASN:HB3	1.90	0.52
1:DH:96:LYS:HG2	1:DH:107:TYR:HB2	1.91	0.52
1:AM:19:LEU:HD11	1:AN:17:LEU:HD22	1.90	0.52
1:AP:19:LEU:HD11	1:AQ:17:LEU:HD22	1.90	0.52
1:AX:94:TRP:NE1	1:CT:6:ILE:HG22	2.25	0.52
1:BU:96:LYS:HG2	1:BU:107:TYR:HB2	1.91	0.52
1:DH:37:THR:HG23	1:DH:58:ASN:HB3	1.90	0.52
1:AF:84:ARG:HD2	1:BV:156:ILE:O	2.10	0.52
1:BU:37:THR:HG23	1:BU:58:ASN:HB3	1.90	0.52
1:AK:96:LYS:HG2	1:AK:107:TYR:HB2	1.91	0.52
1:AV:17:LEU:HD22	1:AW:19:LEU:HD11	1.92	0.52
1:BI:130:ILE:O	1:BI:133:ILE:HG22	2.10	0.52
1:BK:17:LEU:HD22	1:BL:19:LEU:HD11	1.92	0.52
1:BK:94:TRP:CE2	1:BK:111:GLN:HG3	2.45	0.52
1:CF:94:TRP:CE2	1:CF:111:GLN:HG3	2.45	0.52
1:DD:94:TRP:CE2	1:DD:111:GLN:HG3	2.45	0.52
1:AA:17:LEU:HD22	1:AB:19:LEU:HD11	1.92	0.52
1:AB:96:LYS:HG2	1:AB:107:TYR:HB2	1.91	0.52
1:AD:94:TRP:CE2	1:AD:111:GLN:HG3	2.45	0.52
1:BF:96:LYS:HG2	1:BF:107:TYR:HB2	1.91	0.52
1:CX:94:TRP:CE2	1:CX:111:GLN:HG3	2.45	0.52
1:CY:130:ILE:O	1:CY:133:ILE:HG22	2.10	0.52
1:DB:96:LYS:HG2	1:DB:107:TYR:HB2	1.91	0.52
1:DJ:94:TRP:CE2	1:DJ:111:GLN:HG3	2.45	0.52
1:AD:17:LEU:HD22	1:AE:19:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:17:LEU:HD22	1:AQ:19:LEU:HD11	1.92	0.51
1:AQ:130:ILE:O	1:AQ:133:ILE:HG22	2.10	0.51
1:AW:130:ILE:O	1:AW:133:ILE:HG22	2.10	0.51
1:BC:130:ILE:O	1:BC:133:ILE:HG22	2.10	0.51
1:BM:7:ASN:HD21	1:DI:46:ASP:H	1.58	0.51
1:BU:130:ILE:O	1:BU:133:ILE:HG22	2.10	0.51
1:CC:94:TRP:CE2	1:CC:111:GLN:HG3	2.45	0.51
1:CG:130:ILE:O	1:CG:133:ILE:HG22	2.10	0.51
1:CO:17:LEU:HD22	1:CP:19:LEU:HD11	1.92	0.51
1:CP:96:LYS:HG2	1:CP:107:TYR:HB2	1.91	0.51
1:CS:130:ILE:O	1:CS:133:ILE:HG22	2.10	0.51
1:CU:94:TRP:CE2	1:CU:111:GLN:HG3	2.45	0.51
1:CX:17:LEU:HD22	1:CY:19:LEU:HD11	1.92	0.51
1:AN:130:ILE:O	1:AN:133:ILE:HG22	2.10	0.51
1:BT:17:LEU:HD22	1:BU:19:LEU:HD11	1.92	0.51
1:CA:96:LYS:HG2	1:CA:107:TYR:HB2	1.91	0.51
1:CS:96:LYS:HG2	1:CS:107:TYR:HB2	1.91	0.51
1:CU:17:LEU:HD22	1:CV:19:LEU:HD11	1.92	0.51
1:DJ:19:LEU:HD11	1:DK:17:LEU:HD22	1.90	0.51
1:AB:130:ILE:O	1:AB:133:ILE:HG22	2.10	0.51
1:AE:130:ILE:O	1:AE:133:ILE:HG22	2.10	0.51
1:AF:157:ASP:CG	1:BT:52:ARG:HH22	2.13	0.51
1:AM:34:ASN:ND2	1:CP:30:VAL:HA	2.24	0.51
1:BC:96:LYS:HG2	1:BC:107:TYR:HB2	1.91	0.51
1:BQ:94:TRP:CE2	1:BQ:111:GLN:HG3	2.45	0.51
1:BR:130:ILE:O	1:BR:133:ILE:HG22	2.10	0.51
1:BX:130:ILE:O	1:BX:133:ILE:HG22	2.10	0.51
1:CD:130:ILE:O	1:CD:133:ILE:HG22	2.10	0.51
1:DJ:17:LEU:HD22	1:DK:19:LEU:HD11	1.92	0.51
1:AC:161:ARG:HD2	1:BP:34:ASN:HB3	1.91	0.51
1:AM:94:TRP:CE2	1:AM:111:GLN:HG3	2.45	0.51
1:BJ:153:GLN:OE1	1:DF:127:ALA:HB2	2.11	0.51
1:BL:130:ILE:O	1:BL:133:ILE:HG22	2.10	0.51
1:BO:130:ILE:O	1:BO:133:ILE:HG22	2.10	0.51
1:CA:130:ILE:O	1:CA:133:ILE:HG22	2.10	0.51
1:CL:17:LEU:HD22	1:CM:19:LEU:HD11	1.92	0.51
1:CO:94:TRP:CE2	1:CO:111:GLN:HG3	2.45	0.51
1:DH:130:ILE:O	1:DH:133:ILE:HG22	2.10	0.51
1:AA:94:TRP:CE2	1:AA:111:GLN:HG3	2.45	0.51
1:AG:94:TRP:CE2	1:AG:111:GLN:HG3	2.45	0.51
1:AL:159:LEU:HD13	1:BZ:28:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:94:TRP:CE2	1:AS:111:GLN:HG3	2.45	0.51
1:AV:94:TRP:CE2	1:AV:111:GLN:HG3	2.45	0.51
1:AY:94:TRP:CE2	1:AY:111:GLN:HG3	2.45	0.51
1:BB:17:LEU:HD22	1:BC:19:LEU:HD11	1.92	0.51
1:CN:95:ARG:NH2	1:CN:108:THR:OG1	2.44	0.51
1:CR:94:TRP:CE2	1:CR:111:GLN:HG3	2.45	0.51
1:DK:130:ILE:O	1:DK:133:ILE:HG22	2.10	0.51
1:AC:34:ASN:HB3	1:BP:161:ARG:HD2	1.91	0.51
1:AC:159:LEU:HD13	1:BN:28:VAL:HG11	1.93	0.51
1:AH:130:ILE:O	1:AH:133:ILE:HG22	2.10	0.51
1:AJ:17:LEU:HD22	1:AK:19:LEU:HD11	1.92	0.51
1:AM:17:LEU:HD22	1:AN:19:LEU:HD11	1.92	0.51
1:AP:94:TRP:CE2	1:AP:111:GLN:HG3	2.45	0.51
1:AT:121:VAL:HG13	1:AT:125:THR:HB	1.93	0.51
1:AZ:130:ILE:O	1:AZ:133:ILE:HG22	2.10	0.51
1:BE:94:TRP:CE2	1:BE:111:GLN:HG3	2.45	0.51
1:BQ:17:LEU:HD22	1:BR:19:LEU:HD11	1.92	0.51
1:CF:17:LEU:HD22	1:CG:19:LEU:HD11	1.92	0.51
1:CJ:130:ILE:O	1:CJ:133:ILE:HG22	2.10	0.51
1:CL:19:LEU:HD11	1:CM:17:LEU:HD22	1.90	0.51
1:CM:130:ILE:O	1:CM:133:ILE:HG22	2.10	0.51
1:CV:121:VAL:HG13	1:CV:125:THR:HB	1.93	0.51
1:DC:95:ARG:NH2	1:DC:108:THR:OG1	2.44	0.51
1:DE:130:ILE:O	1:DE:133:ILE:HG22	2.10	0.51
1:AJ:94:TRP:CE2	1:AJ:111:GLN:HG3	2.45	0.51
1:AQ:121:VAL:HG13	1:AQ:125:THR:HB	1.93	0.51
1:AT:96:LYS:HG2	1:AT:107:TYR:HB2	1.91	0.51
1:BD:95:ARG:NH2	1:BD:108:THR:OG1	2.44	0.51
1:BK:52:ARG:HH22	1:DI:157:ASP:CG	2.13	0.51
1:BM:95:ARG:NH2	1:BM:108:THR:OG1	2.44	0.51
1:BO:96:LYS:HG2	1:BO:107:TYR:HB2	1.91	0.51
1:BV:95:ARG:NH2	1:BV:108:THR:OG1	2.44	0.51
1:CI:17:LEU:HD22	1:CJ:19:LEU:HD11	1.92	0.51
1:DI:95:ARG:NH2	1:DI:108:THR:OG1	2.44	0.51
1:AK:130:ILE:O	1:AK:133:ILE:HG22	2.10	0.51
1:BF:130:ILE:O	1:BF:133:ILE:HG22	2.10	0.51
1:BH:94:TRP:CE2	1:BH:111:GLN:HG3	2.45	0.51
1:BM:159:LEU:HD13	1:DG:28:VAL:HG11	1.93	0.51
1:BU:121:VAL:HG13	1:BU:125:THR:HB	1.93	0.51
1:BW:6:ILE:O	1:BW:6:ILE:HG13	2.11	0.51
1:CA:121:VAL:HG13	1:CA:125:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CJ:121:VAL:HG13	1:CJ:125:THR:HB	1.93	0.51
1:CQ:95:ARG:NH2	1:CQ:108:THR:OG1	2.44	0.51
1:DA:6:ILE:O	1:DA:6:ILE:HG13	2.11	0.51
1:DE:121:VAL:HG13	1:DE:125:THR:HB	1.93	0.51
1:DG:17:LEU:HD22	1:DH:19:LEU:HD11	1.92	0.51
1:DG:94:TRP:CE2	1:DG:111:GLN:HG3	2.45	0.51
1:AG:6:ILE:O	1:AG:6:ILE:HG13	2.11	0.51
1:AN:96:LYS:HG2	1:AN:107:TYR:HB2	1.91	0.51
1:AR:95:ARG:NH2	1:AR:108:THR:OG1	2.44	0.51
1:BK:6:ILE:HG13	1:BK:6:ILE:O	2.11	0.51
1:BN:17:LEU:HD22	1:BO:19:LEU:HD11	1.92	0.51
1:BN:94:TRP:CE2	1:BN:111:GLN:HG3	2.45	0.51
1:CZ:95:ARG:NH2	1:CZ:108:THR:OG1	2.44	0.51
1:DA:94:TRP:CE2	1:DA:111:GLN:HG3	2.45	0.51
1:DL:95:ARG:NH2	1:DL:108:THR:OG1	2.44	0.51
1:AE:121:VAL:HG13	1:AE:125:THR:HB	1.93	0.51
1:AS:17:LEU:HD22	1:AT:19:LEU:HD11	1.92	0.51
1:BA:95:ARG:NH2	1:BA:108:THR:OG1	2.44	0.51
1:BL:121:VAL:HG13	1:BL:125:THR:HB	1.93	0.51
1:BP:95:ARG:NH2	1:BP:108:THR:OG1	2.44	0.51
1:BQ:6:ILE:O	1:BQ:6:ILE:HG13	2.11	0.51
1:BW:17:LEU:HD22	1:BX:19:LEU:HD11	1.92	0.51
1:BY:95:ARG:NH2	1:BY:108:THR:OG1	2.44	0.51
1:BZ:94:TRP:CE2	1:BZ:111:GLN:HG3	2.45	0.51
1:CT:95:ARG:NH2	1:CT:108:THR:OG1	2.44	0.51
1:AF:95:ARG:NH2	1:AF:108:THR:OG1	2.44	0.50
1:AM:6:ILE:O	1:AM:6:ILE:HG13	2.11	0.50
1:AO:24:ALA:HA	1:CE:163:PHE:CD2	2.44	0.50
1:AU:95:ARG:NH2	1:AU:108:THR:OG1	2.44	0.50
1:AY:6:ILE:HG13	1:AY:6:ILE:O	2.11	0.50
1:BB:6:ILE:HG13	1:BB:6:ILE:O	2.11	0.50
1:CB:95:ARG:NH2	1:CB:108:THR:OG1	2.44	0.50
1:CC:17:LEU:HD22	1:CD:19:LEU:HD11	1.92	0.50
1:CI:94:TRP:CE2	1:CI:111:GLN:HG3	2.45	0.50
1:CR:6:ILE:HG13	1:CR:6:ILE:O	2.11	0.50
1:AC:157:ASP:CG	1:BN:52:ARG:HH22	2.14	0.50
1:AS:6:ILE:O	1:AS:6:ILE:HG13	2.11	0.50
1:BG:2:TYR:CE1	1:DC:97:ALA:HA	2.47	0.50
1:BG:95:ARG:NH2	1:BG:108:THR:OG1	2.44	0.50
1:BI:121:VAL:HG13	1:BI:125:THR:HB	1.93	0.50
1:BJ:34:ASN:HB3	1:DF:161:ARG:HD2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BN:6:ILE:O	1:BN:6:ILE:HG13	2.11	0.50
1:BW:94:TRP:CE2	1:BW:111:GLN:HG3	2.45	0.50
1:CK:95:ARG:NH2	1:CK:108:THR:OG1	2.44	0.50
1:CY:121:VAL:HG13	1:CY:125:THR:HB	1.93	0.50
1:DF:95:ARG:NH2	1:DF:108:THR:OG1	2.44	0.50
1:AA:6:ILE:O	1:AA:6:ILE:HG13	2.11	0.50
1:AC:95:ARG:NH2	1:AC:108:THR:OG1	2.44	0.50
1:AI:95:ARG:NH2	1:AI:108:THR:OG1	2.44	0.50
1:AR:40:TYR:CZ	1:CK:163:PHE:HB2	2.45	0.50
1:BH:28:VAL:HG11	1:DF:159:LEU:HD13	1.93	0.50
1:BZ:6:ILE:O	1:BZ:6:ILE:HG13	2.11	0.50
1:CC:6:ILE:O	1:CC:6:ILE:HG13	2.11	0.50
1:CG:121:VAL:HG13	1:CG:125:THR:HB	1.93	0.50
1:DA:17:LEU:HD22	1:DB:19:LEU:HD11	1.92	0.50
1:DB:130:ILE:O	1:DB:133:ILE:HG22	2.10	0.50
1:AL:95:ARG:NH2	1:AL:108:THR:OG1	2.44	0.50
1:BH:17:LEU:HD22	1:BI:19:LEU:HD11	1.92	0.50
1:BJ:95:ARG:NH2	1:BJ:108:THR:OG1	2.44	0.50
1:BZ:17:LEU:HD22	1:CA:19:LEU:HD11	1.92	0.50
1:AC:57:PHE:CE1	1:BP:162:ILE:HD12	2.47	0.50
1:AL:163:PHE:HD2	1:CB:24:ALA:HA	1.77	0.50
1:AN:121:VAL:HG13	1:AN:125:THR:HB	1.93	0.50
1:CF:6:ILE:HG13	1:CF:6:ILE:O	2.11	0.50
1:CH:95:ARG:NH2	1:CH:108:THR:OG1	2.44	0.50
1:CV:130:ILE:O	1:CV:133:ILE:HG22	2.10	0.50
1:DH:121:VAL:HG13	1:DH:125:THR:HB	1.93	0.50
1:AD:161:ARG:NH1	1:BG:25:GLU:O	2.44	0.50
1:AR:84:ARG:HD2	1:CK:156:ILE:O	2.11	0.50
1:AT:130:ILE:O	1:AT:133:ILE:HG22	2.10	0.50
1:BH:6:ILE:HG13	1:BH:6:ILE:O	2.11	0.50
1:BS:95:ARG:NH2	1:BS:108:THR:OG1	2.44	0.50
1:BT:94:TRP:CE2	1:BT:111:GLN:HG3	2.45	0.50
1:CP:130:ILE:O	1:CP:133:ILE:HG22	2.10	0.50
1:CW:95:ARG:NH2	1:CW:108:THR:OG1	2.44	0.50
1:AD:6:ILE:O	1:AD:6:ILE:HG13	2.12	0.50
1:BC:121:VAL:HG13	1:BC:125:THR:HB	1.93	0.50
1:BJ:98:ASP:HB3	1:DF:1:SER:C	2.32	0.50
1:CL:6:ILE:HG13	1:CL:6:ILE:O	2.11	0.50
1:CS:121:VAL:HG13	1:CS:125:THR:HB	1.93	0.50
1:CX:6:ILE:HG13	1:CX:6:ILE:O	2.11	0.50
1:DJ:6:ILE:O	1:DJ:6:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:95:ARG:NH2	1:AO:108:THR:OG1	2.44	0.50
1:AP:6:ILE:O	1:AP:6:ILE:HG13	2.11	0.50
1:AV:6:ILE:HG13	1:AV:6:ILE:O	2.12	0.50
1:AW:121:VAL:HG13	1:AW:125:THR:HB	1.93	0.50
1:AZ:121:VAL:HG13	1:AZ:125:THR:HB	1.93	0.50
1:BB:52:ARG:HH22	1:CZ:157:ASP:CG	2.14	0.50
1:BS:86:PHE:CE1	1:BS:117:LEU:HD23	2.47	0.50
1:CI:6:ILE:HG13	1:CI:6:ILE:O	2.11	0.50
1:CL:94:TRP:CE2	1:CL:111:GLN:HG3	2.45	0.50
1:CT:86:PHE:CE1	1:CT:117:LEU:HD23	2.47	0.50
1:DD:6:ILE:O	1:DD:6:ILE:HG13	2.11	0.50
1:AJ:6:ILE:O	1:AJ:6:ILE:HG13	2.11	0.50
1:BB:94:TRP:CE2	1:BB:111:GLN:HG3	2.45	0.50
1:BG:57:PHE:CE1	1:DC:162:ILE:HD12	2.47	0.50
1:CU:6:ILE:HG13	1:CU:6:ILE:O	2.11	0.50
1:DL:86:PHE:CE1	1:DL:117:LEU:HD23	2.47	0.50
1:AB:121:VAL:HG13	1:AB:125:THR:HB	1.93	0.49
1:AI:86:PHE:CE1	1:AI:117:LEU:HD23	2.47	0.49
1:BD:86:PHE:CE1	1:BD:117:LEU:HD23	2.47	0.49
1:BX:121:VAL:HG13	1:BX:125:THR:HB	1.93	0.49
1:CD:121:VAL:HG13	1:CD:125:THR:HB	1.93	0.49
1:CO:6:ILE:HG13	1:CO:6:ILE:O	2.11	0.49
1:CP:121:VAL:HG13	1:CP:125:THR:HB	1.93	0.49
1:CQ:86:PHE:CE1	1:CQ:117:LEU:HD23	2.47	0.49
1:AF:94:TRP:NE1	1:BV:6:ILE:HG22	2.27	0.49
1:AO:86:PHE:CE1	1:AO:117:LEU:HD23	2.47	0.49
1:AR:17:LEU:HD22	1:CK:19:LEU:HD11	1.94	0.49
1:AX:86:PHE:CE1	1:AX:117:LEU:HD23	2.47	0.49
1:AX:95:ARG:NH2	1:AX:108:THR:OG1	2.44	0.49
1:BJ:86:PHE:CE1	1:BJ:117:LEU:HD23	2.47	0.49
1:BO:121:VAL:HG13	1:BO:125:THR:HB	1.93	0.49
1:BT:6:ILE:O	1:BT:6:ILE:HG13	2.11	0.49
