Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 10:32 PM EDT

PDB ID	:	6YFK
Title	:	Virus-like particle of bacteriophage ESE007
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

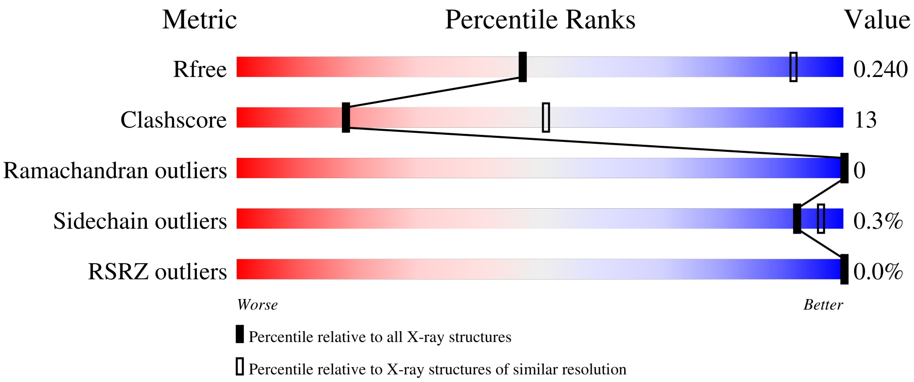
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	137	71% 29%
1	AB	137	60% 40%
1	AC	137	77% 22% •
1	AD	137	64% 36%
1	AE	137	64% 36%

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Mol	Chain	Length	Quality of chain
1	AF	137	71% 28% •
1	AG	137	74% 26%
1	AH	137	63% 37%
1	AI	137	73% 26% •
1	AJ	137	69% 31%
1	AK	137	62% 38%
1	AL	137	74% 26% •
1	AM	137	70% 30%
1	AN	137	64% 36%
1	AO	137	75% 24% •
1	AP	137	70% 30%
1	AQ	137	58% 42%
1	AR	137	70% 29% •
1	AS	137	69% 31%
1	AT	137	63% 37%
1	AU	137	74% 25% •
1	AV	137	68% 32%
1	AW	137	68% 32%
1	AX	137	74% 26% •
1	AY	137	69% 31%
1	AZ	137	68% 32%
1	BA	137	74% 26% •
1	BB	137	72% 28%
1	BC	137	59% 41%
1	BD	137	74% 25% •

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Mol	Chain	Length	Quality of chain
1	BE	137	72% 28%
1	BF	137	61% 39%
1	BG	137	77% 23% •
1	BH	137	64% 36%
1	BI	137	61% 39%
1	BJ	137	71% 28% •
1	BK	137	% 66% 34%
1	BL	137	69% 31%
1	BM	137	% 74% 26% •
1	BN	137	74% 26%
1	BO	137	59% 41%
1	BP	137	73% 26% •
1	BQ	137	72% 28%
1	BR	137	64% 36%
1	BS	137	74% 25% •
1	BT	137	69% 31%
1	BU	137	68% 32%
1	BV	137	74% 26% •
1	BW	137	68% 32%
1	BX	137	64% 36%
1	BY	137	74% 25% •
1	BZ	137	69% 31%
1	CA	137	61% 39%
1	CB	137	73% 26% •
1	CC	137	72% 28%

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Mol	Chain	Length	Quality of chain
1	CD	137	63% 37%
1	CE	137	74% 26% •
1	CF	137	70% 30%
1	CG	137	64% 36%
1	CH	137	74% 25% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 62180 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	137	1036	656	178	200	2	0	0	0
1	AB	137	1036	656	178	200	2	0	0	0
1	AC	137	1036	656	178	200	2	0	0	0
1	AD	137	1036	656	178	200	2	0	0	0
1	AE	137	1036	656	178	200	2	0	0	0
1	AF	137	1036	656	178	200	2	0	0	0
1	AG	137	1036	656	178	200	2	0	0	0
1	AH	137	1036	656	178	200	2	0	0	0
1	AI	137	1036	656	178	200	2	0	0	0
1	AJ	137	1036	656	178	200	2	0	0	0
1	AK	137	1036	656	178	200	2	0	0	0
1	AL	137	1036	656	178	200	2	0	0	0
1	AM	137	1036	656	178	200	2	0	0	0
1	AN	137	1036	656	178	200	2	0	0	0
1	AO	137	1036	656	178	200	2	0	0	0
1	AP	137	1036	656	178	200	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AR	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AS	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AT	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AU	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AV	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AW	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AX	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AY	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	AZ	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BA	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BB	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BC	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BD	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BE	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BF	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BG	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BH	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BI	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BJ	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BK	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BM	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BN	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BO	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BP	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BQ	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BR	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BS	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BT	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BU	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BV	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BW	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BX	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BY	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	BZ	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	CA	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	CB	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	CC	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	CD	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	CE	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	CF	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0
1	CH	137	Total 1036	C 656	N 178	O 200	S 2	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AF	1	Total 1	Ca 1	0	0
2	AG	1	Total 1	Ca 1	0	0
2	AJ	1	Total 1	Ca 1	0	0
2	AL	1	Total 1	Ca 1	0	0
2	AO	1	Total 1	Ca 1	0	0
2	AP	1	Total 1	Ca 1	0	0
2	AU	1	Total 1	Ca 1	0	0
2	AX	1	Total 1	Ca 1	0	0
2	BA	1	Total 1	Ca 1	0	0
2	BB	1	Total 1	Ca 1	0	0
2	BD	1	Total 1	Ca 1	0	0
2	BJ	1	Total 1	Ca 1	0	0
2	BM	1	Total 1	Ca 1	0	0
2	BN	1	Total 1	Ca 1	0	0
2	BP	1	Total 1	Ca 1	0	0
2	BV	1	Total 1	Ca 1	0	0
2	BY	1	Total 1	Ca 1	0	0

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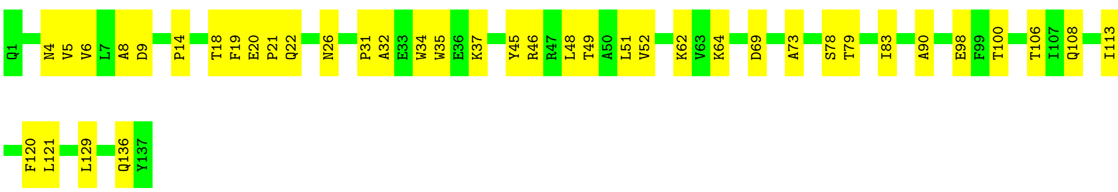
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BZ	1	Total Ca 1 1	0	0
2	CC	1	Total Ca 1 1	0	0
2	CH	1	Total Ca 1 1	0	0

3 Residue-property plots

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.

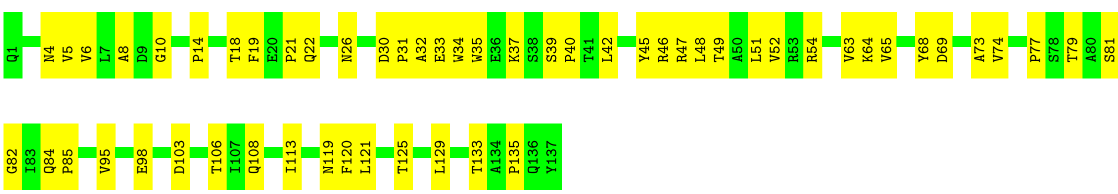
• Molecule 1: coat protein

Chain AA:

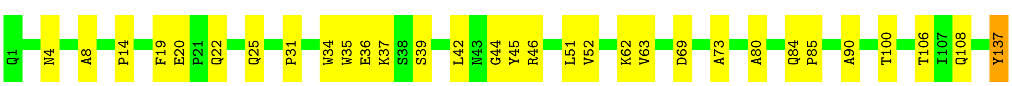
• Molecule 1: coat protein

Chain AB:

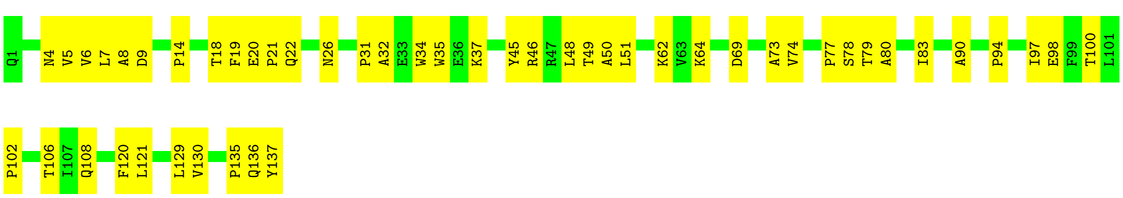
• Molecule 1: coat protein

Chain AC:

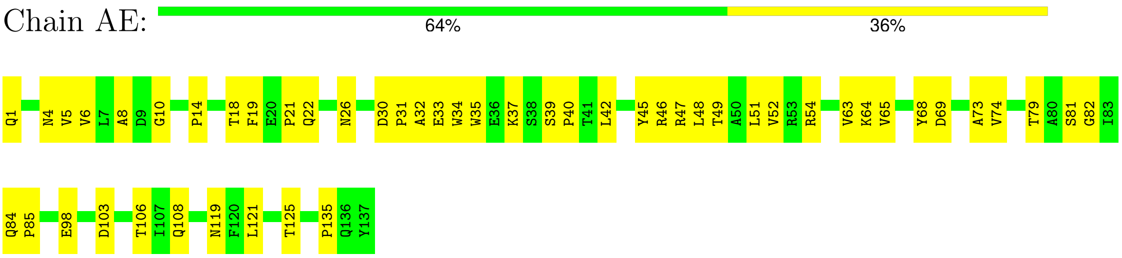
• Molecule 1: coat protein

Chain AD:

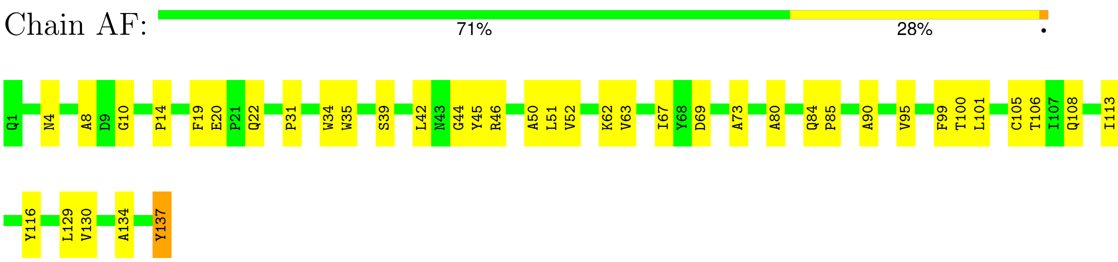
• Molecule 1: coat protein

Chain AE:



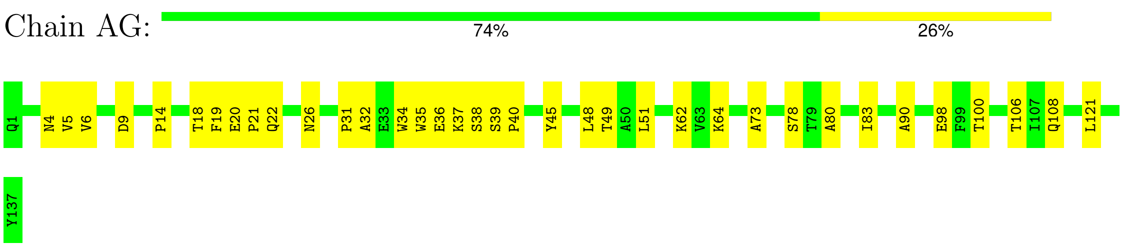
• Molecule 1: coat protein

Chain AF:



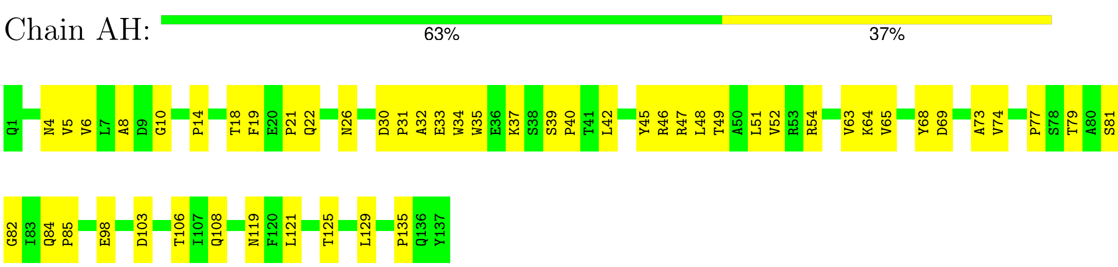
• Molecule 1: coat protein

Chain AG:



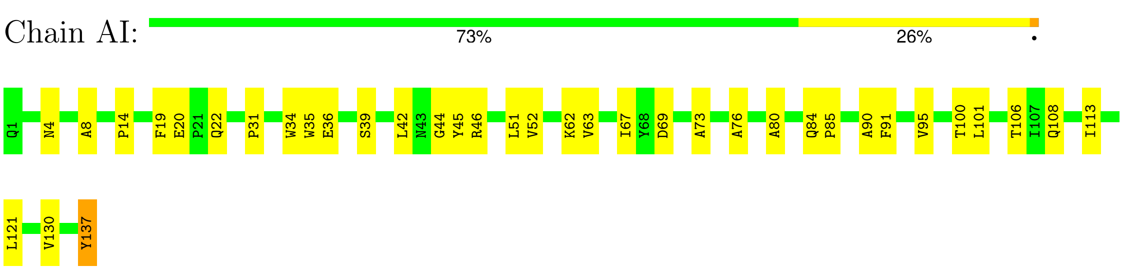
• Molecule 1: coat protein

Chain AH:



• Molecule 1: coat protein

Chain AI:



• Molecule 1: coat protein

Chain AJ:

69% 31%

Q1 N4 V5 V6 D9 P14 T18 F19 E20 P21 Q22 N26 P31 A32 E33 W34 W35 E36 K37 Y45 R46 R47 L48 T49 A50 L51 K62 V63 K64 D69 A73 V74 P77 S78 T79 A80 S81 G82 I83 Q84 A90 V95 E98 F99 T100 T106 I107 Q108 I113 L121 N132 Y137

• Molecule 1: coat protein

Chain AK:

62% 38%

Q1 N4 V5 V6 L7 A8 D9 G10 P14 T18 F19 E20 P21 Q22 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 Y68 D69 A73 V74 T75 A76 P77 S78 T79 A80 S81 G82 I83 Q84 P85 E98 D103 T106 I107 Q108 N119 F120 L121 T125 P135 Q136 Y137

• Molecule 1: coat protein

Chain AL:

74% 26% •

Q1 N4 A8 P14 F19 E20 P21 Q22 Q25 P31 W34 W35 E36 S39 L42 N43 G44 Y45 R46 L51 V52 K62 V63 D69 A73 V74 T75 A76 A80 Q84 P85 A90 V95 T100 L101 T106 I107 Q108 I113 L114 Y137

• Molecule 1: coat protein

Chain AM:

70% 30%

Q1 N4 V5 V6 L7 A8 D9 P14 T18 F19 E20 P21 Q22 N26 P31 A32 E33 W34 W35 E36 K37 Y45 L48 T49 A50 L51 V52 K62 V63 K64 V65 A73 P77 S78 T79 A80 I83 A90 V95 E98 F99 T100 C105 T106 I107 Q108 L121 Q136 Y137

• Molecule 1: coat protein

Chain AN:

64% 36%

Q1 N4 V5 V6 L7 A8 D9 G10 P14 T18 F19 E20 P21 Q22 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 D69 A73 V74 T75 A76 P77 S78 T79 A80 S81 G82 I83 Q84 P85 V95 E98 D103 T106 I107 Q108 I113 L121 T125 Q136 Y137