1:BU:30:VAL:HA	1:DG:34:ASN:ND2	2.27	0.49
1:AC:86:PHE:CE1	1:AC:117:LEU:HD23	2.47	0.49
1:AJ:52:ARG:HH22	1:CB:157:ASP:CG	2.15	0.49
1:BJ:127:ALA:HB2	1:DF:153:GLN:OE1	2.11	0.49
1:BM:86:PHE:CE1	1:BM:117:LEU:HD23	2.47	0.49
1:BV:86:PHE:CE1	1:BV:117:LEU:HD23	2.47	0.49
1:CE:95:ARG:NH2	1:CE:108:THR:OG1	2.44	0.49
1:AH:121:VAL:HG13	1:AH:125:THR:HB	1.93	0.49
1:BF:121:VAL:HG13	1:BF:125:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:86:PHE:CE2	1:CC:117:LEU:HD23	2.48	0.49
1:DG:86:PHE:CE2	1:DG:117:LEU:HD23	2.48	0.49
1:BA:86:PHE:CE1	1:BA:117:LEU:HD23	2.47	0.49
1:DB:121:VAL:HG13	1:DB:125:THR:HB	1.93	0.49
1:AI:159:LEU:HD13	1:BW:28:VAL:HG11	1.94	0.49
1:AU:86:PHE:CE1	1:AU:117:LEU:HD23	2.47	0.49
1:BP:86:PHE:CE1	1:BP:117:LEU:HD23	2.47	0.49
1:CI:86:PHE:CE2	1:CI:117:LEU:HD23	2.48	0.49
1:CM:121:VAL:HG13	1:CM:125:THR:HB	1.93	0.49
1:CN:86:PHE:CE1	1:CN:117:LEU:HD23	2.47	0.49
1:DA:86:PHE:CE2	1:DA:117:LEU:HD23	2.48	0.49
1:DI:86:PHE:CE1	1:DI:117:LEU:HD23	2.47	0.49
1:AM:86:PHE:CE2	1:AM:117:LEU:HD23	2.48	0.49
1:AO:163:PHE:HD2	1:CE:24:ALA:HA	1.77	0.49
1:BG:86:PHE:CE1	1:BG:117:LEU:HD23	2.47	0.49
1:CF:86:PHE:CE2	1:CF:117:LEU:HD23	2.48	0.49
1:CW:86:PHE:CE1	1:CW:117:LEU:HD23	2.47	0.49
1:DC:86:PHE:CE1	1:DC:117:LEU:HD23	2.47	0.49
1:DG:6:ILE:O	1:DG:6:ILE:HG13	2.12	0.49
1:AR:44:GLY:HA3	1:CK:9:SER:OG	2.13	0.49
1:BE:86:PHE:CE2	1:BE:117:LEU:HD23	2.48	0.49
1:BH:86:PHE:CE2	1:BH:117:LEU:HD23	2.48	0.49
1:DF:86:PHE:CE1	1:DF:117:LEU:HD23	2.47	0.49
1:DJ:86:PHE:CE2	1:DJ:117:LEU:HD23	2.48	0.49
1:AY:86:PHE:CE2	1:AY:117:LEU:HD23	2.48	0.49
1:BH:34:ASN:HD22	1:BL:30:VAL:HA	1.74	0.49
1:BW:86:PHE:CE2	1:BW:117:LEU:HD23	2.48	0.49
1:CH:86:PHE:CE1	1:CH:117:LEU:HD23	2.47	0.49
1:CU:86:PHE:CE2	1:CU:117:LEU:HD23	2.48	0.49
1:DD:86:PHE:CE2	1:DD:117:LEU:HD23	2.48	0.49
1:DK:121:VAL:HG13	1:DK:125:THR:HB	1.93	0.49
1:AD:86:PHE:CE2	1:AD:117:LEU:HD23	2.48	0.49
1:AG:52:ARG:HH22	1:BY:157:ASP:CG	2.16	0.49
1:AO:6:ILE:HG22	1:CE:94:TRP:NE1	2.28	0.49
1:AR:86:PHE:CE1	1:AR:117:LEU:HD23	2.47	0.49
1:AS:153:GLN:OE1	1:AT:127:ALA:HB2	2.13	0.49
1:BY:86:PHE:CE1	1:BY:117:LEU:HD23	2.47	0.49
1:BZ:153:GLN:OE1	1:CA:127:ALA:HB2	2.13	0.49
1:CE:86:PHE:CE1	1:CE:117:LEU:HD23	2.47	0.49
1:CK:86:PHE:CE1	1:CK:117:LEU:HD23	2.47	0.49
1:AK:121:VAL:HG13	1:AK:125:THR:HB	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:86:PHE:CE2	1:AS:117:LEU:HD23	2.48	0.48
1:AU:157:ASP:CG	1:CL:52:ARG:HH22	2.17	0.48
1:BM:163:PHE:HD2	1:DI:24:ALA:HA	1.78	0.48
1:CX:153:GLN:OE1	1:CY:127:ALA:HB2	2.13	0.48
1:DJ:153:GLN:OE1	1:DK:127:ALA:HB2	2.13	0.48
1:AF:86:PHE:CE1	1:AF:117:LEU:HD23	2.47	0.48
1:AP:86:PHE:CE2	1:AP:117:LEU:HD23	2.48	0.48
1:BB:40:TYR:OH	1:BC:164:GLY:O	2.28	0.48
1:BB:86:PHE:CE2	1:BB:117:LEU:HD23	2.48	0.48
1:BE:153:GLN:OE1	1:BF:127:ALA:HB2	2.13	0.48
1:BK:153:GLN:OE1	1:BL:127:ALA:HB2	2.13	0.48
1:BR:121:VAL:HG13	1:BR:125:THR:HB	1.93	0.48
1:CL:153:GLN:OE1	1:CM:127:ALA:HB2	2.13	0.48
1:CO:153:GLN:OE1	1:CP:127:ALA:HB2	2.13	0.48
1:AD:153:GLN:OE1	1:AE:127:ALA:HB2	2.14	0.48
1:AL:86:PHE:CE1	1:AL:117:LEU:HD23	2.47	0.48
1:BE:6:ILE:HG13	1:BE:6:ILE:O	2.11	0.48
1:BN:86:PHE:CE2	1:BN:117:LEU:HD23	2.48	0.48
1:CI:153:GLN:OE1	1:CJ:127:ALA:HB2	2.13	0.48
1:CZ:86:PHE:CE1	1:CZ:117:LEU:HD23	2.47	0.48
1:AX:57:PHE:CE1	1:CT:162:ILE:HD12	2.49	0.48
1:BQ:153:GLN:OE1	1:BR:127:ALA:HB2	2.13	0.48
1:BZ:86:PHE:CE2	1:BZ:117:LEU:HD23	2.48	0.48
1:CB:86:PHE:CE1	1:CB:117:LEU:HD23	2.47	0.48
1:CL:86:PHE:CE2	1:CL:117:LEU:HD23	2.48	0.48
1:CU:153:GLN:OE1	1:CV:127:ALA:HB2	2.13	0.48
1:AH:50:LEU:HD11	1:CC:82:VAL:HG13	1.96	0.48
1:AU:57:PHE:CE1	1:CN:162:ILE:HD12	2.49	0.48
1:BQ:7:ASN:ND2	1:BR:46:ASP:H	2.12	0.48
1:CM:30:VAL:HA	1:CX:34:ASN:ND2	2.28	0.48
1:CO:86:PHE:CE2	1:CO:117:LEU:HD23	2.48	0.48
1:AG:153:GLN:OE1	1:AH:127:ALA:HB2	2.13	0.48
1:AM:153:GLN:OE1	1:AN:127:ALA:HB2	2.13	0.48
1:BB:153:GLN:OE1	1:BC:127:ALA:HB2	2.13	0.48
1:BT:7:ASN:ND2	1:BU:46:ASP:H	2.12	0.48
1:BZ:96:LYS:HB3	1:CA:4:ILE:HD13	1.96	0.48
1:AB:30:VAL:HA	1:AS:34:ASN:ND2	2.28	0.48
1:AJ:86:PHE:CE2	1:AJ:117:LEU:HD23	2.48	0.48
1:AV:86:PHE:CE2	1:AV:117:LEU:HD23	2.48	0.48
1:AY:153:GLN:OE1	1:AZ:127:ALA:HB2	2.14	0.48
1:BN:153:GLN:OE1	1:BO:127:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CR:7:ASN:ND2	1:CS:46:ASP:H	2.12	0.48
1:DJ:7:ASN:ND2	1:DK:46:ASP:H	2.12	0.48
1:BK:86:PHE:CE2	1:BK:117:LEU:HD23	2.48	0.48
1:BT:153:GLN:OE1	1:BU:127:ALA:HB2	2.13	0.48
1:CO:96:LYS:HB3	1:CP:4:ILE:HD13	1.96	0.48
1:DG:153:GLN:OE1	1:DH:127:ALA:HB2	2.13	0.48
1:AJ:153:GLN:OE1	1:AK:127:ALA:HB2	2.13	0.48
1:AS:57:PHE:CD1	1:AT:162:ILE:HD12	2.49	0.48
1:AT:50:LEU:HD11	1:AV:82:VAL:HG13	1.96	0.48
1:AX:16:ASN:OD1	1:CT:18:VAL:HG22	2.13	0.48
1:BA:40:TYR:CE1	1:CW:163:PHE:HB2	2.49	0.48
1:BG:78:ASP:HA	1:DC:107:TYR:CD1	2.49	0.48
1:BH:96:LYS:HB3	1:BI:4:ILE:HD13	1.96	0.48
1:BK:7:ASN:ND2	1:BL:46:ASP:H	2.12	0.48
1:BT:57:PHE:CD1	1:BU:162:ILE:HD12	2.49	0.48
1:DD:153:GLN:OE1	1:DE:127:ALA:HB2	2.13	0.48
1:AD:7:ASN:ND2	1:AE:46:ASP:H	2.12	0.48
1:AP:153:GLN:OE1	1:AQ:127:ALA:HB2	2.13	0.48
1:AV:7:ASN:ND2	1:AW:46:ASP:H	2.12	0.48
1:AY:96:LYS:HB3	1:AZ:4:ILE:HD13	1.96	0.48
1:BH:153:GLN:OE1	1:BI:127:ALA:HB2	2.13	0.48
1:BT:157:ASP:OD1	1:DI:47:ASN:OD1	2.31	0.48
1:CF:7:ASN:ND2	1:CG:46:ASP:H	2.12	0.48
1:CF:57:PHE:CD1	1:CG:162:ILE:HD12	2.49	0.48
1:CR:57:PHE:CD1	1:CS:162:ILE:HD12	2.49	0.48
1:CU:57:PHE:CD1	1:CV:162:ILE:HD12	2.49	0.48
1:CU:96:LYS:HB3	1:CV:4:ILE:HD13	1.96	0.48
1:DA:96:LYS:HB3	1:DB:4:ILE:HD13	1.96	0.48
1:DA:153:GLN:OE1	1:DB:127:ALA:HB2	2.13	0.48
1:DJ:96:LYS:HB3	1:DK:4:ILE:HD13	1.96	0.48
1:AM:57:PHE:CD1	1:AN:162:ILE:HD12	2.49	0.47
1:AM:96:LYS:HB3	1:AN:4:ILE:HD13	1.96	0.47
1:BN:96:LYS:HB3	1:BO:4:ILE:HD13	1.96	0.47
1:BT:86:PHE:CE2	1:BT:117:LEU:HD23	2.48	0.47
1:BW:153:GLN:OE1	1:BX:127:ALA:HB2	2.13	0.47
1:CC:96:LYS:HB3	1:CD:4:ILE:HD13	1.96	0.47
1:CI:57:PHE:CD1	1:CJ:162:ILE:HD12	2.49	0.47
1:CL:96:LYS:HB3	1:CM:4:ILE:HD13	1.96	0.47
1:CX:96:LYS:HB3	1:CY:4:ILE:HD13	1.96	0.47
1:BE:57:PHE:CD1	1:BF:162:ILE:HD12	2.49	0.47
1:BJ:2:TYR:CD1	1:DF:96:LYS:HE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:7:ASN:ND2	1:CJ:46:ASP:H	2.12	0.47
1:DA:7:ASN:ND2	1:DB:46:ASP:H	2.12	0.47
1:DD:96:LYS:HB3	1:DE:4:ILE:HD13	1.96	0.47
1:DG:57:PHE:CD1	1:DH:162:ILE:HD12	2.49	0.47
1:AA:57:PHE:CD1	1:AB:162:ILE:HD12	2.49	0.47
1:AA:153:GLN:OE1	1:AB:127:ALA:HB2	2.13	0.47
1:AS:96:LYS:HB3	1:AT:4:ILE:HD13	1.96	0.47
1:AV:153:GLN:OE1	1:AW:127:ALA:HB2	2.13	0.47
1:BE:157:ASP:OD1	1:BS:47:ASN:OD1	2.32	0.47
1:BQ:57:PHE:CD1	1:BR:162:ILE:HD12	2.49	0.47
1:BQ:86:PHE:CE2	1:BQ:117:LEU:HD23	2.48	0.47
1:BW:57:PHE:CD1	1:BX:162:ILE:HD12	2.49	0.47
1:BW:96:LYS:HB3	1:BX:4:ILE:HD13	1.96	0.47
1:CC:153:GLN:OE1	1:CD:127:ALA:HB2	2.13	0.47
1:DJ:57:PHE:CD1	1:DK:162:ILE:HD12	2.49	0.47
1:AD:57:PHE:CD1	1:AE:162:ILE:HD12	2.49	0.47
1:AG:57:PHE:CD1	1:AH:162:ILE:HD12	2.49	0.47
1:AP:96:LYS:HB3	1:AQ:4:ILE:HD13	1.96	0.47
1:BQ:96:LYS:HB3	1:BR:4:ILE:HD13	1.96	0.47
1:CF:153:GLN:OE1	1:CG:127:ALA:HB2	2.13	0.47
1:DA:57:PHE:CD1	1:DB:162:ILE:HD12	2.49	0.47
1:AJ:57:PHE:CD1	1:AK:162:ILE:HD12	2.49	0.47
1:AU:162:ILE:HD12	1:CN:57:PHE:CE1	2.49	0.47
1:AV:96:LYS:HB3	1:AW:4:ILE:HD13	1.96	0.47
1:BA:111:GLN:OE1	1:CW:119:SER:HB2	2.14	0.47
1:BQ:23:PRO:O	1:BQ:26:PRO:HD2	2.15	0.47
1:CO:7:ASN:ND2	1:CP:46:ASP:H	2.12	0.47
1:DD:57:PHE:CD1	1:DE:162:ILE:HD12	2.49	0.47
1:AA:23:PRO:O	1:AA:26:PRO:HD2	2.15	0.47
1:AA:86:PHE:CE2	1:AA:117:LEU:HD23	2.48	0.47
1:AE:86:PHE:HE1	1:AE:117:LEU:HD23	1.80	0.47
1:AF:46:ASP:H	1:BV:7:ASN:HD21	1.62	0.47
1:AG:7:ASN:ND2	1:AH:46:ASP:H	2.12	0.47
1:AK:86:PHE:HE1	1:AK:117:LEU:HD23	1.80	0.47
1:CC:7:ASN:ND2	1:CD:46:ASP:H	2.12	0.47
1:CD:86:PHE:HE1	1:CD:117:LEU:HD23	1.80	0.47
1:CF:23:PRO:O	1:CF:26:PRO:HD2	2.15	0.47
1:CO:57:PHE:CD1	1:CP:162:ILE:HD12	2.49	0.47
1:CR:153:GLN:OE1	1:CS:127:ALA:HB2	2.13	0.47
1:CX:23:PRO:O	1:CX:26:PRO:HD2	2.15	0.47
1:DA:23:PRO:O	1:DA:26:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:163:PHE:HD2	1:BY:24:ALA:HA	1.78	0.47
1:AN:86:PHE:HE1	1:AN:117:LEU:HD23	1.80	0.47
1:AP:7:ASN:ND2	1:AQ:46:ASP:H	2.12	0.47
1:AP:57:PHE:CD1	1:AQ:162:ILE:HD12	2.49	0.47
1:AV:57:PHE:CD1	1:AW:162:ILE:HD12	2.49	0.47
1:AY:57:PHE:CD1	1:AZ:162:ILE:HD12	2.49	0.47
1:BB:23:PRO:O	1:BB:26:PRO:HD2	2.15	0.47
1:BE:23:PRO:O	1:BE:26:PRO:HD2	2.15	0.47
1:BE:96:LYS:HB3	1:BF:4:ILE:HD13	1.96	0.47
1:BH:52:ARG:HH22	1:DF:157:ASP:CG	2.17	0.47
1:BH:57:PHE:CD1	1:BI:162:ILE:HD12	2.49	0.47
1:BM:24:ALA:HA	1:DI:163:PHE:CD2	2.50	0.47
1:BW:23:PRO:O	1:BW:26:PRO:HD2	2.15	0.47
1:CI:23:PRO:O	1:CI:26:PRO:HD2	2.15	0.47
1:CO:23:PRO:O	1:CO:26:PRO:HD2	2.15	0.47
1:CX:86:PHE:CE2	1:CX:117:LEU:HD23	2.48	0.47
1:AA:52:ARG:HH22	1:BP:157:ASP:CG	2.18	0.47
1:BB:96:LYS:HB3	1:BC:4:ILE:HD13	1.96	0.47
1:BF:86:PHE:HE1	1:BF:117:LEU:HD23	1.80	0.47
1:BJ:96:LYS:HE2	1:DF:2:TYR:CD1	2.49	0.47
1:BJ:96:LYS:HA	1:DF:3:THR:O	2.14	0.47
1:BN:57:PHE:CD1	1:BO:162:ILE:HD12	2.49	0.47
1:BT:96:LYS:HB3	1:BU:4:ILE:HD13	1.96	0.47
1:CS:86:PHE:HE1	1:CS:117:LEU:HD23	1.80	0.47
1:AA:7:ASN:ND2	1:AB:46:ASP:H	2.12	0.47
1:AH:30:VAL:HA	1:CC:34:ASN:HD22	1.78	0.47
1:AJ:96:LYS:HB3	1:AK:4:ILE:HD13	1.96	0.47
1:BB:57:PHE:CD1	1:BC:162:ILE:HD12	2.49	0.47
1:BG:155:LEU:HD13	1:DC:86:PHE:CD2	2.50	0.47
1:BK:57:PHE:CD1	1:BL:162:ILE:HD12	2.49	0.47
1:CC:57:PHE:CD1	1:CD:162:ILE:HD12	2.49	0.47
1:AF:7:ASN:O	1:BV:53:PRO:HG2	2.14	0.47
1:AG:86:PHE:CE2	1:AG:117:LEU:HD23	2.48	0.47
1:AR:94:TRP:CD1	1:CK:6:ILE:HA	2.50	0.47
1:BJ:162:ILE:HD12	1:DF:57:PHE:CE1	2.50	0.47
1:BK:96:LYS:HB3	1:BL:4:ILE:HD13	1.96	0.47
1:BP:46:ASP:OD2	1:BP:48:SER:OG	2.27	0.47
1:CA:86:PHE:HE1	1:CA:117:LEU:HD23	1.80	0.47
1:CL:57:PHE:CD1	1:CM:162:ILE:HD12	2.49	0.47
1:CU:23:PRO:O	1:CU:26:PRO:HD2	2.15	0.47
1:CW:155:LEU:HD23	1:CW:155:LEU:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DE:86:PHE:HE1	1:DE:117:LEU:HD23	1.80	0.47
1:DG:33:ASP:HB2	1:DG:36:SER:H	1.80	0.47
1:AD:23:PRO:O	1:AD:26:PRO:HD2	2.15	0.46
1:AF:111:GLN:OE1	1:BV:119:SER:HB2	2.15	0.46
1:AH:86:PHE:HE1	1:AH:117:LEU:HD23	1.80	0.46
1:AR:30:VAL:HG21	1:AR:41:LEU:HB2	1.98	0.46
1:AR:57:PHE:CE1	1:CK:162:ILE:HD12	2.50	0.46
1:AS:33:ASP:HB2	1:AS:36:SER:H	1.81	0.46
1:AU:40:TYR:CE1	1:CN:163:PHE:HB2	2.50	0.46
1:BH:7:ASN:ND2	1:BI:46:ASP:H	2.12	0.46
1:BI:86:PHE:HE1	1:BI:117:LEU:HD23	1.80	0.46
1:BZ:23:PRO:O	1:BZ:26:PRO:HD2	2.15	0.46
1:CJ:86:PHE:HE1	1:CJ:117:LEU:HD23	1.80	0.46
1:AG:96:LYS:HB3	1:AH:4:ILE:HD13	1.96	0.46
1:AI:30:VAL:HG21	1:AI:41:LEU:HB2	1.98	0.46
1:AY:23:PRO:O	1:AY:26:PRO:HD2	2.15	0.46
1:BA:162:ILE:HD12	1:CW:57:PHE:CE1	2.50	0.46
1:BJ:161:ARG:HD2	1:DF:34:ASN:HB3	1.97	0.46
1:BM:119:SER:HB2	1:DI:111:GLN:OE1	2.15	0.46
1:BU:29:HIS:O	1:DG:34:ASN:ND2	2.48	0.46
1:BV:30:VAL:HG21	1:BV:41:LEU:HB2	1.98	0.46
1:BW:7:ASN:ND2	1:BX:46:ASP:H	2.12	0.46
1:DD:23:PRO:O	1:DD:26:PRO:HD2	2.15	0.46
1:DK:86:PHE:HE1	1:DK:117:LEU:HD23	1.80	0.46
1:AG:23:PRO:O	1:AG:26:PRO:HD2	2.15	0.46
1:AO:34:ASN:HB3	1:CE:161:ARG:HD2	1.97	0.46
1:AV:23:PRO:O	1:AV:26:PRO:HD2	2.15	0.46
1:BA:24:ALA:HA	1:CW:163:PHE:HD2	1.80	0.46
1:BC:86:PHE:HE1	1:BC:117:LEU:HD23	1.80	0.46
1:BD:30:VAL:HG21	1:BD:41:LEU:HB2	1.97	0.46
1:BN:7:ASN:ND2	1:BO:46:ASP:H	2.12	0.46
1:BP:30:VAL:HG21	1:BP:41:LEU:HB2	1.98	0.46
1:BT:23:PRO:O	1:BT:26:PRO:HD2	2.15	0.46
1:BZ:57:PHE:CD1	1:CA:162:ILE:HD12	2.49	0.46
1:CC:33:ASP:HB2	1:CC:36:SER:H	1.81	0.46
1:CI:96:LYS:HB3	1:CJ:4:ILE:HD13	1.96	0.46
1:CO:33:ASP:HB2	1:CO:36:SER:H	1.81	0.46
1:CR:86:PHE:CE2	1:CR:117:LEU:HD23	2.48	0.46
1:CZ:30:VAL:HG21	1:CZ:41:LEU:HB2	1.98	0.46
1:DJ:23:PRO:O	1:DJ:26:PRO:HD2	2.15	0.46
1:AJ:23:PRO:O	1:AJ:26:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:7:ASN:ND2	1:AT:46:ASP:H	2.12	0.46
1:AY:33:ASP:HB2	1:AY:36:SER:H	1.81	0.46
1:BG:38:ILE:HG22	1:DC:160:PRO:HB2	1.97	0.46
1:CX:57:PHE:CD1	1:CY:162:ILE:HD12	2.49	0.46
1:AD:96:LYS:HB3	1:AE:4:ILE:HD13	1.96	0.46
1:AM:23:PRO:O	1:AM:26:PRO:HD2	2.15	0.46
1:BK:23:PRO:O	1:BK:26:PRO:HD2	2.15	0.46
1:CE:30:VAL:HG21	1:CE:41:LEU:HB2	1.98	0.46
1:CG:155:LEU:HD11	1:CG:162:ILE:HD11	1.98	0.46
1:CL:23:PRO:O	1:CL:26:PRO:HD2	2.15	0.46
1:CR:23:PRO:O	1:CR:26:PRO:HD2	2.15	0.46
1:CX:7:ASN:ND2	1:CY:46:ASP:H	2.12	0.46
1:DL:30:VAL:HG21	1:DL:41:LEU:HB2	1.98	0.46
1:AA:96:LYS:HB3	1:AB:4:ILE:HD13	1.96	0.46
1:AD:28:VAL:HG11	1:BV:159:LEU:HD13	1.98	0.46
1:AD:33:ASP:HB2	1:AD:36:SER:H	1.81	0.46
1:AF:161:ARG:HD2	1:BV:34:ASN:HB3	1.97	0.46
1:AP:23:PRO:O	1:AP:26:PRO:HD2	2.15	0.46
1:AT:155:LEU:HD11	1:AT:162:ILE:HD11	1.98	0.46
1:BN:23:PRO:O	1:BN:26:PRO:HD2	2.15	0.46
1:CC:23:PRO:O	1:CC:26:PRO:HD2	2.15	0.46
1:CG:86:PHE:HE1	1:CG:117:LEU:HD23	1.80	0.46
1:CV:86:PHE:HE1	1:CV:117:LEU:HD23	1.80	0.46
1:DG:7:ASN:ND2	1:DH:46:ASP:H	2.12	0.46
1:DI:30:VAL:HG21	1:DI:41:LEU:HB2	1.98	0.46
1:AF:30:VAL:HG21	1:AF:41:LEU:HB2	1.98	0.46
1:AM:33:ASP:HB2	1:AM:36:SER:H	1.81	0.46
1:AP:33:ASP:HB2	1:AP:36:SER:H	1.81	0.46
1:BF:155:LEU:HD11	1:BF:162:ILE:HD11	1.98	0.46
1:BM:30:VAL:HG21	1:BM:41:LEU:HB2	1.98	0.46
1:BZ:33:ASP:HB2	1:BZ:36:SER:H	1.81	0.46
1:CB:30:VAL:HG21	1:CB:41:LEU:HB2	1.98	0.46
1:CF:96:LYS:HB3	1:CG:4:ILE:HD13	1.96	0.46
1:AB:155:LEU:HD11	1:AB:162:ILE:HD11	1.98	0.46
1:AO:119:SER:HB2	1:CE:111:GLN:OE1	2.15	0.46
1:AS:23:PRO:O	1:AS:26:PRO:HD2	2.15	0.46
1:AY:28:VAL:HG11	1:CW:159:LEU:HD13	1.98	0.46
1:BB:7:ASN:ND2	1:BC:46:ASP:H	2.12	0.46
1:BH:23:PRO:O	1:BH:26:PRO:HD2	2.15	0.46
1:BJ:24:ALA:HA	1:DF:163:PHE:HD2	1.80	0.46
1:BN:33:ASP:HB2	1:BN:36:SER:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:33:ASP:HB2	1:BW:36:SER:H	1.81	0.46
1:BY:30:VAL:HG21	1:BY:41:LEU:HB2	1.98	0.46
1:CK:30:VAL:HG21	1:CK:41:LEU:HB2	1.97	0.46
1:CM:86:PHE:HE1	1:CM:117:LEU:HD23	1.80	0.46
1:DE:37:THR:HG23	1:DE:58:ASN:HD22	1.81	0.46
1:DF:30:VAL:HG21	1:DF:41:LEU:HB2	1.97	0.46
1:DG:96:LYS:HB3	1:DH:4:ILE:HD13	1.96	0.46
1:DJ:33:ASP:HB2	1:DJ:36:SER:H	1.81	0.46
1:AC:46:ASP:OD2	1:AC:48:SER:OG	2.27	0.46
1:AT:37:THR:HG23	1:AT:58:ASN:HD22	1.81	0.46
1:BC:155:LEU:HD11	1:BC:162:ILE:HD11	1.98	0.46
1:BJ:94:TRP:CD1	1:DF:6:ILE:HA	2.51	0.46
1:BK:33:ASP:HB2	1:BK:36:SER:H	1.81	0.46
1:BL:86:PHE:HE1	1:BL:117:LEU:HD23	1.80	0.46
1:CD:37:THR:HG23	1:CD:58:ASN:HD22	1.81	0.46
1:CR:96:LYS:HB3	1:CS:4:ILE:HD13	1.96	0.46
1:DA:33:ASP:HB2	1:DA:36:SER:H	1.81	0.46
1:DC:30:VAL:HG21	1:DC:41:LEU:HB2	1.98	0.46
1:AJ:7:ASN:ND2	1:AK:46:ASP:H	2.12	0.46
1:AK:155:LEU:HD11	1:AK:162:ILE:HD11	1.98	0.46
1:AL:163:PHE:HB2	1:CB:40:TYR:CE1	2.50	0.46
1:BA:30:VAL:HG21	1:BA:41:LEU:HB2	1.98	0.46
1:BF:37:THR:HG23	1:BF:58:ASN:HD22	1.81	0.46
1:BJ:86:PHE:CD2	1:DF:155:LEU:HD13	2.51	0.46
1:BR:37:THR:HG23	1:BR:58:ASN:HD22	1.81	0.46
1:CR:33:ASP:HB2	1:CR:36:SER:H	1.81	0.46
1:DG:23:PRO:O	1:DG:26:PRO:HD2	2.15	0.46
1:AC:162:ILE:HD12	1:BP:57:PHE:CE1	2.51	0.45
1:AH:37:THR:HG23	1:AH:58:ASN:HD22	1.81	0.45
1:AO:7:ASN:HD21	1:CE:46:ASP:H	1.64	0.45
1:BA:84:ARG:HD2	1:CW:156:ILE:O	2.16	0.45
1:BA:163:PHE:HB2	1:CW:40:TYR:CE1	2.51	0.45
1:BH:33:ASP:HB2	1:BH:36:SER:H	1.81	0.45
1:BX:155:LEU:HD11	1:BX:162:ILE:HD11	1.98	0.45
1:CD:155:LEU:HD11	1:CD:162:ILE:HD11	1.98	0.45
1:CG:37:THR:HG23	1:CG:58:ASN:HD22	1.81	0.45
1:CI:33:ASP:HB2	1:CI:36:SER:H	1.81	0.45
1:CL:7:ASN:ND2	1:CM:46:ASP:H	2.12	0.45
1:CM:155:LEU:HD11	1:CM:162:ILE:HD11	1.98	0.45
1:CS:37:THR:HG23	1:CS:58:ASN:HD22	1.81	0.45
1:AA:33:ASP:HB2	1:AA:36:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:33:ASP:HB2	1:AJ:36:SER:H	1.81	0.45
1:AL:57:PHE:CE1	1:CB:162:ILE:HD12	2.51	0.45
1:AQ:155:LEU:HD11	1:AQ:162:ILE:HD11	1.98	0.45
1:AY:7:ASN:ND2	1:AZ:46:ASP:H	2.12	0.45
1:BE:7:ASN:ND2	1:BF:46:ASP:H	2.12	0.45
1:BN:155:LEU:HG	1:BN:162:ILE:HD11	1.99	0.45
1:BS:30:VAL:HG21	1:BS:41:LEU:HB2	1.98	0.45
1:CA:37:THR:HG23	1:CA:58:ASN:HD22	1.81	0.45
1:DB:155:LEU:HD11	1:DB:162:ILE:HD11	1.98	0.45
1:AC:30:VAL:HG21	1:AC:41:LEU:HB2	1.98	0.45
1:AW:86:PHE:HE1	1:AW:117:LEU:HD23	1.80	0.45
1:AW:155:LEU:HD11	1:AW:162:ILE:HD11	1.98	0.45
1:BJ:30:VAL:HG21	1:BJ:41:LEU:HB2	1.98	0.45
1:BO:151:LYS:HE3	1:BO:162:ILE:HG23	1.99	0.45
1:BT:155:LEU:HG	1:BT:162:ILE:HD11	1.99	0.45
1:CI:155:LEU:HG	1:CI:162:ILE:HD11	1.99	0.45
1:CX:155:LEU:HG	1:CX:162:ILE:HD11	1.99	0.45
1:DD:33:ASP:HB2	1:DD:36:SER:H	1.81	0.45
1:AE:37:THR:HG23	1:AE:58:ASN:HD22	1.81	0.45
1:AL:86:PHE:HE1	1:AL:117:LEU:HD23	1.82	0.45
1:AP:155:LEU:HG	1:AP:162:ILE:HD11	1.99	0.45
1:AZ:155:LEU:HD11	1:AZ:162:ILE:HD11	1.98	0.45
1:BB:155:LEU:HG	1:BB:162:ILE:HD11	1.99	0.45
1:BU:37:THR:HG23	1:BU:58:ASN:HD22	1.81	0.45
1:CF:33:ASP:HB2	1:CF:36:SER:H	1.81	0.45
1:CG:151:LYS:HE3	1:CG:162:ILE:HG23	1.99	0.45
1:CP:151:LYS:HE3	1:CP:162:ILE:HG23	1.99	0.45
1:CV:155:LEU:HD11	1:CV:162:ILE:HD11	1.98	0.45
1:CZ:86:PHE:HE1	1:CZ:117:LEU:HD23	1.82	0.45
1:DC:86:PHE:HE1	1:DC:117:LEU:HD23	1.82	0.45
1:DH:155:LEU:HD11	1:DH:162:ILE:HD11	1.98	0.45
1:AB:86:PHE:HE1	1:AB:117:LEU:HD23	1.80	0.45
1:AE:155:LEU:HD11	1:AE:162:ILE:HD11	1.98	0.45
1:AK:37:THR:HG23	1:AK:58:ASN:HD22	1.81	0.45
1:AT:86:PHE:HE1	1:AT:117:LEU:HD23	1.80	0.45
1:AU:30:VAL:HG21	1:AU:41:LEU:HB2	1.98	0.45
1:AU:111:GLN:OE1	1:CN:119:SER:HB2	2.16	0.45
1:AX:86:PHE:HE1	1:AX:117:LEU:HD23	1.82	0.45
1:AZ:86:PHE:HE1	1:AZ:117:LEU:HD23	1.80	0.45
1:BC:37:THR:HG23	1:BC:58:ASN:HD22	1.81	0.45
1:BG:86:PHE:HE1	1:BG:117:LEU:HD23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:151:LYS:HE3	1:BL:162:ILE:HG23	1.99	0.45
1:BM:86:PHE:HE1	1:BM:117:LEU:HD23	1.82	0.45
1:BR:151:LYS:HE3	1:BR:162:ILE:HG23	1.99	0.45
1:DE:151:LYS:HE3	1:DE:162:ILE:HG23	1.99	0.45
1:DK:155:LEU:HD11	1:DK:162:ILE:HD11	1.98	0.45
1:AH:155:LEU:HD11	1:AH:162:ILE:HD11	1.98	0.45
1:AJ:155:LEU:HG	1:AJ:162:ILE:HD11	1.99	0.45
1:AZ:37:THR:HG23	1:AZ:58:ASN:HD22	1.81	0.45
1:BA:86:PHE:HE1	1:BA:117:LEU:HD23	1.82	0.45
1:BB:33:ASP:HB2	1:BB:36:SER:H	1.81	0.45
1:BD:7:ASN:HD21	1:CZ:46:ASP:H	1.65	0.45
1:BG:24:ALA:HA	1:DC:163:PHE:CD2	2.52	0.45
1:BG:30:VAL:HG21	1:BG:41:LEU:HB2	1.98	0.45
1:BJ:86:PHE:HE1	1:BJ:117:LEU:HD23	1.82	0.45
1:BK:155:LEU:HG	1:BK:162:ILE:HD11	1.99	0.45
1:BL:37:THR:HG23	1:BL:58:ASN:HD22	1.81	0.45
1:BL:155:LEU:HD11	1:BL:162:ILE:HD11	1.98	0.45
1:BT:33:ASP:HB2	1:BT:36:SER:H	1.81	0.45
1:CB:86:PHE:HE1	1:CB:117:LEU:HD23	1.82	0.45
1:CC:155:LEU:HG	1:CC:162:ILE:HD11	1.98	0.45
1:CH:86:PHE:HE1	1:CH:117:LEU:HD23	1.82	0.45
1:CJ:37:THR:HG23	1:CJ:58:ASN:HD22	1.81	0.45
1:CM:151:LYS:HE3	1:CM:162:ILE:HG23	1.99	0.45
1:CR:155:LEU:HG	1:CR:162:ILE:HD11	1.98	0.45
1:CU:33:ASP:HB2	1:CU:36:SER:H	1.81	0.45
1:CY:155:LEU:HD11	1:CY:162:ILE:HD11	1.98	0.45
1:AE:151:LYS:HE3	1:AE:162:ILE:HG23	1.99	0.45
1:AF:155:LEU:HA	1:AF:155:LEU:HD23	1.77	0.45
1:AO:1:SER:C	1:CE:98:ASP:HB3	2.36	0.45
1:AO:30:VAL:HG21	1:AO:41:LEU:HB2	1.98	0.45
1:AO:163:PHE:HB2	1:CE:40:TYR:CE1	2.51	0.45
1:AU:40:TYR:OH	1:CN:164:GLY:O	2.31	0.45
1:BE:33:ASP:HB2	1:BE:36:SER:H	1.81	0.45
1:BF:151:LYS:HE3	1:BF:162:ILE:HG23	1.99	0.45
1:BJ:57:PHE:CE1	1:DF:162:ILE:HD12	2.52	0.45
1:BU:155:LEU:HD11	1:BU:162:ILE:HD11	1.98	0.45
1:BX:86:PHE:HE1	1:BX:117:LEU:HD23	1.80	0.45
1:BX:151:LYS:HE3	1:BX:162:ILE:HG23	1.99	0.45
1:CO:155:LEU:HG	1:CO:162:ILE:HD11	1.99	0.45
1:CQ:30:VAL:HG21	1:CQ:41:LEU:HB2	1.98	0.45
1:DE:155:LEU:HD11	1:DE:162:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DJ:155:LEU:HG	1:DJ:162:ILE:HD11	1.99	0.45
1:AL:30:VAL:HG21	1:AL:41:LEU:HB2	1.98	0.45
1:AQ:37:THR:HG23	1:AQ:58:ASN:HD22	1.81	0.45
1:AR:86:PHE:HE1	1:AR:117:LEU:HD23	1.82	0.45
1:AR:111:GLN:OE1	1:CK:119:SER:HB2	2.16	0.45
1:BH:155:LEU:HG	1:BH:162:ILE:HD11	1.99	0.45
1:BI:37:THR:HG23	1:BI:58:ASN:HD22	1.81	0.45
1:CA:151:LYS:HE3	1:CA:162:ILE:HG23	1.99	0.45
1:CD:151:LYS:HE3	1:CD:162:ILE:HG23	1.99	0.45
1:CE:86:PHE:HE1	1:CE:117:LEU:HD23	1.82	0.45
1:CJ:155:LEU:HD11	1:CJ:162:ILE:HD11	1.98	0.45
1:DD:155:LEU:HG	1:DD:162:ILE:HD11	1.99	0.45
1:DG:155:LEU:HG	1:DG:162:ILE:HD11	1.99	0.45
1:DL:86:PHE:HE1	1:DL:117:LEU:HD23	1.82	0.45
1:AB:37:THR:HG23	1:AB:58:ASN:HD22	1.81	0.45
1:AD:155:LEU:HG	1:AD:162:ILE:HD11	1.99	0.45
1:AG:33:ASP:HB2	1:AG:36:SER:H	1.81	0.45
1:AI:7:ASN:HD21	1:BY:46:ASP:H	1.65	0.45
1:AU:163:PHE:CD2	1:CN:24:ALA:HA	2.49	0.45
1:AX:7:ASN:O	1:CT:53:PRO:HG2	2.16	0.45