• Molecule 1: coat protein

Chain AO: 75% 24% •

Q1 N4 A8 P14 F19 E20 P21 Q22 P31 W34 W35 E36 K37 S38 S39 L42 N43 G44 Y45 R46 A50 L51 V52 K62 V63 D69 A73 A76 A80 Q84 P85 A90 T100 T106 I107 Q108 N119 L129 Y137

• Molecule 1: coat protein

Chain AP: 70% 30%

Q1 N4 V5 V6 L7 A8 D9 P14 T18 F19 E20 P21 Q22 N26 P31 A32 E33 W34 W35 E36 K37 Y45 L48 T49 A50 L51 V52 K62 V63 K64 T71 L72 A73 V74 S78 T79 A80 I83 A90 V95 E98 F99 T100 C105 T106 I107 Q108 I113 Y116 N132 Y137

• Molecule 1: coat protein

Chain AQ: 58% 42%

Q1 N4 V5 V6 L7 A8 D9 G10 P14 T18 F19 E20 P21 Q22 Q25 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 Y68 D69 A73 V74 T79 A80 S81 G82 I83 Q84 P85 F91 P94 V95 F96 I97 E98 F99 T100 D103 T106 I107 Q108 Y116 N119 F120 L121 T125 L129 Y137

• Molecule 1: coat protein

Chain AR: 70% 29% •

Q1 I2 A3 N4 A8 D9 G10 P14 F19 E20 P21 Q22 P31 W34 W35 E36 S39 L42 N43 G44 Y45 R46 L51 V52 K62 V63 D69 A73 V74 T75 A76 A80 S81 G82 I83 Q84 P85 A90 T100 T106 I107 Q108 N119 F120 L121 T127 D128 L129 Y137

• Molecule 1: coat protein

Chain AS: 69% 31%

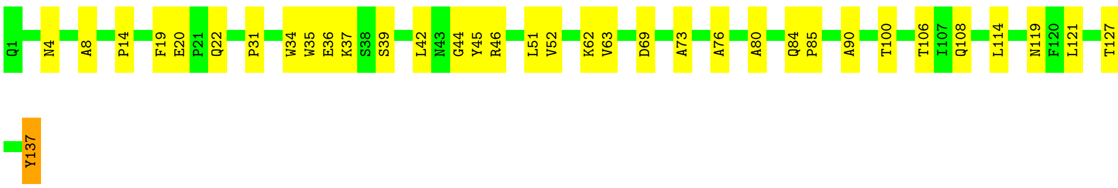
Q1 N4 V5 V6 L7 A8 D9 P14 T18 F19 E20 P21 Q22 N26 P31 A32 E33 W34 W35 E36 K37 Y45 R46 R47 L48 T49 A50 L51 V52 K62 V63 K64 D69 A73 P77 S78 T79 A80 I83 A90 E98 F99 T100 C105 T106 I107 Q108 I113 L121 Q136 Y137

• Molecule 1: coat protein

Chain AT: 63% 37%

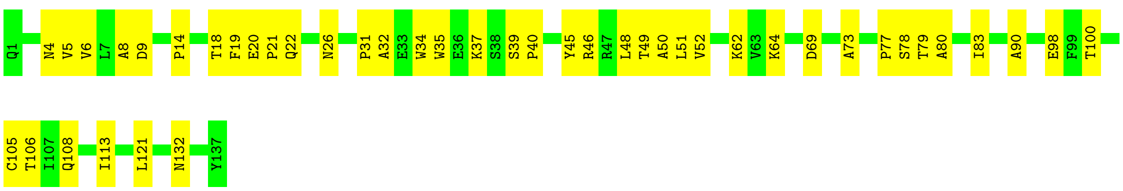
• Molecule 1: coat protein

Chain AU:



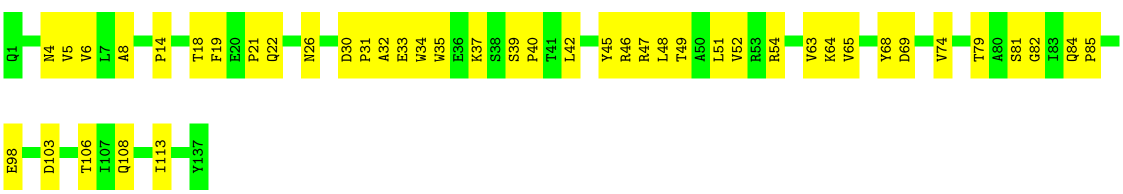
• Molecule 1: coat protein

Chain AV:



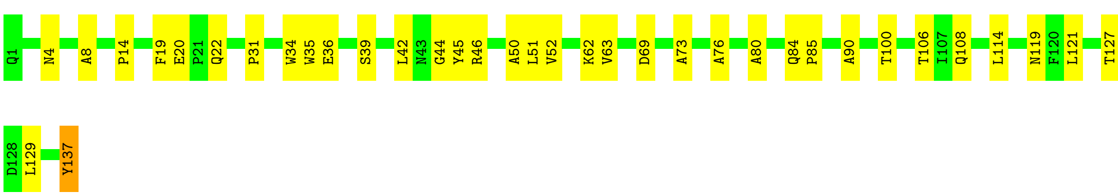
• Molecule 1: coat protein

Chain AW:



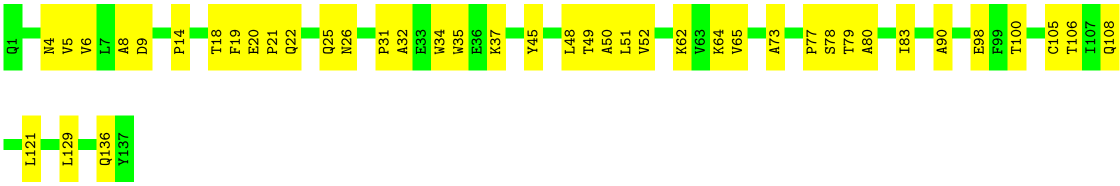
• Molecule 1: coat protein

Chain AX:



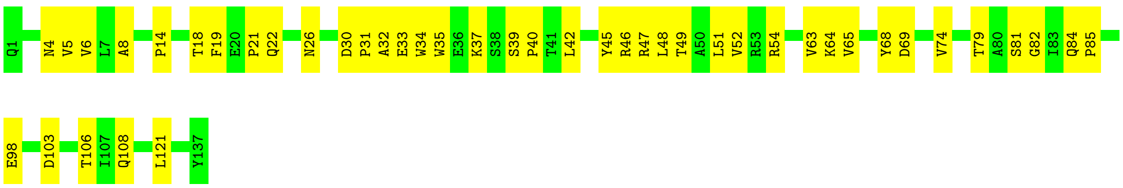
• Molecule 1: coat protein

Chain AY:



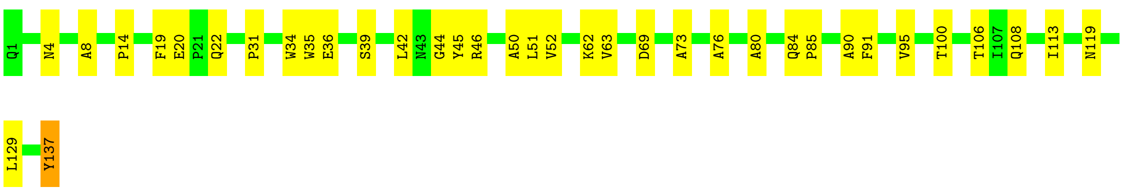
• Molecule 1: coat protein

Chain AZ:



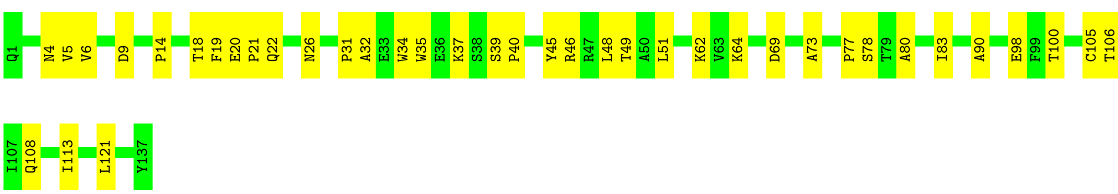
• Molecule 1: coat protein

Chain BA:



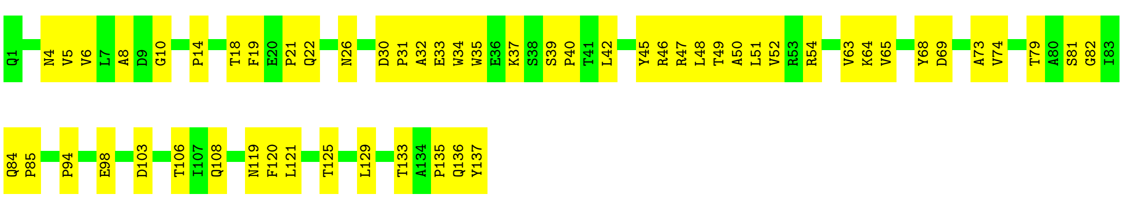
• Molecule 1: coat protein

Chain BB:



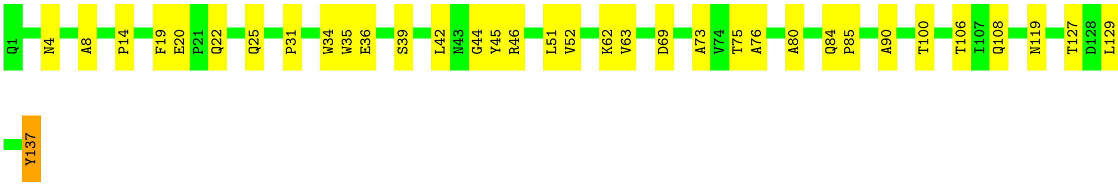
• Molecule 1: coat protein

Chain BC:



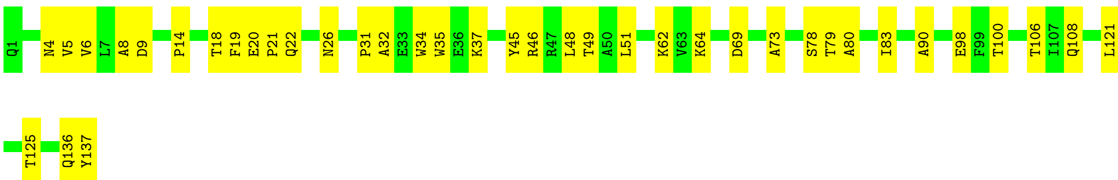
• Molecule 1: coat protein

Chain BD:



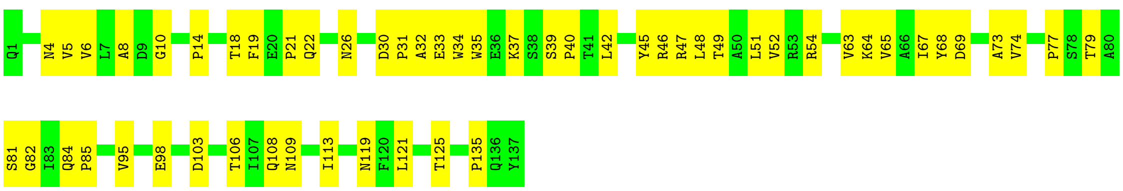
• Molecule 1: coat protein

Chain BE:



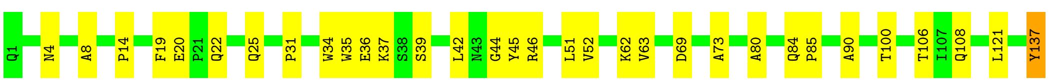
• Molecule 1: coat protein

Chain BF:



• Molecule 1: coat protein

Chain BG:

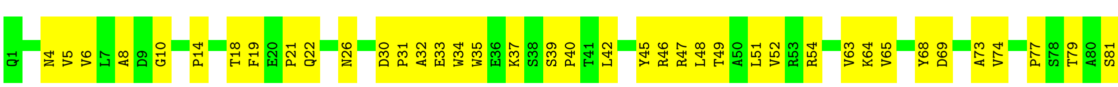


• Molecule 1: coat protein

Chain BH:

• Molecule 1: coat protein

Chain BI:



G82 I83 Q84 P85 E98 D103 T106 I107 Q108 I113 N119 F120 L121 T125 L129 P135 Q136 Y137

• Molecule 1: coat protein

Chain BJ: 71% 28% •

Q1 N4 A8 P14 F19 E20 P21 Q22 P31 W34 W35 E36 S39 L42 N43 G44 Y45 R46 A50 L51 V52 K62 V63 I67 Y68 D69 A73 A76 A80 Q84 P85 A90 F91 V95 T100 L101 T106 I107 Q108 I113 Y116 L121 L129 V130 Y137

• Molecule 1: coat protein

Chain BK: % 66% 34%

Q1 N4 V5 V6 L7 A8 D9 A12 A13 P14 T18 F19 E20 P21 Q22 Q25 N26 P31 A32 E33 W34 W35 E36 K37 Y45 R46 R47 L48 T49 A50 L51 V52 K62 V63 K64 V65 D69 A73 P77 S78 T79 A80 I83 A90 E98 F99 T100 C105 T106 I107 Q108 I113 L129 N132 Q136 Y137

• Molecule 1: coat protein

Chain BL: 69% 31%

Q1 N4 V5 V6 L7 A8 P14 T18 F19 E20 P21 Q22 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 Y68 D69 V74 T79 A80 S81 G82 I83 Q84 P85 E98 D103 T106 I107 Q108 Y137

• Molecule 1: coat protein

Chain BM: % 74% 26% •

Q1 N4 A8 P14 F19 E20 P21 Q22 P31 W34 W35 E36 S39 L42 N43 G44 Y45 R46 L51 V52 K62 V63 D69 A73 P77 A80 Q84 P85 A90 V95 T100 L101 C105 T106 I107 Q108 I113 Y116 L121 V130 Y137

• Molecule 1: coat protein

Chain BN: 74% 26%

Q1 N4 V5 V6 D9 P14 T18 F19 E20 P21 Q22 N26 P31 A32 E33 W34 W35 E36 K37 Y45 R46 R47 L48 T49 A50 L51 K62 V63 K64 D69 A73 P77 S78 T79 A80 S81 G82 I83 A90 E98 F99 T100 T106 I107 Q108

L121 Y137

- Molecule 1: coat protein

Chain BO: 59% 41%

Q1 N4 V5 V6 L7 A8 D9 G10 P14 T18 F19 E20 P21 Q22 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 Y68 D69 A73 V74 P77 S78 T79 A80 S81

G82 I83 Q84 P85 E98 D103 T106 I107 Q108 N119 F120 L121 T125 L129 T133 A134 P135 Q136 Y137

- Molecule 1: coat protein

Chain BP: 73% 26% •

Q1 I2 A3 N4 A8 P14 F19 E20 P21 Q22 P31 W34 W35 E36 K37 S38 S39 L42 N43 G44 Y45 R46 L51 V52 K62 V63 D69 A73 V74 T75 A76 A80 Q84 P85 A90 T100 T106 I107 Q108 I113 T127 V130

Y137

- Molecule 1: coat protein

Chain BQ: 72% 28%

Q1 N4 V5 V6 L7 A8 D9 P14 T18 F19 E20 P21 Q22 N26 P31 A32 E33 W34 W35 E36 K37 Y45 L48 T49 A50 L51 V52 K62 V63 K64 A73 P77 S78 T79 A80 I83 A90 E98 F99 T100 T106 I107 Q108 L121