1:AZ:151:LYS:HE3	1:AZ:162:ILE:HG23	1.99	0.45
1:CH:30:VAL:HG21	1:CH:41:LEU:HB2	1.98	0.45
1:CT:30:VAL:HG21	1:CT:41:LEU:HB2	1.98	0.45
1:CV:37:THR:HG23	1:CV:58:ASN:HD22	1.81	0.45
1:CX:33:ASP:HB2	1:CX:36:SER:H	1.81	0.45
1:AK:151:LYS:HE3	1:AK:162:ILE:HG23	1.99	0.45
1:AR:94:TRP:CD1	1:CK:6:ILE:HG22	2.50	0.45
1:AU:46:ASP:H	1:CN:7:ASN:HD21	1.65	0.45
1:BC:151:LYS:HE3	1:BC:162:ILE:HG23	1.99	0.45
1:BI:155:LEU:HD11	1:BI:162:ILE:HD11	1.98	0.45
1:CK:86:PHE:HE1	1:CK:117:LEU:HD23	1.82	0.45
1:CU:53:PRO:HG2	1:CV:7:ASN:O	2.17	0.45
1:CU:155:LEU:HG	1:CU:162:ILE:HD11	1.99	0.45
1:CW:30:VAL:HG21	1:CW:41:LEU:HB2	1.98	0.45
1:CW:86:PHE:HE1	1:CW:117:LEU:HD23	1.82	0.45
1:DB:37:THR:HG23	1:DB:58:ASN:HD22	1.81	0.45
1:AA:53:PRO:HG2	1:AB:7:ASN:O	2.18	0.44
1:AI:86:PHE:HE1	1:AI:117:LEU:HD23	1.82	0.44
1:AV:53:PRO:HG2	1:AW:7:ASN:O	2.18	0.44
1:BQ:33:ASP:HB2	1:BQ:36:SER:H	1.81	0.44
1:BQ:155:LEU:HG	1:BQ:162:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BY:86:PHE:HE1	1:BY:117:LEU:HD23	1.82	0.44
1:BZ:7:ASN:ND2	1:CA:46:ASP:H	2.12	0.44
1:CA:155:LEU:HD11	1:CA:162:ILE:HD11	1.98	0.44
1:CJ:151:LYS:HE3	1:CJ:162:ILE:HG23	1.99	0.44
1:CO:53:PRO:HG2	1:CP:7:ASN:O	2.17	0.44
1:CS:151:LYS:HE3	1:CS:162:ILE:HG23	1.99	0.44
1:CV:151:LYS:HE3	1:CV:162:ILE:HG23	1.99	0.44
1:CY:37:THR:HG23	1:CY:58:ASN:HD22	1.81	0.44
1:DH:37:THR:HG23	1:DH:58:ASN:HD22	1.81	0.44
1:AG:53:PRO:HG2	1:AH:7:ASN:O	2.18	0.44
1:AM:7:ASN:ND2	1:AN:46:ASP:H	2.12	0.44
1:AN:37:THR:HG23	1:AN:58:ASN:HD22	1.81	0.44
1:AR:57:PHE:CD1	1:CK:162:ILE:HD12	2.52	0.44
1:AS:155:LEU:HG	1:AS:162:ILE:HD11	1.99	0.44
1:AU:86:PHE:HE1	1:AU:117:LEU:HD23	1.82	0.44
1:AV:33:ASP:HB2	1:AV:36:SER:H	1.81	0.44
1:AX:30:VAL:HG21	1:AX:41:LEU:HB2	1.97	0.44
1:AY:53:PRO:HG2	1:AZ:7:ASN:O	2.18	0.44
1:BO:37:THR:HG23	1:BO:58:ASN:HD22	1.81	0.44
1:BO:155:LEU:HD11	1:BO:162:ILE:HD11	1.98	0.44
1:CJ:30:VAL:HA	1:DA:34:ASN:ND2	2.32	0.44
1:CN:30:VAL:HG21	1:CN:41:LEU:HB2	1.98	0.44
1:CP:86:PHE:HE1	1:CP:117:LEU:HD23	1.80	0.44
1:CP:155:LEU:HD11	1:CP:162:ILE:HD11	1.98	0.44
1:DD:53:PRO:HG2	1:DE:7:ASN:O	2.17	0.44
1:AA:155:LEU:HG	1:AA:162:ILE:HD11	1.99	0.44
1:AO:86:PHE:HE1	1:AO:117:LEU:HD23	1.82	0.44
1:BH:53:PRO:HG2	1:BI:7:ASN:O	2.18	0.44
1:BR:86:PHE:HE1	1:BR:117:LEU:HD23	1.80	0.44
1:BR:155:LEU:HD11	1:BR:162:ILE:HD11	1.98	0.44
1:BS:33:ASP:OD1	1:BS:33:ASP:N	2.51	0.44
1:BW:53:PRO:HG2	1:BX:7:ASN:O	2.18	0.44
1:CS:155:LEU:HD11	1:CS:162:ILE:HD11	1.98	0.44
1:CW:33:ASP:OD1	1:CW:33:ASP:N	2.51	0.44
1:DH:151:LYS:HE3	1:DH:162:ILE:HG23	1.99	0.44
1:AE:63:GLN:HG3	1:BG:50:LEU:HD22	1.99	0.44
1:AJ:53:PRO:HG2	1:AK:7:ASN:O	2.18	0.44
1:BD:33:ASP:OD1	1:BD:33:ASP:N	2.51	0.44
1:BG:2:TYR:N	1:DC:98:ASP:HB3	2.32	0.44
1:BG:33:ASP:OD1	1:BG:33:ASP:N	2.51	0.44
1:BU:31:SER:HA	1:DG:33:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:155:LEU:HG	1:BW:162:ILE:HD11	1.99	0.44
1:CB:33:ASP:OD1	1:CB:33:ASP:N	2.51	0.44
1:CI:53:PRO:HG2	1:CJ:7:ASN:O	2.18	0.44
1:CP:37:THR:HG23	1:CP:58:ASN:HD22	1.81	0.44
1:CQ:86:PHE:HE1	1:CQ:117:LEU:HD23	1.82	0.44
1:AC:155:LEU:HD13	1:BP:86:PHE:CD2	2.53	0.44
1:AD:53:PRO:HG2	1:AE:7:ASN:O	2.18	0.44
1:AF:86:PHE:CD2	1:BV:155:LEU:HD13	2.52	0.44
1:AN:151:LYS:HE3	1:AN:162:ILE:HG23	1.99	0.44
1:AR:96:LYS:HE2	1:CK:2:TYR:CD1	2.52	0.44
1:BP:86:PHE:HE1	1:BP:117:LEU:HD23	1.82	0.44
1:BS:130:ILE:O	1:BS:133:ILE:HG22	2.18	0.44
1:BZ:53:PRO:HG2	1:CA:7:ASN:O	2.17	0.44
1:CF:155:LEU:HG	1:CF:162:ILE:HD11	1.99	0.44
1:CK:33:ASP:OD1	1:CK:33:ASP:N	2.51	0.44
1:CK:130:ILE:O	1:CK:133:ILE:HG22	2.18	0.44
1:CQ:130:ILE:O	1:CQ:133:ILE:HG22	2.18	0.44
1:CY:86:PHE:HE1	1:CY:117:LEU:HD23	1.80	0.44
1:DB:151:LYS:HE3	1:DB:162:ILE:HG23	1.99	0.44
1:DF:33:ASP:OD1	1:DF:33:ASP:N	2.51	0.44
1:AC:86:PHE:HE1	1:AC:117:LEU:HD23	1.82	0.44
1:AG:155:LEU:HG	1:AG:162:ILE:HD11	1.99	0.44
1:AS:11:GLY:HA3	1:AT:21:GLU:HG2	2.00	0.44
1:BA:130:ILE:O	1:BA:133:ILE:HG22	2.18	0.44
1:BD:130:ILE:O	1:BD:133:ILE:HG22	2.18	0.44
1:BE:155:LEU:HG	1:BE:162:ILE:HD11	1.99	0.44
1:BY:155:LEU:HA	1:BY:155:LEU:HD23	1.77	0.44
1:CD:35:LYS:NZ	1:CK:34:ASN:HD21	2.15	0.44
1:CF:53:PRO:HG2	1:CG:7:ASN:O	2.17	0.44
1:CU:7:ASN:ND2	1:CV:46:ASP:H	2.12	0.44
1:DJ:53:PRO:HG2	1:DK:7:ASN:O	2.18	0.44
1:DK:37:THR:HG23	1:DK:58:ASN:HD22	1.81	0.44
1:AB:151:LYS:HE3	1:AB:162:ILE:HG23	1.99	0.44
1:AF:130:ILE:O	1:AF:133:ILE:HG22	2.18	0.44
1:AI:57:PHE:CE1	1:BY:162:ILE:HD12	2.53	0.44
1:AM:155:LEU:HG	1:AM:162:ILE:HD11	1.99	0.44
1:BB:53:PRO:HG2	1:BC:7:ASN:O	2.18	0.44
1:BG:34:ASN:CB	1:DC:161:ARG:HD2	2.42	0.44
1:BG:130:ILE:O	1:BG:133:ILE:HG22	2.18	0.44
1:BM:163:PHE:HB2	1:DI:40:TYR:CE1	2.53	0.44
1:BX:37:THR:HG23	1:BX:58:ASN:HD22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BY:130:ILE:O	1:BY:133:ILE:HG22	2.18	0.44
1:BZ:155:LEU:HG	1:BZ:162:ILE:HD11	1.99	0.44
1:CL:33:ASP:HB2	1:CL:36:SER:H	1.81	0.44
1:CL:155:LEU:HG	1:CL:162:ILE:HD11	1.98	0.44
1:CR:53:PRO:HG2	1:CS:7:ASN:O	2.18	0.44
1:CR:82:VAL:HG13	1:DB:50:LEU:HD11	1.98	0.44
1:AI:130:ILE:O	1:AI:133:ILE:HG22	2.18	0.44
1:AV:155:LEU:HG	1:AV:162:ILE:HD11	1.99	0.44
1:AW:151:LYS:HE3	1:AW:162:ILE:HG23	1.99	0.44
1:BJ:6:ILE:HA	1:DF:94:TRP:CD1	2.53	0.44
1:BJ:33:ASP:OD1	1:BJ:33:ASP:N	2.51	0.44
1:BM:130:ILE:O	1:BM:133:ILE:HG22	2.18	0.44
1:BP:33:ASP:OD1	1:BP:33:ASP:N	2.51	0.44
1:CC:11:GLY:HA3	1:CD:21:GLU:HG2	2.00	0.44
1:CL:40:TYR:OH	1:CM:164:GLY:O	2.28	0.44
1:CM:37:THR:HG23	1:CM:58:ASN:HD22	1.81	0.44
1:CT:33:ASP:OD1	1:CT:33:ASP:N	2.51	0.44
1:CT:155:LEU:HA	1:CT:155:LEU:HD23	1.77	0.44
1:DD:11:GLY:HA3	1:DE:21:GLU:HG2	2.00	0.44
1:DF:130:ILE:O	1:DF:133:ILE:HG22	2.18	0.44
1:DI:130:ILE:O	1:DI:133:ILE:HG22	2.18	0.44
1:AC:130:ILE:O	1:AC:133:ILE:HG22	2.18	0.44
1:AL:6:ILE:HG22	1:CB:94:TRP:NE1	2.33	0.44
1:AR:161:ARG:HD2	1:CK:34:ASN:HB3	1.98	0.44
1:BG:78:ASP:HA	1:DC:107:TYR:CE1	2.53	0.44
1:BG:155:LEU:HD23	1:BG:155:LEU:HA	1.78	0.44
1:BG:163:PHE:HB2	1:DC:40:TYR:CZ	2.52	0.44
1:BN:53:PRO:HG2	1:BO:7:ASN:O	2.18	0.44
1:BS:86:PHE:HE1	1:BS:117:LEU:HD23	1.82	0.44
1:BW:11:GLY:HA3	1:BX:21:GLU:HG2	2.00	0.44
1:CO:11:GLY:HA3	1:CP:21:GLU:HG2	2.00	0.44
1:AL:40:TYR:CE1	1:CB:163:PHE:HB2	2.53	0.43
1:AQ:86:PHE:HE1	1:AQ:117:LEU:HD23	1.80	0.43
1:AR:18:VAL:HG22	1:CK:16:ASN:OD1	2.18	0.43
1:AT:151:LYS:HE3	1:AT:162:ILE:HG23	1.99	0.43
1:AU:24:ALA:HA	1:CN:163:PHE:CD2	2.53	0.43
1:BI:151:LYS:HE3	1:BI:162:ILE:HG23	1.99	0.43
1:BQ:53:PRO:HG2	1:BR:7:ASN:O	2.18	0.43
1:BT:11:GLY:HA3	1:BU:21:GLU:HG2	2.00	0.43
1:CA:35:LYS:NZ	1:CH:34:ASN:HD21	2.16	0.43
1:AD:117:LEU:HD12	1:AE:112:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:33:ASP:OD1	1:AI:33:ASP:N	2.51	0.43
1:AW:37:THR:HG23	1:AW:58:ASN:HD22	1.81	0.43
1:BB:117:LEU:HD12	1:BC:112:SER:O	2.18	0.43
1:BE:53:PRO:HG2	1:BF:7:ASN:O	2.18	0.43
1:BP:155:LEU:HD23	1:BP:155:LEU:HA	1.77	0.43
1:BT:53:PRO:HG2	1:BU:7:ASN:O	2.17	0.43
1:BZ:11:GLY:HA3	1:CA:21:GLU:HG2	2.00	0.43
1:CX:53:PRO:HG2	1:CY:7:ASN:O	2.18	0.43
1:DA:155:LEU:HG	1:DA:162:ILE:HD11	1.99	0.43
1:DL:130:ILE:O	1:DL:133:ILE:HG22	2.18	0.43
1:AE:63:GLN:HG3	1:BG:50:LEU:HD21	1.99	0.43
1:AG:11:GLY:HA3	1:AH:21:GLU:HG2	2.00	0.43
1:AJ:1:SER:C	1:AK:98:ASP:HB3	2.39	0.43
1:AO:33:ASP:OD1	1:AO:33:ASP:N	2.51	0.43
1:AP:117:LEU:HD12	1:AQ:112:SER:O	2.19	0.43
1:AS:117:LEU:HD12	1:AT:112:SER:O	2.18	0.43
1:AU:163:PHE:HB2	1:CN:40:TYR:CE1	2.54	0.43
1:AX:162:ILE:HD12	1:CT:57:PHE:CE1	2.54	0.43
1:BG:2:TYR:CD1	1:DC:97:ALA:HA	2.53	0.43
1:BO:86:PHE:HE1	1:BO:117:LEU:HD23	1.80	0.43
1:BQ:11:GLY:HA3	1:BR:21:GLU:HG2	2.00	0.43
1:CF:1:SER:C	1:CG:98:ASP:HB3	2.39	0.43
1:CO:133:ILE:HD12	1:CP:111:GLN:HB2	2.01	0.43
1:CQ:33:ASP:OD1	1:CQ:33:ASP:N	2.51	0.43
1:CU:11:GLY:HA3	1:CV:21:GLU:HG2	2.00	0.43
1:CY:151:LYS:HE3	1:CY:162:ILE:HG23	1.99	0.43
1:DA:11:GLY:HA3	1:DB:21:GLU:HG2	2.00	0.43
1:DA:53:PRO:HG2	1:DB:7:ASN:O	2.18	0.43
1:DF:86:PHE:HE1	1:DF:117:LEU:HD23	1.82	0.43
1:DI:33:ASP:OD1	1:DI:33:ASP:N	2.51	0.43
1:DI:86:PHE:HE1	1:DI:117:LEU:HD23	1.82	0.43
1:DJ:117:LEU:HD12	1:DK:112:SER:O	2.18	0.43
1:AD:1:SER:C	1:AE:98:ASP:HB3	2.39	0.43
1:AG:1:SER:C	1:AH:98:ASP:HB3	2.39	0.43
1:AJ:121:VAL:HG22	1:AJ:130:ILE:HD11	2.01	0.43
1:AM:1:SER:C	1:AN:98:ASP:HB3	2.39	0.43
1:AN:155:LEU:HD11	1:AN:162:ILE:HD11	1.98	0.43
1:AO:130:ILE:O	1:AO:133:ILE:HG22	2.18	0.43
1:AQ:151:LYS:HE3	1:AQ:162:ILE:HG23	1.99	0.43
1:AX:130:ILE:O	1:AX:133:ILE:HG22	2.18	0.43
1:AY:155:LEU:HG	1:AY:162:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:57:PHE:CE1	1:CZ:162:ILE:HD12	2.53	0.43
1:BH:1:SER:C	1:BI:98:ASP:HB3	2.39	0.43
1:BQ:121:VAL:HG22	1:BQ:130:ILE:HD11	2.01	0.43
1:BZ:117:LEU:HD12	1:CA:112:SER:O	2.19	0.43
1:CC:1:SER:C	1:CD:98:ASP:HB3	2.39	0.43
1:CC:53:PRO:HG2	1:CD:7:ASN:O	2.17	0.43
1:CC:117:LEU:HD12	1:CD:112:SER:O	2.19	0.43
1:CE:130:ILE:O	1:CE:133:ILE:HG22	2.18	0.43
1:CL:53:PRO:HG2	1:CM:7:ASN:O	2.17	0.43
1:CL:133:ILE:HD12	1:CM:111:GLN:HB2	2.01	0.43
1:CO:117:LEU:HD12	1:CP:112:SER:O	2.18	0.43
1:CU:127:ALA:HB2	1:CV:153:GLN:OE1	2.19	0.43
1:CZ:33:ASP:OD1	1:CZ:33:ASP:N	2.51	0.43
1:DA:117:LEU:HD12	1:DB:112:SER:O	2.19	0.43
1:DD:1:SER:C	1:DE:98:ASP:HB3	2.39	0.43
1:DJ:1:SER:C	1:DK:98:ASP:HB3	2.39	0.43
1:AA:121:VAL:HG22	1:AA:130:ILE:HD11	2.01	0.43
1:AM:53:PRO:HG2	1:AN:7:ASN:O	2.18	0.43
1:AS:53:PRO:HG2	1:AT:7:ASN:O	2.18	0.43
1:AS:121:VAL:HG22	1:AS:130:ILE:HD11	2.01	0.43
1:AV:117:LEU:HD12	1:AW:112:SER:O	2.19	0.43
1:AX:111:GLN:HB2	1:CT:133:ILE:HD12	2.00	0.43
1:AY:121:VAL:HG22	1:AY:130:ILE:HD11	2.01	0.43
1:AY:127:ALA:HB2	1:AZ:153:GLN:OE1	2.19	0.43
1:BJ:18:VAL:HG22	1:DF:16:ASN:OD1	2.18	0.43
1:BK:127:ALA:HB2	1:BL:153:GLN:OE1	2.19	0.43
1:BT:133:ILE:HD12	1:BU:111:GLN:HB2	2.01	0.43
1:BU:151:LYS:HE3	1:BU:162:ILE:HG23	1.99	0.43
1:CF:133:ILE:HD12	1:CG:111:GLN:HB2	2.01	0.43
1:CI:1:SER:C	1:CJ:98:ASP:HB3	2.39	0.43
1:CI:11:GLY:HA3	1:CJ:21:GLU:HG2	2.00	0.43
1:CL:127:ALA:HB2	1:CM:153:GLN:OE1	2.19	0.43
1:CO:127:ALA:HB2	1:CP:153:GLN:OE1	2.19	0.43
1:CW:130:ILE:O	1:CW:133:ILE:HG22	2.18	0.43
1:CX:1:SER:C	1:CY:98:ASP:HB3	2.39	0.43
1:DC:130:ILE:O	1:DC:133:ILE:HG22	2.18	0.43
1:DD:7:ASN:ND2	1:DE:46:ASP:H	2.12	0.43
1:DG:11:GLY:HA3	1:DH:21:GLU:HG2	2.00	0.43
1:DJ:133:ILE:HD12	1:DK:111:GLN:HB2	2.01	0.43
1:AJ:127:ALA:HB2	1:AK:153:GLN:OE1	2.19	0.43
1:AL:7:ASN:HD21	1:CB:46:ASP:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:46:ASP:OD2	1:AL:48:SER:OG	2.27	0.43
1:AS:127:ALA:HB2	1:AT:153:GLN:OE1	2.19	0.43
1:AV:121:VAL:HG22	1:AV:130:ILE:HD11	2.01	0.43
1:AV:133:ILE:HD12	1:AW:111:GLN:HB2	2.01	0.43
1:BA:86:PHE:CD2	1:CW:155:LEU:HD13	2.54	0.43
1:BD:119:SER:HB2	1:CZ:111:GLN:OE1	2.19	0.43
1:BH:11:GLY:HA3	1:BI:21:GLU:HG2	2.00	0.43
1:BH:133:ILE:HD12	1:BI:111:GLN:HB2	2.01	0.43
1:BK:53:PRO:HG2	1:BL:7:ASN:O	2.18	0.43
1:BN:1:SER:C	1:BO:98:ASP:HB3	2.39	0.43
1:BQ:1:SER:C	1:BR:98:ASP:HB3	2.39	0.43
1:BV:86:PHE:HE1	1:BV:117:LEU:HD23	1.82	0.43
1:BW:1:SER:C	1:BX:98:ASP:HB3	2.39	0.43
1:CF:127:ALA:HB2	1:CG:153:GLN:OE1	2.19	0.43
1:CH:33:ASP:OD1	1:CH:33:ASP:N	2.51	0.43
1:CI:127:ALA:HB2	1:CJ:153:GLN:OE1	2.19	0.43
1:CI:133:ILE:HD12	1:CJ:111:GLN:HB2	2.01	0.43
1:CN:86:PHE:HE1	1:CN:117:LEU:HD23	1.82	0.43
1:CR:11:GLY:HA3	1:CS:21:GLU:HG2	2.00	0.43
1:CU:121:VAL:HG22	1:CU:130:ILE:HD11	2.01	0.43
1:DD:127:ALA:HB2	1:DE:153:GLN:OE1	2.19	0.43
1:DD:133:ILE:HD12	1:DE:111:GLN:HB2	2.01	0.43
1:DJ:127:ALA:HB2	1:DK:153:GLN:OE1	2.19	0.43
1:AA:117:LEU:HD12	1:AB:112:SER:O	2.19	0.43
1:AL:130:ILE:O	1:AL:133:ILE:HG22	2.18	0.43
1:BD:86:PHE:HE1	1:BD:117:LEU:HD23	1.82	0.43
1:BE:117:LEU:HD12	1:BF:112:SER:O	2.19	0.43
1:BE:121:VAL:HG22	1:BE:130:ILE:HD11	2.01	0.43
1:BE:127:ALA:HB2	1:BF:153:GLN:OE1	2.19	0.43
1:BE:133:ILE:HD12	1:BF:111:GLN:HB2	2.01	0.43
1:BJ:130:ILE:O	1:BJ:133:ILE:HG22	2.18	0.43
1:BP:130:ILE:O	1:BP:133:ILE:HG22	2.18	0.43
1:BQ:117:LEU:HD12	1:BR:112:SER:O	2.19	0.43
1:BX:155:LEU:HD23	1:BX:155:LEU:HA	1.88	0.43
1:CC:127:ALA:HB2	1:CD:153:GLN:OE1	2.19	0.43
1:CI:117:LEU:HD12	1:CJ:112:SER:O	2.19	0.43
1:CR:133:ILE:HD12	1:CS:111:GLN:HB2	2.01	0.43
1:CT:86:PHE:HE1	1:CT:117:LEU:HD23	1.82	0.43
1:CU:117:LEU:HD12	1:CV:112:SER:O	2.19	0.43
1:CX:11:GLY:HA3	1:CY:21:GLU:HG2	2.00	0.43
1:CX:121:VAL:HG22	1:CX:130:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DG:53:PRO:HG2	1:DH:7:ASN:O	2.18	0.43
1:DK:151:LYS:HE3	1:DK:162:ILE:HG23	1.99	0.43
1:DK:155:LEU:HD23	1:DK:155:LEU:HA	1.88	0.43
1:AA:127:ALA:HB2	1:AB:153:GLN:OE1	2.19	0.43
1:AD:11:GLY:HA3	1:AE:21:GLU:HG2	2.00	0.43
1:AD:133:ILE:HD12	1:AE:111:GLN:HB2	2.00	0.43
1:AJ:11:GLY:HA3	1:AK:21:GLU:HG2	2.00	0.43
1:AJ:63:GLN:HG3	1:AJ:64:TYR:CD1	2.54	0.43
1:AP:53:PRO:HG2	1:AQ:7:ASN:O	2.18	0.43
1:AV:11:GLY:HA3	1:AW:21:GLU:HG2	2.00	0.43
1:AY:1:SER:C	1:AZ:98:ASP:HB3	2.39	0.43
1:BK:1:SER:C	1:BL:98:ASP:HB3	2.39	0.43
1:BK:133:ILE:HD12	1:BL:111:GLN:HB2	2.01	0.43
1:BQ:127:ALA:HB2	1:BR:153:GLN:OE1	2.19	0.43
1:CE:33:ASP:OD1	1:CE:33:ASP:N	2.51	0.43
1:CL:11:GLY:HA3	1:CM:21:GLU:HG2	2.00	0.43
1:CO:1:SER:C	1:CP:98:ASP:HB3	2.39	0.43
1:CU:1:SER:C	1:CV:98:ASP:HB3	2.39	0.43
1:CU:133:ILE:HD12	1:CV:111:GLN:HB2	2.01	0.43
1:DG:127:ALA:HB2	1:DH:153:GLN:OE1	2.19	0.43
1:DJ:121:VAL:HG22	1:DJ:130:ILE:HD11	2.01	0.43
1:AF:86:PHE:HE1	1:AF:117:LEU:HD23	1.82	0.43
1:AG:63:GLN:HG3	1:AG:64:TYR:CD1	2.54	0.43
1:AG:133:ILE:HD12	1:AH:111:GLN:HB2	2.01	0.43
1:AH:151:LYS:HE3	1:AH:162:ILE:HG23	1.99	0.43
1:AM:121:VAL:HG22	1:AM:130:ILE:HD11	2.01	0.43
1:AR:153:GLN:OE1	1:CK:127:ALA:HB2	2.18	0.43
1:BC:30:VAL:HA	1:BN:34:ASN:HD22	1.82	0.43
1:BE:1:SER:C	1:BF:98:ASP:HB3	2.39	0.43
1:BH:117:LEU:HD12	1:BI:112:SER:O	2.19	0.43
1:BH:127:ALA:HB2	1:BI:153:GLN:OE1	2.19	0.43
1:BK:63:GLN:HG3	1:BK:64:TYR:CD1	2.54	0.43
1:BT:121:VAL:HG22	1:BT:130:ILE:HD11	2.01	0.43
1:BW:127:ALA:HB2	1:BX:153:GLN:OE1	2.19	0.43
1:BZ:63:GLN:HG3	1:BZ:64:TYR:CD1	2.54	0.43
1:CA:30:VAL:HA	1:CF:34:ASN:HD22	1.81	0.43
1:CT:130:ILE:O	1:CT:133:ILE:HG22	2.18	0.43
1:CW:34:ASN:HD21	1:CY:35:LYS:NZ	2.16	0.43
1:CZ:130:ILE:O	1:CZ:133:ILE:HG22	2.18	0.43
1:DB:86:PHE:HE1	1:DB:117:LEU:HD23	1.80	0.43
1:DD:117:LEU:HD12	1:DE:112:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DG:63:GLN:HG3	1:DG:64:TYR:CD1	2.54	0.43
1:AC:34:ASN:HD21	1:DH:35:LYS:NZ	2.17	0.43
1:AG:34:ASN:HD22	1:CS:30:VAL:HA	1.83	0.43
1:AJ:117:LEU:HD12	1:AK:112:SER:O	2.19	0.43
1:AP:11:GLY:HA3	1:AQ:21:GLU:HG2	2.00	0.43
1:AS:63:GLN:HG3	1:AS:64:TYR:CD1	2.54	0.43
1:AY:133:ILE:HD12	1:AZ:111:GLN:HB2	2.01	0.43
1:BB:63:GLN:HG3	1:BB:64:TYR:CD1	2.54	0.43
1:BE:11:GLY:HA3	1:BF:21:GLU:HG2	2.00	0.43
1:BK:11:GLY:HA3	1:BL:21:GLU:HG2	2.00	0.43
1:BW:133:ILE:HD12	1:BX:111:GLN:HB2	2.01	0.43
1:BZ:121:VAL:HG22	1:BZ:130:ILE:HD11	2.01	0.43
1:BZ:127:ALA:HB2	1:CA:153:GLN:OE1	2.19	0.43
1:BZ:133:ILE:HD12	1:CA:111:GLN:HB2	2.01	0.43
1:CC:121:VAL:HG22	1:CC:130:ILE:HD11	2.01	0.43
1:CH:130:ILE:O	1:CH:133:ILE:HG22	2.18	0.43
1:CH:155:LEU:HD21	1:CH:162:ILE:HD11	2.01	0.43
1:CR:127:ALA:HB2	1:CS:153:GLN:OE1	2.19	0.43
1:DG:1:SER:C	1:DH:98:ASP:HB3	2.39	0.43
1:AA:1:SER:C	1:AB:98:ASP:HB3	2.39	0.42
1:AF:113:CYS:HB2	1:BV:117:LEU:HD13	2.00	0.42
1:AP:63:GLN:HG3	1:AP:64:TYR:CD1	2.54	0.42
1:AP:127:ALA:HB2	1:AQ:153:GLN:OE1	2.19	0.42
1:AS:1:SER:C	1:AT:98:ASP:HB3	2.39	0.42
1:AV:127:ALA:HB2	1:AW:153:GLN:OE1	2.19	0.42
1:AY:57:PHE:CE1	1:AZ:162:ILE:HD12	2.54	0.42
1:BK:117:LEU:HD12	1:BL:112:SER:O	2.19	0.42
1:BN:11:GLY:HA3	1:BO:21:GLU:HG2	2.00	0.42
1:BN:127:ALA:HB2	1:BO:153:GLN:OE1	2.19	0.42
1:BQ:133:ILE:HD12	1:BR:111:GLN:HB2	2.01	0.42
1:BW:63:GLN:HG3	1:BW:64:TYR:CD1	2.54	0.42
1:BY:155:LEU:HD21	1:BY:162:ILE:HD11	2.01	0.42
1:CN:155:LEU:HD21	1:CN:162:ILE:HD11	2.01	0.42
1:CO:63:GLN:HG3	1:CO:64:TYR:CD1	2.54	0.42
1:CR:63:GLN:HG3	1:CR:64:TYR:CD1	2.54	0.42
1:CX:63:GLN:HG3	1:CX:64:TYR:CD1	2.54	0.42
1:CX:117:LEU:HD12	1:CY:112:SER:O	2.19	0.42
1:DA:127:ALA:HB2	1:DB:153:GLN:OE1	2.19	0.42
1:AC:86:PHE:CD2	1:BP:155:LEU:HD13	2.54	0.42
1:AI:155:LEU:HD13	1:BY:86:PHE:CD2	2.54	0.42
1:AR:155:LEU:HA	1:AR:155:LEU:HD23	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AV:63:GLN:HG3	1:AV:64:TYR:CD1	2.54	0.42
1:BB:133:ILE:HD12	1:BC:111:GLN:HB2	2.01	0.42
1:BD:155:LEU:HD21	1:BD:162:ILE:HD11	2.01	0.42
1:BH:57:PHE:CE1	1:BI:162:ILE:HD12	2.55	0.42
1:BQ:63:GLN:HG3	1:BQ:64:TYR:CD1	2.54	0.42
1:CB:130:ILE:O	1:CB:133:ILE:HG22	2.18	0.42
1:CF:63:GLN:HG3	1:CF:64:TYR:CD1	2.54	0.42
1:CL:1:SER:C	1:CM:98:ASP:HB3	2.39	0.42
1:CS:155:LEU:HD23	1:CS:155:LEU:HA	1.88	0.42
1:DA:1:SER:C	1:DB:98:ASP:HB3	2.39	0.42
1:DA:133:ILE:HD12	1:DB:111:GLN:HB2	2.00	0.42
1:DG:57:PHE:CE1	1:DH:162:ILE:HD12	2.55	0.42
1:DG:117:LEU:HD12	1:DH:112:SER:O	2.18	0.42
1:DJ:11:GLY:HA3	1:DK:21:GLU:HG2	2.00	0.42
1:AC:155:LEU:HD23	1:AC:155:LEU:HA	1.77	0.42
1:AD:57:PHE:CE1	1:AE:162:ILE:HD12	2.54	0.42
1:AD:63:GLN:HG3	1:AD:64:TYR:CD1	2.54	0.42
1:AI:155:LEU:HD23	1:AI:155:LEU:HA	1.77	0.42
1:AM:11:GLY:HA3	1:AN:21:GLU:HG2	2.00	0.42
1:AM:63:GLN:HG3	1:AM:64:TYR:CD1	2.54	0.42
1:AM:133:ILE:HD12	1:AN:111:GLN:HB2	2.01	0.42
1:AP:57:PHE:CE1	1:AQ:162:ILE:HD12	2.55	0.42
1:AR:130:ILE:O	1:AR:133:ILE:HG22	2.18	0.42
1:BN:117:LEU:HD12	1:BO:112:SER:O	2.19	0.42
1:BT:57:PHE:CE1	1:BU:162:ILE:HD12	2.55	0.42
1:BT:117:LEU:HD12	1:BU:112:SER:O	2.19	0.42
1:BZ:1:SER:C	1:CA:98:ASP:HB3	2.39	0.42
1:CA:50:LEU:HD11	1:CF:82:VAL:HG13	2.00	0.42
1:CI:57:PHE:CE1	1:CJ:162:ILE:HD12	2.55	0.42
1:CL:63:GLN:HG3	1:CL:64:TYR:CD1	2.54	0.42
1:CN:130:ILE:O	1:CN:133:ILE:HG22	2.18	0.42
1:CO:121:VAL:HG22	1:CO:130:ILE:HD11	2.01	0.42
1:DA:57:PHE:CE1	1:DB:162:ILE:HD12	2.55	0.42
1:DA:63:GLN:HG3	1:DA:64:TYR:CD1	2.54	0.42
1:DG:121:VAL:HG22	1:DG:130:ILE:HD11	2.01	0.42
1:DH:86:PHE:HE1	1:DH:117:LEU:HD23	1.80	0.42
1:DJ:63:GLN:HG3	1:DJ:64:TYR:CD1	2.54	0.42
1:DL:155:LEU:HD21	1:DL:162:ILE:HD11	2.01	0.42
1:AA:57:PHE:CE1	1:AB:162:ILE:HD12	2.55	0.42
1:AD:34:ASN:HD22	1:DE:30:VAL:HA	1.84	0.42
1:AG:127:ALA:HB2	1:AH:153:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:155:LEU:HD23	1:AO:155:LEU:HA	1.78	0.42
1:AR:98:ASP:HB3	1:CK:2:TYR:N	2.35	0.42
1:AR:162:ILE:HD12	1:CK:57:PHE:CE1	2.55	0.42
1:AS:133:ILE:HD12	1:AT:111:GLN:HB2	2.01	0.42
1:AX:155:LEU:HD21	1:AX:162:ILE:HD11	2.01	0.42
1:AY:63:GLN:HG3	1:AY:64:TYR:CD1	2.54	0.42
1:BE:63:GLN:HG3	1:BE:64:TYR:CD1	2.54	0.42
1:BG:157:ASP:CG	1:DA:52:ARG:NH2	2.68	0.42
1:BH:121:VAL:HG22	1:BH:130:ILE:HD11	2.01	0.42
1:BJ:40:TYR:CE1	1:DF:163:PHE:HB2	2.54	0.42
1:BM:155:LEU:HD21	1:BM:162:ILE:HD11	2.01	0.42
1:BT:63:GLN:HG3	1:BT:64:TYR:CD1	2.54	0.42
1:BW:121:VAL:HG22	1:BW:130:ILE:HD11	2.01	0.42
1:CI:63:GLN:HG3	1:CI:64:TYR:CD1	2.54	0.42
1:CL:117:LEU:HD12	1:CM:112:SER:O	2.19	0.42
1:CU:57:PHE:CE1	1:CV:162:ILE:HD12	2.55	0.42
1:CX:127:ALA:HB2	1:CY:153:GLN:OE1	2.19	0.42
1:CZ:155:LEU:HD21	1:CZ:162:ILE:HD11	2.01	0.42
1:DI:155:LEU:HD21	1:DI:162:ILE:HD11	2.01	0.42
1:AA:63:GLN:HG3	1:AA:64:TYR:CD1	2.54	0.42
1:AA:133:ILE:HD12	1:AB:111:GLN:HB2	2.01	0.42
1:AC:155:LEU:HD21	1:AC:162:ILE:HD11	2.01	0.42
1:AI:155:LEU:HD21	1:AI:162:ILE:HD11	2.01	0.42
1:AL:162:ILE:HD12	1:CB:57:PHE:CE1	2.54	0.42
1:AM:117:LEU:HD12	1:AN:112:SER:O	2.19	0.42
1:AO:57:PHE:CE1	1:CE:162:ILE:HD12	2.55	0.42
1:AR:33:ASP:OD1	1:AR:33:ASP:N	2.51	0.42
1:AU:7:ASN:HD21	1:CN:46:ASP:H	1.67	0.42
1:AU:17:LEU:HD22	1:CN:19:LEU:HD11	2.01	0.42
1:AU:130:ILE:O	1:AU:133:ILE:HG22	2.18	0.42
1:AV:1:SER:C	1:AW:98:ASP:HB3	2.39	0.42
1:AY:117:LEU:HD12	1:AZ:112:SER:O	2.19	0.42
1:BH:63:GLN:HG3	1:BH:64:TYR:CD1	2.54	0.42
1:BN:133:ILE:HD12	1:BO:111:GLN:HB2	2.01	0.42
1:BT:1:SER:C	1:BU:98:ASP:HB3	2.39	0.42
1:BT:127:ALA:HB2	1:BU:153:GLN:OE1	2.19	0.42
1:CF:117:LEU:HD12	1:CG:112:SER:O	2.19	0.42
1:CF:155:LEU:HD23	1:CF:155:LEU:HA	1.92	0.42
1:DD:121:VAL:HG22	1:DD:130:ILE:HD11	2.01	0.42
1:DD:155:LEU:HD23	1:DD:155:LEU:HA	1.92	0.42
1:AI:119:SER:HB2	1:BY:111:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:133:ILE:HD12	1:AK:111:GLN:HB2	2.01	0.42
1:AR:57:PHE:HE2	1:CK:163:PHE:CE1	2.37	0.42
1:AR:155:LEU:HD21	1:AR:162:ILE:HD11	2.01	0.42
1:AX:33:ASP:OD1	1:AX:33:ASP:N	2.51	0.42
1:BB:1:SER:C	1:BC:98:ASP:HB3	2.39	0.42
1:BO:155:LEU:HD23	1:BO:155:LEU:HA	1.88	0.42
1:BQ:57:PHE:CE1	1:BR:162:ILE:HD12	2.55	0.42
1:BS:155:LEU:HD21	1:BS:162:ILE:HD11	2.01	0.42
1:BU:86:PHE:HE1	1:BU:117:LEU:HD23	1.80	0.42