Q136 Y137

- Molecule 1: coat protein

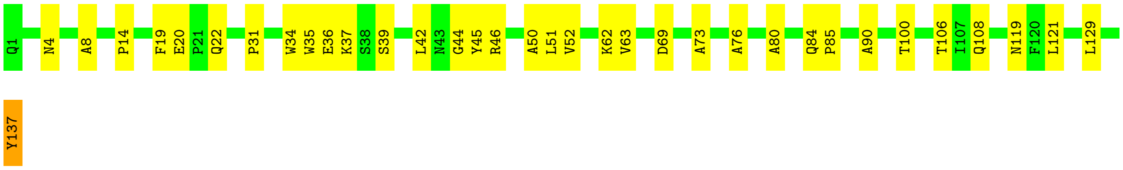
Chain BR: 64% 36%

Q1 N4 V5 V6 L7 A8 D9 G10 P14 T18 F19 E20 P21 Q22 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 Y68 D69 A73 V74 P77 S78 T79 A80 S81

G82 I83 Q84 P85 V95 E98 D103 T106 I107 Q108 L121 T125 P135 Q136 Y137

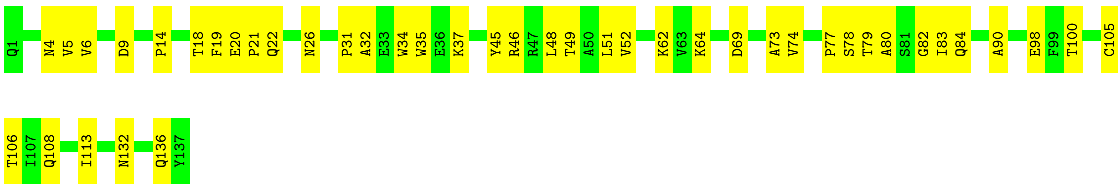
- Molecule 1: coat protein

Chain BS: 74% 25% •



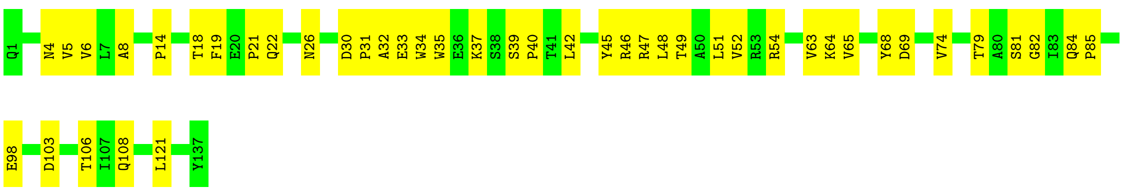
• Molecule 1: coat protein

Chain BT:



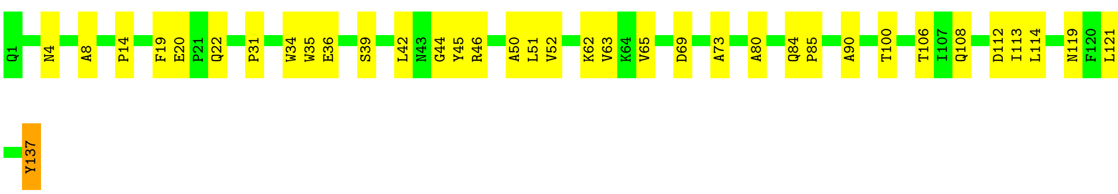
• Molecule 1: coat protein

Chain BU:



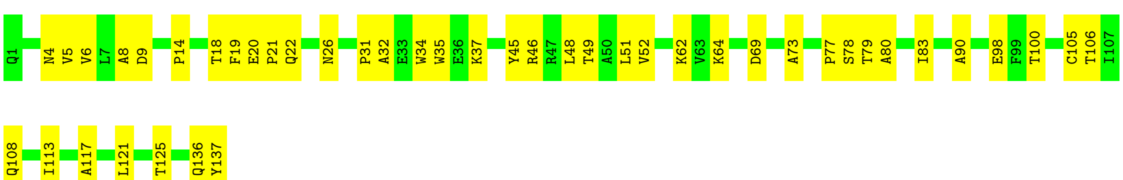
• Molecule 1: coat protein

Chain BV:



• Molecule 1: coat protein

Chain BW:



• Molecule 1: coat protein

Chain BX:

Q1 N4 V5 V6 L7 A8 D9 G10 P14 T18 F19 E20 P21 Q22 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 Y68 D69 A73 V74 T79 A80 S81 G82 I83

Q84 P85 P94 E98 D103 T106 I107 Q108 N119 F120 L121 T125 L129 Y137

- Molecule 1: coat protein

Chain BY: 74% 25% •

Q1 N4 A8 P14 F19 E20 P21 Q22 P31 W34 W35 E36 S39 L42 N43 G44 Y45 R46 L51 V52 K62 V63 D69 A73 A76 A80 S81 Q84 P85 A90 T100 T106 I107 Q108 L114 N119 F120 L121 T127

Y137

- Molecule 1: coat protein

Chain BZ: 69% 31%

Q1 N4 V5 V6 L7 A8 D9 P14 T18 F19 E20 P21 Q22 N26 P31 A32 E33 W34 W35 E36 K37 Y45 R46 R47 L48 T49 A50 L51 V52 K62 V63 K64 V65 D69 A73 P77 S78 T79 A80 I83 A90 V95 E98 F99 T100