1:BV:130:ILE:O	1:BV:133:ILE:HG22	2.18	0.42
1:CC:133:ILE:HD12	1:CD:111:GLN:HB2	2.01	0.42
1:DD:63:GLN:HG3	1:DD:64:TYR:CD1	2.54	0.42
1:AA:11:GLY:HA3	1:AB:21:GLU:HG2	2.00	0.42
1:AL:119:SER:HB2	1:CB:111:GLN:OE1	2.19	0.42
1:AM:52:ARG:HH22	1:CE:157:ASP:CG	2.23	0.42
1:AP:133:ILE:HD12	1:AQ:111:GLN:HB2	2.01	0.42
1:AU:155:LEU:HD23	1:AU:155:LEU:HA	1.78	0.42
1:BB:127:ALA:HB2	1:BC:153:GLN:OE1	2.19	0.42
1:BE:57:PHE:CE1	1:BF:162:ILE:HD12	2.55	0.42
1:BM:57:PHE:CE1	1:DI:162:ILE:HD12	2.55	0.42
1:BN:121:VAL:HG22	1:BN:130:ILE:HD11	2.01	0.42
1:BW:57:PHE:CE1	1:BX:162:ILE:HD12	2.55	0.42
1:CC:57:PHE:CE1	1:CD:162:ILE:HD12	2.55	0.42
1:CC:63:GLN:HG3	1:CC:64:TYR:CD1	2.54	0.42
1:CF:57:PHE:CE1	1:CG:162:ILE:HD12	2.55	0.42
1:CU:63:GLN:HG3	1:CU:64:TYR:CD1	2.54	0.42
1:CY:155:LEU:HD23	1:CY:155:LEU:HA	1.88	0.42
1:DC:155:LEU:HD21	1:DC:162:ILE:HD11	2.01	0.42
1:DD:57:PHE:CE1	1:DE:162:ILE:HD12	2.55	0.42
1:DJ:57:PHE:CE1	1:DK:162:ILE:HD12	2.55	0.42
1:AD:127:ALA:HB2	1:AE:153:GLN:OE1	2.19	0.42
1:AF:40:TYR:CZ	1:BV:163:PHE:HB2	2.55	0.42
1:AG:117:LEU:HD12	1:AH:112:SER:O	2.19	0.42
1:AJ:57:PHE:CE1	1:AK:162:ILE:HD12	2.54	0.42
1:AK:30:VAL:HA	1:BW:34:ASN:HD22	1.83	0.42
1:AS:155:LEU:HD13	1:AT:86:PHE:CD2	2.55	0.42
1:BB:121:VAL:HG22	1:BB:130:ILE:HD11	2.01	0.42
1:BD:24:ALA:HA	1:CZ:163:PHE:CD2	2.52	0.42
1:BD:155:LEU:HD23	1:BD:155:LEU:HA	1.77	0.42
1:BK:121:VAL:HG22	1:BK:130:ILE:HD11	2.01	0.42
1:BZ:57:PHE:CE1	1:CA:162:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CL:57:PHE:CE1	1:CM:162:ILE:HD12	2.55	0.42
1:CV:58:ASN:OD1	1:CV:87:TYR:HB3	2.20	0.42
1:CX:57:PHE:CE1	1:CY:162:ILE:HD12	2.55	0.42
1:DA:121:VAL:HG22	1:DA:130:ILE:HD11	2.01	0.42
1:AD:121:VAL:HG22	1:AD:130:ILE:HD11	2.01	0.42
1:AE:58:ASN:OD1	1:AE:87:TYR:HB3	2.20	0.42
1:AF:33:ASP:OD1	1:AF:33:ASP:N	2.51	0.42
1:AG:121:VAL:HG22	1:AG:130:ILE:HD11	2.01	0.42
1:AJ:34:ASN:HD22	1:CV:30:VAL:HA	1.84	0.42
1:AL:94:TRP:NE1	1:CB:6:ILE:HG22	2.35	0.42
1:AT:58:ASN:OD1	1:AT:87:TYR:HB3	2.20	0.42
1:AW:58:ASN:OD1	1:AW:87:TYR:HB3	2.20	0.42
1:AY:11:GLY:HA3	1:AZ:21:GLU:HG2	2.00	0.42
1:BB:57:PHE:CE1	1:BC:162:ILE:HD12	2.55	0.42
1:BD:162:ILE:HD12	1:CZ:57:PHE:CE1	2.55	0.42
1:BE:155:LEU:HD13	1:BF:86:PHE:CD2	2.55	0.42
1:BH:155:LEU:HD13	1:BI:86:PHE:CD2	2.55	0.42
1:BK:57:PHE:CE1	1:BL:162:ILE:HD12	2.55	0.42
1:BP:155:LEU:HD21	1:BP:162:ILE:HD11	2.01	0.42
1:BT:155:LEU:HD13	1:BU:86:PHE:CD2	2.55	0.42
1:CF:11:GLY:HA3	1:CG:21:GLU:HG2	2.00	0.42
1:CR:1:SER:C	1:CS:98:ASP:HB3	2.39	0.42
1:AB:155:LEU:HD23	1:AB:155:LEU:HA	1.88	0.42
1:AC:24:ALA:HA	1:BP:163:PHE:CD2	2.53	0.42
1:AG:155:LEU:HD13	1:AH:86:PHE:CD2	2.55	0.42
1:AK:45:SER:HB3	1:AK:53:PRO:HD2	2.02	0.42
1:AM:127:ALA:HB2	1:AN:153:GLN:OE1	2.19	0.42
1:AV:57:PHE:CE1	1:AW:162:ILE:HD12	2.55	0.42
1:BH:82:VAL:HG11	1:BL:50:LEU:HD21	2.01	0.42
1:CC:155:LEU:HD13	1:CD:86:PHE:CD2	2.55	0.42
1:CL:121:VAL:HG22	1:CL:130:ILE:HD11	2.01	0.42
1:CP:155:LEU:HD23	1:CP:155:LEU:HA	1.88	0.42
1:CQ:155:LEU:HD21	1:CQ:162:ILE:HD11	2.01	0.42
1:CR:57:PHE:CE1	1:CS:162:ILE:HD12	2.55	0.42
1:CR:121:VAL:HG22	1:CR:130:ILE:HD11	2.01	0.42
1:DA:155:LEU:HD13	1:DB:86:PHE:CD2	2.55	0.42
1:DI:155:LEU:HA	1:DI:155:LEU:HD23	1.77	0.42
1:AJ:155:LEU:HD13	1:AK:86:PHE:CD2	2.55	0.41
1:AL:155:LEU:HD21	1:AL:162:ILE:HD11	2.01	0.41
1:AO:155:LEU:HD21	1:AO:162:ILE:HD11	2.01	0.41
1:AO:162:ILE:HD12	1:CE:57:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:1:SER:C	1:AQ:98:ASP:HB3	2.39	0.41
1:AW:45:SER:HB3	1:AW:53:PRO:HD2	2.02	0.41
1:BC:45:SER:HB3	1:BC:53:PRO:HD2	2.02	0.41
1:BG:19:LEU:HD11	1:DC:17:LEU:HD22	2.02	0.41
1:BN:63:GLN:HG3	1:BN:64:TYR:CD1	2.54	0.41
1:BV:155:LEU:HD21	1:BV:162:ILE:HD11	2.01	0.41
1:BW:117:LEU:HD12	1:BX:112:SER:O	2.19	0.41
1:BW:155:LEU:HD13	1:BX:86:PHE:CD2	2.55	0.41
1:CA:155:LEU:HD23	1:CA:155:LEU:HA	1.88	0.41
1:CO:155:LEU:HD13	1:CP:86:PHE:CD2	2.55	0.41
1:CR:117:LEU:HD12	1:CS:112:SER:O	2.19	0.41
1:CW:155:LEU:HD21	1:CW:162:ILE:HD11	2.01	0.41
1:CX:133:ILE:HD12	1:CY:111:GLN:HB2	2.01	0.41
1:DD:155:LEU:HD13	1:DE:86:PHE:CD2	2.55	0.41
1:DE:58:ASN:OD1	1:DE:87:TYR:HB3	2.20	0.41
1:DG:155:LEU:HD13	1:DH:86:PHE:CD2	2.55	0.41
1:AH:155:LEU:HD23	1:AH:155:LEU:HA	1.88	0.41
1:AM:155:LEU:HD13	1:AN:86:PHE:CD2	2.55	0.41
1:AO:155:LEU:HD13	1:CE:86:PHE:CD2	2.55	0.41
1:AP:121:VAL:HG22	1:AP:130:ILE:HD11	2.01	0.41
1:AP:155:LEU:HD13	1:AQ:86:PHE:CD2	2.55	0.41
1:AQ:58:ASN:OD1	1:AQ:87:TYR:HB3	2.20	0.41
1:AR:40:TYR:CD2	1:CK:163:PHE:HD1	2.38	0.41
1:AU:119:SER:HB2	1:CN:111:GLN:OE1	2.19	0.41
1:AU:155:LEU:HD21	1:AU:162:ILE:HD11	2.01	0.41
1:AV:155:LEU:HD13	1:AW:86:PHE:CD2	2.55	0.41
1:BB:11:GLY:HA3	1:BC:21:GLU:HG2	2.00	0.41
1:BZ:155:LEU:HD13	1:CA:86:PHE:CD2	2.55	0.41
1:CG:58:ASN:OD1	1:CG:87:TYR:HB3	2.20	0.41
1:CI:121:VAL:HG22	1:CI:130:ILE:HD11	2.01	0.41
1:CK:155:LEU:HD21	1:CK:162:ILE:HD11	2.01	0.41
1:CS:58:ASN:OD1	1:CS:87:TYR:HB3	2.20	0.41
1:CT:155:LEU:HD21	1:CT:162:ILE:HD11	2.01	0.41
1:DH:58:ASN:OD1	1:DH:87:TYR:HB3	2.20	0.41
1:DJ:155:LEU:HD13	1:DK:86:PHE:CD2	2.55	0.41
1:AA:82:VAL:HG13	1:DH:50:LEU:HD11	2.03	0.41
1:AF:155:LEU:HD21	1:AF:162:ILE:HD11	2.01	0.41
1:AG:155:LEU:HD23	1:AG:155:LEU:HA	1.92	0.41
1:AQ:45:SER:HB3	1:AQ:53:PRO:HD2	2.02	0.41
1:AT:45:SER:HB3	1:AT:53:PRO:HD2	2.02	0.41
1:AU:33:ASP:OD1	1:AU:33:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:40:TYR:CE1	1:CZ:163:PHE:HB2	2.55	0.41
1:BF:58:ASN:OD1	1:BF:87:TYR:HB3	2.20	0.41
1:BG:155:LEU:HD21	1:BG:162:ILE:HD11	2.01	0.41
1:BJ:155:LEU:HD21	1:BJ:162:ILE:HD11	2.01	0.41
1:BO:45:SER:HB3	1:BO:53:PRO:HD2	2.02	0.41
1:BQ:155:LEU:HD13	1:BR:86:PHE:CD2	2.55	0.41
1:CE:22:ILE:HD13	1:CE:22:ILE:HA	1.92	0.41
1:CE:155:LEU:HA	1:CE:155:LEU:HD23	1.77	0.41
1:CE:155:LEU:HD21	1:CE:162:ILE:HD11	2.01	0.41
1:CU:155:LEU:HD13	1:CV:86:PHE:CD2	2.55	0.41
1:DB:58:ASN:OD1	1:DB:87:TYR:HB3	2.20	0.41
1:DG:133:ILE:HD12	1:DH:111:GLN:HB2	2.01	0.41
1:DK:45:SER:HB3	1:DK:53:PRO:HD2	2.02	0.41
1:AA:155:LEU:HD13	1:AB:86:PHE:CD2	2.55	0.41
1:AG:57:PHE:CE1	1:AH:162:ILE:HD12	2.55	0.41
1:AM:57:PHE:CE1	1:AN:162:ILE:HD12	2.55	0.41
1:BA:163:PHE:CD2	1:CW:24:ALA:HA	2.52	0.41
1:BD:163:PHE:HB2	1:CZ:40:TYR:CE1	2.54	0.41
1:BD:163:PHE:CD2	1:CZ:24:ALA:HA	2.53	0.41
1:BM:163:PHE:CD2	1:DI:24:ALA:HA	2.56	0.41
1:BN:155:LEU:HD13	1:BO:86:PHE:CD2	2.55	0.41
1:BR:50:LEU:HD23	1:BR:50:LEU:HA	1.89	0.41
1:CA:60:VAL:HB	1:CA:85:GLU:HG3	2.03	0.41
1:CD:45:SER:HB3	1:CD:53:PRO:HD2	2.03	0.41
1:CM:58:ASN:OD1	1:CM:87:TYR:HB3	2.20	0.41
1:CO:57:PHE:CE1	1:CP:162:ILE:HD12	2.55	0.41
1:DB:45:SER:HB3	1:DB:53:PRO:HD2	2.02	0.41
1:DF:155:LEU:HD21	1:DF:162:ILE:HD11	2.01	0.41
1:AB:58:ASN:OD1	1:AB:87:TYR:HB3	2.20	0.41
1:AH:45:SER:HB3	1:AH:53:PRO:HD2	2.02	0.41
1:AH:58:ASN:OD1	1:AH:87:TYR:HB3	2.20	0.41
1:AI:94:TRP:NE1	1:BY:6:ILE:HG22	2.36	0.41
1:AK:60:VAL:HB	1:AK:85:GLU:HG3	2.03	0.41
1:AL:24:ALA:HA	1:CB:163:PHE:CD2	2.53	0.41
1:AR:98:ASP:HB3	1:CK:1:SER:O	2.20	0.41
1:AZ:58:ASN:OD1	1:AZ:87:TYR:HB3	2.20	0.41
1:BA:155:LEU:HD21	1:BA:162:ILE:HD11	2.01	0.41
1:BI:155:LEU:HD23	1:BI:155:LEU:HA	1.88	0.41
1:CM:45:SER:HB3	1:CM:53:PRO:HD2	2.02	0.41
1:AD:155:LEU:HD13	1:AE:86:PHE:CD2	2.55	0.41
1:AE:35:LYS:HZ1	1:BG:34:ASN:HD21	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:45:SER:HB3	1:AE:53:PRO:HD2	2.02	0.41
1:AI:6:ILE:HG22	1:BY:94:TRP:NE1	2.34	0.41
1:AU:19:LEU:HD11	1:CN:17:LEU:HD22	2.03	0.41
1:AY:155:LEU:HD13	1:AZ:86:PHE:CD2	2.55	0.41
1:BF:45:SER:HB3	1:BF:53:PRO:HD2	2.02	0.41
1:BI:45:SER:HB3	1:BI:53:PRO:HD2	2.03	0.41
1:CB:155:LEU:HD21	1:CB:162:ILE:HD11	2.01	0.41
1:CF:155:LEU:HD13	1:CG:86:PHE:CD2	2.55	0.41
1:AA:155:LEU:HD23	1:AA:155:LEU:HA	1.92	0.41
1:AK:58:ASN:OD1	1:AK:87:TYR:HB3	2.20	0.41
1:AO:19:LEU:HD11	1:CE:17:LEU:HD22	2.02	0.41
1:AT:60:VAL:HB	1:AT:85:GLU:HG3	2.03	0.41
1:AX:96:LYS:HE2	1:CT:2:TYR:CD1	2.56	0.41
1:BR:58:ASN:OD1	1:BR:87:TYR:HB3	2.20	0.41
1:BU:58:ASN:OD1	1:BU:87:TYR:HB3	2.20	0.41
1:BX:58:ASN:OD1	1:BX:87:TYR:HB3	2.20	0.41
1:CF:121:VAL:HG22	1:CF:130:ILE:HD11	2.01	0.41
1:CJ:58:ASN:OD1	1:CJ:87:TYR:HB3	2.20	0.41
1:CN:155:LEU:HD23	1:CN:155:LEU:HA	1.77	0.41
1:AI:163:PHE:HB2	1:BY:40:TYR:CE1	2.55	0.41
1:AL:155:LEU:HD13	1:CB:86:PHE:CD2	2.55	0.41
1:AN:60:VAL:HB	1:AN:85:GLU:HG3	2.03	0.41
1:AQ:60:VAL:HB	1:AQ:85:GLU:HG3	2.03	0.41
1:BK:155:LEU:HD13	1:BL:86:PHE:CD2	2.55	0.41
1:BL:45:SER:HB3	1:BL:53:PRO:HD2	2.02	0.41
1:BX:30:VAL:HA	1:CL:34:ASN:HD22	1.85	0.41
1:CA:58:ASN:OD1	1:CA:87:TYR:HB3	2.20	0.41
1:CR:155:LEU:HD13	1:CS:86:PHE:CD2	2.55	0.41
1:DJ:155:LEU:HD23	1:DJ:155:LEU:HA	1.92	0.41
1:AB:60:VAL:HB	1:AB:85:GLU:HG3	2.03	0.41
1:AG:94:TRP:NE1	1:AH:6:ILE:HG22	2.36	0.41
1:AK:50:LEU:HD11	1:BW:82:VAL:HG13	2.03	0.41
1:AK:155:LEU:HA	1:AK:155:LEU:HD23	1.88	0.41
1:AL:155:LEU:HA	1:AL:155:LEU:HD23	1.77	0.41
1:AN:58:ASN:OD1	1:AN:87:TYR:HB3	2.20	0.41
1:AS:94:TRP:NE1	1:AT:6:ILE:HG22	2.36	0.41
1:AV:94:TRP:NE1	1:AW:6:ILE:HG22	2.36	0.41
1:AX:98:ASP:HB3	1:CT:1:SER:C	2.41	0.41
1:BA:164:GLY:O	1:CW:40:TYR:OH	2.31	0.41
1:BB:80:LEU:HA	1:BB:80:LEU:HD23	1.87	0.41
1:BB:94:TRP:NE1	1:BC:6:ILE:HG22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:155:LEU:HD13	1:BC:86:PHE:CD2	2.55	0.41
1:BF:60:VAL:HB	1:BF:85:GLU:HG3	2.03	0.41
1:BI:58:ASN:OD1	1:BI:87:TYR:HB3	2.20	0.41
1:BN:57:PHE:CE1	1:BO:162:ILE:HD12	2.55	0.41
1:BT:94:TRP:NE1	1:BU:6:ILE:HG22	2.36	0.41
1:CD:58:ASN:OD1	1:CD:87:TYR:HB3	2.20	0.41
1:CG:60:VAL:HB	1:CG:85:GLU:HG3	2.03	0.41
1:CG:155:LEU:HD23	1:CG:155:LEU:HA	1.88	0.41
1:CI:94:TRP:NE1	1:CJ:6:ILE:HG22	2.36	0.41
1:CJ:45:SER:HB3	1:CJ:53:PRO:HD2	2.02	0.41
1:CJ:155:LEU:HA	1:CJ:155:LEU:HD23	1.88	0.41
1:CU:94:TRP:NE1	1:CV:6:ILE:HG22	2.36	0.41
1:CY:58:ASN:OD1	1:CY:87:TYR:HB3	2.20	0.41
1:DG:94:TRP:NE1	1:DH:6:ILE:HG22	2.36	0.41
1:DL:155:LEU:HD23	1:DL:155:LEU:HA	1.78	0.41
1:AA:94:TRP:NE1	1:AB:6:ILE:HG22	2.36	0.41
1:AJ:94:TRP:NE1	1:AK:6:ILE:HG22	2.36	0.41
1:AS:155:LEU:HD23	1:AS:155:LEU:HA	1.93	0.41
1:AW:60:VAL:HB	1:AW:85:GLU:HG3	2.03	0.41
1:BA:155:LEU:HA	1:BA:155:LEU:HD23	1.77	0.41
1:BD:46:ASP:H	1:CZ:7:ASN:HD21	1.69	0.41
1:BQ:155:LEU:HD23	1:BQ:155:LEU:HA	1.92	0.41
1:CD:60:VAL:HB	1:CD:85:GLU:HG3	2.03	0.41
1:CK:22:ILE:HD13	1:CK:22:ILE:HA	1.92	0.41
1:CP:60:VAL:HB	1:CP:85:GLU:HG3	2.03	0.41
1:CS:45:SER:HB3	1:CS:53:PRO:HD2	2.02	0.41
1:CV:60:VAL:HB	1:CV:85:GLU:HG3	2.03	0.41
1:DB:50:LEU:HD23	1:DB:50:LEU:HA	1.89	0.41
1:DJ:94:TRP:NE1	1:DK:6:ILE:HG22	2.36	0.41
1:AB:94:TRP:CE2	1:AB:111:GLN:HG3	2.57	0.40
1:BC:50:LEU:HD23	1:BC:50:LEU:HA	1.89	0.40
1:BC:58:ASN:OD1	1:BC:87:TYR:HB3	2.20	0.40
1:BE:94:TRP:NE1	1:BF:6:ILE:HG22	2.36	0.40
1:BL:94:TRP:CE2	1:BL:111:GLN:HG3	2.57	0.40
1:CA:45:SER:HB3	1:CA:53:PRO:HD2	2.02	0.40
1:CC:94:TRP:NE1	1:CD:6:ILE:HG22	2.36	0.40
1:CG:45:SER:HB3	1:CG:53:PRO:HD2	2.03	0.40
1:CI:155:LEU:HD13	1:CJ:86:PHE:CD2	2.55	0.40
1:DA:80:LEU:HA	1:DA:80:LEU:HD23	1.87	0.40
1:AB:45:SER:HB3	1:AB:53:PRO:HD2	2.02	0.40
1:AC:7:ASN:HD21	1:BP:46:ASP:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:94:TRP:NE1	1:AE:6:ILE:HG22	2.36	0.40
1:AF:42:ASP:OD2	1:BV:9:SER:N	2.52	0.40
1:AP:94:TRP:NE1	1:AQ:6:ILE:HG22	2.36	0.40
1:AS:57:PHE:CE1	1:AT:162:ILE:HD12	2.55	0.40
1:AX:111:GLN:OE1	1:CT:119:SER:HB2	2.21	0.40
1:BA:33:ASP:OD1	1:BA:33:ASP:N	2.51	0.40
1:BR:45:SER:HB3	1:BR:53:PRO:HD2	2.03	0.40
1:BX:94:TRP:CE2	1:BX:111:GLN:HG3	2.57	0.40
1:CP:94:TRP:CE2	1:CP:111:GLN:HG3	2.57	0.40
1:CR:94:TRP:NE1	1:CS:6:ILE:HG22	2.36	0.40
1:CZ:155:LEU:HD23	1:CZ:155:LEU:HA	1.77	0.40
1:DH:60:VAL:HB	1:DH:85:GLU:HG3	2.03	0.40
1:AD:40:TYR:OH	1:AE:164:GLY:O	2.28	0.40
1:AH:60:VAL:HB	1:AH:85:GLU:HG3	2.03	0.40
1:AK:94:TRP:CE2	1:AK:111:GLN:HG3	2.57	0.40
1:AM:80:LEU:HA	1:AM:80:LEU:HD23	1.87	0.40
1:AT:94:TRP:CE2	1:AT:111:GLN:HG3	2.57	0.40
1:AZ:45:SER:HB3	1:AZ:53:PRO:HD2	2.02	0.40
1:BJ:22:ILE:HD13	1:BJ:22:ILE:HA	1.92	0.40
1:BM:40:TYR:CE1	1:DI:163:PHE:HB2	2.56	0.40
1:BM:155:LEU:HD23	1:BM:155:LEU:HA	1.77	0.40
1:BO:58:ASN:OD1	1:BO:87:TYR:HB3	2.20	0.40
1:BU:45:SER:HB3	1:BU:53:PRO:HD2	2.02	0.40
1:BU:94:TRP:CE2	1:BU:111:GLN:HG3	2.57	0.40
1:CL:155:LEU:HD13	1:CM:86:PHE:CD2	2.55	0.40
1:CM:94:TRP:CE2	1:CM:111:GLN:HG3	2.57	0.40
1:CO:94:TRP:NE1	1:CP:6:ILE:HG22	2.36	0.40
1:CY:60:VAL:HB	1:CY:85:GLU:HG3	2.03	0.40
1:DH:45:SER:HB3	1:DH:53:PRO:HD2	2.02	0.40
1:DK:58:ASN:OD1	1:DK:87:TYR:HB3	2.20	0.40
1:AE:60:VAL:HB	1:AE:85:GLU:HG3	2.03	0.40
1:AE:94:TRP:CE2	1:AE:111:GLN:HG3	2.57	0.40
1:AF:135:LEU:HD22	1:BV:19:LEU:HD23	2.03	0.40
1:AR:112:SER:O	1:CK:117:LEU:HD12	2.22	0.40
1:AT:50:LEU:HD23	1:AT:50:LEU:HA	1.89	0.40
1:AV:40:TYR:OH	1:AW:164:GLY:O	2.28	0.40
1:AY:94:TRP:NE1	1:AZ:6:ILE:HG22	2.36	0.40
1:BC:60:VAL:HB	1:BC:85:GLU:HG3	2.03	0.40
1:BE:155:LEU:HD23	1:BE:155:LEU:HA	1.92	0.40
1:BG:40:TYR:OH	1:DC:164:GLY:O	2.31	0.40
1:BK:94:TRP:NE1	1:BL:6:ILE:HG22	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:94:TRP:NE1	1:BX:6:ILE:HG22	2.36	0.40
1:CL:94:TRP:NE1	1:CM:6:ILE:HG22	2.36	0.40
1:CP:58:ASN:OD1	1:CP:87:TYR:HB3	2.20	0.40
1:CU:82:VAL:HG13	1:CY:50:LEU:HD11	2.04	0.40
1:DE:60:VAL:HB	1:DE:85:GLU:HG3	2.03	0.40
1:AD:119:SER:HB2	1:AE:111:GLN:OE1	2.22	0.40
1:AH:94:TRP:CE2	1:AH:111:GLN:HG3	2.57	0.40
1:AM:119:SER:HB2	1:AN:111:GLN:OE1	2.22	0.40
1:AN:94:TRP:CE2	1:AN:111:GLN:HG3	2.57	0.40
1:AP:28:VAL:HG11	1:CK:159:LEU:HD13	2.03	0.40
1:AW:94:TRP:CE2	1:AW:111:GLN:HG3	2.57	0.40
1:BH:119:SER:HB2	1:BI:111:GLN:OE1	2.22	0.40
1:BI:60:VAL:HB	1:BI:85:GLU:HG3	2.03	0.40
1:BL:58:ASN:OD1	1:BL:87:TYR:HB3	2.20	0.40
1:BR:94:TRP:CE2	1:BR:111:GLN:HG3	2.57	0.40
1:BU:30:VAL:HA	1:DG:34:ASN:HD22	1.87	0.40
1:BY:33:ASP:OD1	1:BY:33:ASP:N	2.51	0.40
1:CF:119:SER:HB2	1:CG:111:GLN:OE1	2.22	0.40
1:CG:94:TRP:CE2	1:CG:111:GLN:HG3	2.57	0.40
1:CU:34:ASN:HD22	1:CY:30:VAL:HA	1.85	0.40
1:CV:45:SER:HB3	1:CV:53:PRO:HD2	2.02	0.40
1:CX:119:SER:HB2	1:CY:111:GLN:OE1	2.22	0.40
1:CX:155:LEU:HD13	1:CY:86:PHE:CD2	2.55	0.40
1:CZ:46:ASP:OD2	1:CZ:48:SER:OG	2.27	0.40
1:DA:119:SER:HB2	1:DB:111:GLN:OE1	2.22	0.40
1:DJ:119:SER:HB2	1:DK:111:GLN:OE1	2.22	0.40
1:DK:60:VAL:HB	1:DK:85:GLU:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:149:TRP:CD1	1:BQ:12:ASP:OD2[1_554]	1.99	0.21

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	AA	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AB	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AC	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AD	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AE	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AF	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AG	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AH	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AI	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AJ	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AK	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AL	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AM	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AN	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AO	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AP	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AQ	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AR	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AS	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AT	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AU	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AV	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AW	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AX	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	AY	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	AZ	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BA	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BB	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BC	162/164 (99%)	161 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BD	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BE	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BF	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BG	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BH	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BI	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BJ	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BK	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BL	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BM	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BN	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BO	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BP	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BQ	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BR	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BS	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BT	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BU	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BV	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BW	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	BX	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BY	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	BZ	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CA	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CB	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CC	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CD	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CE	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CF	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CG	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CH	162/164 (99%)	161 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CJ	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CK	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CL	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CM	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CN	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CO	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CP	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CQ	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CR	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CS	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CT	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CU	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CV	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CW	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CX	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	CY	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	CZ	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DA	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	DB	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DC	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DD	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	DE	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DF	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DG	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	DH	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DI	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DJ	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	DK	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	DL	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
All	All	14580/14760 (99%)	14430 (99%)	150 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	145/145 (100%)	145 (100%)	0	100	100
1	AB	145/145 (100%)	145 (100%)	0	100	100
1	AC	145/145 (100%)	145 (100%)	0	100	100
1	AD	145/145 (100%)	145 (100%)	0	100	100
1	AE	145/145 (100%)	145 (100%)	0	100	100
1	AF	145/145 (100%)	145 (100%)	0	100	100
1	AG	145/145 (100%)	145 (100%)	0	100	100
1	AH	145/145 (100%)	145 (100%)	0	100	100
1	AI	145/145 (100%)	145 (100%)	0	100	100
1	AJ	145/145 (100%)	145 (100%)	0	100	100
1	AK	145/145 (100%)	145 (100%)	0	100	100
1	AL	145/145 (100%)	145 (100%)	0	100	100
1	AM	145/145 (100%)	145 (100%)	0	100	100
1	AN	145/145 (100%)	145 (100%)	0	100	100
1	AO	145/145 (100%)	145 (100%)	0	100	100
1	AP	145/145 (100%)	145 (100%)	0	100	100
1	AQ	145/145 (100%)	145 (100%)	0	100	100
1	AR	145/145 (100%)	145 (100%)	0	100	100
1	AS	145/145 (100%)	145 (100%)	0	100	100
1	AT	145/145 (100%)	145 (100%)	0	100	100
1	AU	145/145 (100%)	145 (100%)	0	100	100
1	AV	145/145 (100%)	145 (100%)	0	100	100
1	AW	145/145 (100%)	145 (100%)	0	100	100
1	AX	145/145 (100%)	145 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AY	145/145 (100%)	145 (100%)	0	100	100
1	AZ	145/145 (100%)	145 (100%)	0	100	100
1	BA	145/145 (100%)	145 (100%)	0	100	100
1	BB	145/145 (100%)	145 (100%)	0	100	100
1	BC	145/145 (100%)	145 (100%)	0	100	100
1	BD	145/145 (100%)	145 (100%)	0	100	100
1	BE	145/145 (100%)	145 (100%)	0	100	100
1	BF	145/145 (100%)	145 (100%)	0	100	100
1	BG	145/145 (100%)	145 (100%)	0	100	100
1	BH	145/145 (100%)	145 (100%)	0	100	100
1	BI	145/145 (100%)	145 (100%)	0	100	100
1	BJ	145/145 (100%)	145 (100%)	0	100	100
1	BK	145/145 (100%)	145 (100%)	0	100	100
1	BL	145/145 (100%)	145 (100%)	0	100	100
1	BM	145/145 (100%)	145 (100%)	0	100	100
1	BN	145/145 (100%)	145 (100%)	0	100	100
1	BO	145/145 (100%)	145 (100%)	0	100	100
1	BP	145/145 (100%)	145 (100%)	0	100	100
1	BQ	145/145 (100%)	145 (100%)	0	100	100
1	BR	145/145 (100%)	145 (100%)	0	100	100
1	BS	145/145 (100%)	145 (100%)	0	100	100
1	BT	145/145 (100%)	145 (100%)	0	100	100
1	BU	145/145 (100%)	145 (100%)	0	100	100
1	BV	145/145 (100%)	145 (100%)	0	100	100
1	BW	145/145 (100%)	145 (100%)	0	100	100
1	BX	145/145 (100%)	145 (100%)	0	100	100
1	BY	145/145 (100%)	145 (100%)	0	100	100
1	BZ	145/145 (100%)	145 (100%)	0	100	100
1	CA	145/145 (100%)	145 (100%)	0	100	100
1	CB	145/145 (100%)	145 (100%)	0	100	100
1	CC	145/145 (100%)	145 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	145/145 (100%)	145 (100%)	0	100	100
1	CE	145/145 (100%)	145 (100%)	0	100	100
1	CF	145/145 (100%)	145 (100%)	0	100	100
1	CG	145/145 (100%)	145 (100%)	0	100	100
1	CH	145/145 (100%)	145 (100%)	0	100	100
1	CI	145/145 (100%)	145 (100%)	0	100	100
1	CJ	145/145 (100%)	145 (100%)	0	100	100
1	CK	145/145 (100%)	145 (100%)	0	100	100
1	CL	145/145 (100%)	145 (100%)	0	100	100
1	CM	145/145 (100%)	145 (100%)	0	100	100
1	CN	145/145 (100%)	145 (100%)	0	100	100
1	CO	145/145 (100%)	145 (100%)	0	100	100
1	CP	145/145 (100%)	145 (100%)	0	100	100
1	CQ	145/145 (100%)	145 (100%)	0	100	100
1	CR	145/145 (100%)	145 (100%)	0	100	100
1	CS	145/145 (100%)	145 (100%)	0	100	100
1	CT	145/145 (100%)	145 (100%)	0	100	100
1	CU	145/145 (100%)	145 (100%)	0	100	100
1	CV	145/145 (100%)	145 (100%)	0	100	100
1	CW	145/145 (100%)	145 (100%)	0	100	100
1	CX	145/145 (100%)	145 (100%)	0	100	100
1	CY	145/145 (100%)	145 (100%)	0	100	100
1	CZ	145/145 (100%)	145 (100%)	0	100	100
1	DA	145/145 (100%)	145 (100%)	0	100	100
1	DB	145/145 (100%)	145 (100%)	0	100	100
1	DC	145/145 (100%)	145 (100%)	0	100	100
1	DD	145/145 (100%)	145 (100%)	0	100	100
1	DE	145/145 (100%)	145 (100%)	0	100	100
1	DF	145/145 (100%)	145 (100%)	0	100	100
1	DG	145/145 (100%)	145 (100%)	0	100	100
1	DH	145/145 (100%)	145 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DI	145/145 (100%)	145 (100%)	0	100	100
1	DJ	145/145 (100%)	145 (100%)	0	100	100
1	DK	145/145 (100%)	145 (100%)	0	100	100
1	DL	145/145 (100%)	145 (100%)	0	100	100
All	All	13050/13050 (100%)	13050 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	AC	34	ASN
1	AD	47	ASN
1	AG	47	ASN
1	AI	47	ASN
1	AJ	47	ASN
1	AL	47	ASN
1	AM	47	ASN
1	AO	47	ASN
1	AP	47	ASN
1	AU	47	ASN
1	AV	47	ASN
1	AX	47	ASN
1	AY	47	ASN
1	BB	47	ASN
1	BG	34	ASN
1	BH	47	ASN
1	BJ	47	ASN
1	BK	47	ASN
1	BP	47	ASN
1	BS	47	ASN
1	BT	47	ASN
1	BV	34	ASN
1	BV	47	ASN
1	BW	47	ASN
1	BY	47	ASN
1	BZ	47	ASN
1	CB	47	ASN
1	CC	47	ASN
1	CE	47	ASN

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Mol	Chain	Res	Type
1	CH	34	ASN
1	CH	47	ASN
1	CI	47	ASN
1	CK	34	ASN
1	CK	47	ASN
1	CN	47	ASN
1	CR	47	ASN
1	CT	34	ASN
1	CU	47	ASN
1	CW	34	ASN
1	CX	47	ASN
1	CZ	47	ASN
1	DA	47	ASN
1	DC	47	ASN
1	DD	47	ASN
1	DG	47	ASN
1	DI	47	ASN
1	DL	47	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	164/164 (100%)	-0.41	0	100	100	21, 41, 68, 76	0
1	AB	164/164 (100%)	-0.36	0	100	100	21, 41, 67, 89	0
1	AC	164/164 (100%)	-0.31	1 (0%)	89	78	24, 42, 71, 98	0
1	AD	164/164 (100%)	-0.41	0	100	100	21, 41, 68, 76	0
1	AE	164/164 (100%)	-0.37	0	100	100	21, 41, 67, 89	0
1	AF	164/164 (100%)	-0.18	0	100	100	24, 42, 71, 98	0
1	AG	164/164 (100%)	-0.38	0	100	100	21, 41, 68, 76	0
1	AH	164/164 (100%)	-0.38	0	100	100	21, 41, 67, 89	0
1	AI	164/164 (100%)	-0.30	1 (0%)	89	78	24, 42, 71, 98	0
1	AJ	164/164 (100%)	-0.41	0	100	100	21, 41, 68, 76	0
1	AK	164/164 (100%)	-0.35	0	100	100	21, 41, 67, 89	0
1	AL	164/164 (100%)	-0.27	2 (1%)	79	61	24, 42, 71, 98	0
1	AM	164/164 (100%)	-0.41	0	100	100	21, 41, 68, 76	0
1	AN	164/164 (100%)	-0.35	1 (0%)	89	78	21, 41, 67, 89	0
1	AO	164/164 (100%)	-0.33	2 (1%)	79	61	24, 42, 71, 98	0
1	AP	164/164 (100%)	-0.49	0	100	100	21, 41, 68, 76	0
1	AQ	164/164 (100%)	-0.46	0	100	100	21, 41, 67, 89	0
1	AR	164/164 (100%)	-0.30	0	100	100	24, 42, 71, 98	0
1	AS	164/164 (100%)	-0.38	0	100	100	21, 41, 68, 76	0
1	AT	164/164 (100%)	-0.47	0	100	100	21, 41, 67, 89	0
1	AU	164/164 (100%)	-0.32	0	100	100	24, 42, 71, 98	0
1	AV	164/164 (100%)	-0.43	0	100	100	21, 41, 68, 76	0
1	AW	164/164 (100%)	-0.39	0	100	100	21, 41, 67, 89	0
1	AX	164/164 (100%)	-0.38	0	100	100	24, 42, 71, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AY	164/164 (100%)	-0.46	0	100	100	21, 41, 68, 76	0
1	AZ	164/164 (100%)	-0.43	0	100	100	21, 41, 67, 89	0
1	BA	164/164 (100%)	-0.24	1 (0%)	89	78	24, 42, 71, 98	0
1	BB	164/164 (100%)	-0.44	0	100	100	21, 41, 68, 76	0
1	BC	164/164 (100%)	-0.40	0	100	100	21, 41, 67, 89	0
1	BD	164/164 (100%)	-0.29	1 (0%)	89	78	24, 42, 71, 98	0
1	BE	164/164 (100%)	-0.36	0	100	100	21, 41, 68, 76	0
1	BF	164/164 (100%)	-0.35	0	100	100	21, 41, 67, 89	0
1	BG	164/164 (100%)	-0.14	1 (0%)	89	78	24, 42, 71, 98	0
1	BH	164/164 (100%)	-0.49	0	100	100	21, 41, 68, 76	0
1	BI	164/164 (100%)	-0.40	0	100	100	21, 41, 67, 89	0
1	BJ	164/164 (100%)	-0.44	0	100	100	24, 42, 71, 98	0
1	BK	164/164 (100%)	-0.44	0	100	100	21, 41, 68, 76	0
1	BL	164/164 (100%)	-0.43	0	100	100	21, 41, 67, 89	0
1	BM	164/164 (100%)	-0.34	1 (0%)	89	78	24, 42, 71, 98	0
1	BN	164/164 (100%)	-0.41	0	100	100	21, 41, 68, 76	0
1	BO	164/164 (100%)	-0.46	0	100	100	21, 41, 67, 89	0
1	BP	164/164 (100%)	-0.32	0	100	100	24, 42, 71, 98	0
1	BQ	164/164 (100%)	-0.44	0	100	100	21, 41, 68, 76	0
1	BR	164/164 (100%)	-0.40	0	100	100	21, 41, 67, 89	0
1	BS	164/164 (100%)	-0.45	1 (0%)	89	78	24, 42, 71, 98	0
1	BT	164/164 (100%)	-0.31	0	100	100	21, 41, 68, 76	0
1	BU	164/164 (100%)	-0.23	0	100	100	21, 41, 67, 89	0
1	BV	164/164 (100%)	-0.07	2 (1%)	79	61	24, 42, 71, 98	0
1	BW	164/164 (100%)	-0.38	0	100	100	21, 41, 68, 76	0
1	BX	164/164 (100%)	-0.41	0	100	100	21, 41, 67, 89	0
1	BY	164/164 (100%)	-0.35	1 (0%)	89	78	24, 42, 71, 98	0
1	BZ	164/164 (100%)	-0.44	0	100	100	21, 41, 68, 76	0
1	CA	164/164 (100%)	-0.49	0	100	100	21, 41, 67, 89	0
1	CB	164/164 (100%)	-0.38	0	100	100	24, 42, 71, 98	0
1	CC	164/164 (100%)	-0.45	0	100	100	21, 41, 68, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	CD	164/164 (100%)	-0.46	0	100	100	21, 41, 67, 89	0
1	CE	164/164 (100%)	-0.35	0	100	100	24, 42, 71, 98	0
1	CF	164/164 (100%)	-0.44	0	100	100	21, 41, 68, 76	0
1	CG	164/164 (100%)	-0.45	0	100	100	21, 41, 67, 89	0
1	CH	164/164 (100%)	-0.39	1 (0%)	89	78	24, 42, 71, 98	0
1	CI	164/164 (100%)	-0.34	0	100	100	21, 41, 68, 76	0
1	CJ	164/164 (100%)	-0.29	0	100	100	21, 41, 67, 89	0
1	CK	164/164 (100%)	-0.27	3 (1%)	68	47	24, 42, 71, 98	0
1	CL	164/164 (100%)	-0.42	0	100	100	21, 41, 68, 76	0
1	CM	164/164 (100%)	-0.35	0	100	100	21, 41, 67, 89	0
1	CN	164/164 (100%)	-0.31	0	100	100	24, 42, 71, 98	0
1	CO	164/164 (100%)	-0.46	0	100	100	21, 41, 68, 76	0
1	CP	164/164 (100%)	-0.47	0	100	100	21, 41, 67, 89	0
1	CQ	164/164 (100%)	-0.44	1 (0%)	89	78	24, 42, 71, 98	0
1	CR	164/164 (100%)	-0.46	0	100	100	21, 41, 68, 76	0
1	CS	164/164 (100%)	-0.43	0	100	100	21, 41, 67, 89	0
1	CT	164/164 (100%)	-0.35	0	100	100	24, 42, 71, 98	0
1	CU	164/164 (100%)	-0.38	0	100	100	21, 41, 68, 76	0
1	CV	164/164 (100%)	-0.45	0	100	100	21, 41, 67, 89	0
1	CW	164/164 (100%)	-0.36	0	100	100	24, 42, 71, 98	0
1	CX	164/164 (100%)	-0.44	0	100	100	21, 41, 68, 76	0
1	CY	164/164 (100%)	-0.38	0	100	100	21, 41, 67, 89	0
1	CZ	164/164 (100%)	-0.39	1 (0%)	89	78	24, 42, 71, 98	0
1	DA	164/164 (100%)	-0.35	0	100	100	21, 41, 68, 76	0
1	DB	164/164 (100%)	-0.40	0	100	100	21, 41, 67, 89	0
1	DC	164/164 (100%)	-0.27	1 (0%)	89	78	24, 42, 71, 98	0
1	DD	164/164 (100%)	-0.44	0	100	100	21, 41, 68, 76	0
1	DE	164/164 (100%)	-0.37	0	100	100	21, 41, 67, 89	0
1	DF	164/164 (100%)	-0.40	0	100	100	24, 42, 71, 98	0
1	DG	164/164 (100%)	-0.43	0	100	100	21, 41, 68, 76	0
1	DH	164/164 (100%)	-0.42	0	100	100	21, 41, 67, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	DI	164/164 (100%)	-0.31	2 (1%) 79 61	24, 42, 71, 98	0
1	DJ	164/164 (100%)	-0.44	0 100 100	21, 41, 68, 76	0
1	DK	164/164 (100%)	-0.47	0 100 100	21, 41, 67, 89	0
1	DL	164/164 (100%)	-0.46	0 100 100	24, 42, 71, 98	0
All	All	14760/14760 (100%)	-0.38	24 (0%) 95 90	21, 42, 71, 98	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BV	35	LYS	3.5
1	CK	34	ASN	3.4
1	BG	35	LYS	3.0
1	BM	35	LYS	3.0
1	BA	34	ASN	2.8
1	DI	31	SER	2.8
1	AC	36	SER	2.7
1	AI	34	ASN	2.7
1	BV	34	ASN	2.7
1	BY	34	ASN	2.7
1	AL	34	ASN	2.7
1	AL	35	LYS	2.6
1	CK	36	SER	2.5
1	CZ	34	ASN	2.5
1	AO	35	LYS	2.3
1	CQ	34	ASN	2.3
1	DI	34	ASN	2.2
1	CH	35	LYS	2.2
1	CK	35	LYS	2.1
1	DC	34	ASN	2.1
1	AO	34	ASN	2.1
1	BD	34	ASN	2.1
1	AN	103	ASP	2.0
1	BS	34	ASN	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 monosaccharides 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.