C105 T106 I107 Q108 I113 N132 Y137

- Molecule 1: coat protein

Chain CA: 61% 39%

Q1 N4 V5 V6 L7 A8 D9 G10 P14 T18 F19 E20 P21 Q22 N26 D30 P31 A32 E33 W34 W35 E36 K37 S38 S39 P40 T41 L42 Y45 R46 R47 L48 T49 A50 L51 V52 R53 R54 V63 K64 V65 Y68 D69 V74 T79 A80 S81 G82 I83 Q84

P85 F91 P94 V95 F96 I97 E98 D103 T106 I107 Q108 N119 F120 L121 T125 L129 Q136 Y137

- Molecule 1: coat protein

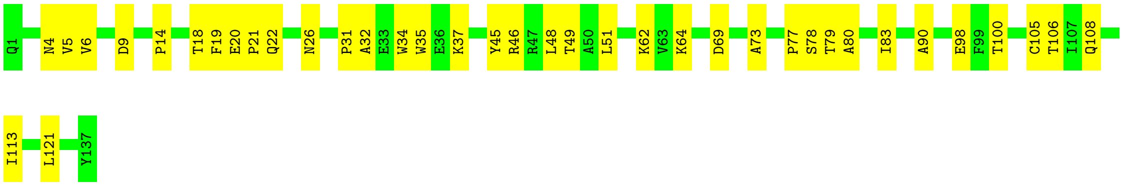
Chain CB: 73% 26% •

Q1 N4 A8 P14 F19 E20 P21 Q22 P31 W34 W35 S39 L42 N43 G44 Y45 R46 A50 L51 V52 K62 V63 D69 A73 A76 A80 S81 G82 I83 Q84 P85 A90 T100 T106 I107 Q108 L114 N119 F120 L121

T127 D128 L129 Y137

- Molecule 1: coat protein

Chain CC: 72% 28%

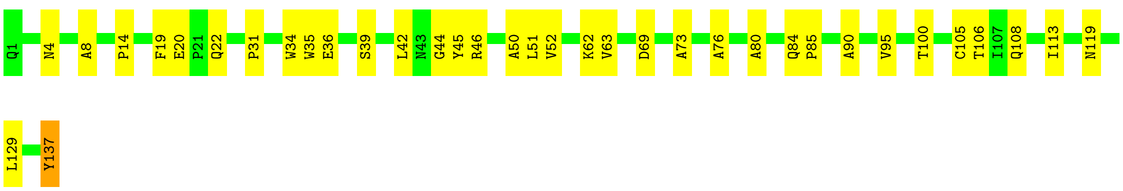


• Molecule 1: coat protein

Chain CD: 63% 37%

• Molecule 1: coat protein

Chain CE: 74% 26% •

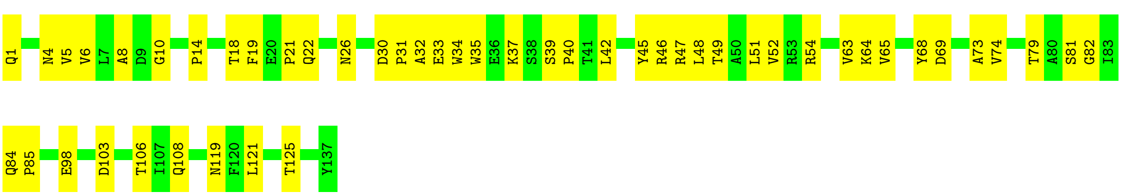


• Molecule 1: coat protein

Chain CF: 70% 30%

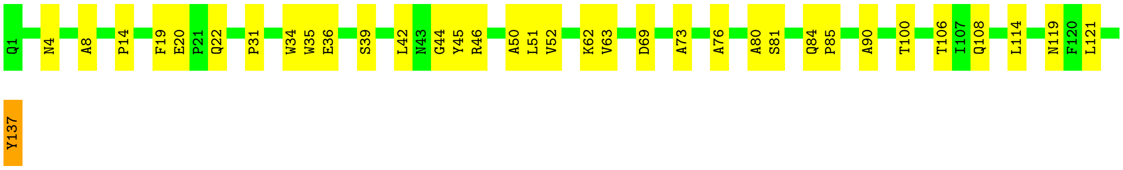
• Molecule 1: coat protein

Chain CG: 64% 36%



• Molecule 1: coat protein

Chain CH: 74% 25% •


Q1
N4
A8
P14
F19
E20
P21
Q22
P31
W34
W35
E36
S39
L42
N43
G44
Y45
R46
A50
L51
V52
K62
V63
D69
A73
A76
A80
S81
Q84
P85
A90
T100
T106
I107
Q108
L114
N119
F120
L121
Y137

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	278.20Å 278.20Å 661.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.00 – 3.70 38.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	64.8 (38.00-3.70) 64.9 (38.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.235 , 0.237 0.238 , 0.240	Depositor DCC
R_{free} test set	5033 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 25.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.026 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.024 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.027 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.024 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.029 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.024 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.043 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	62180	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.32	0/1059	0.53	0/1451
1	AB	0.34	0/1059	0.54	0/1451
1	AC	0.34	0/1059	0.55	0/1451
1	AD	0.33	0/1059	0.53	0/1451
1	AE	0.34	0/1059	0.54	0/1451
1	AF	0.34	0/1059	0.56	0/1451
1	AG	0.33	0/1059	0.53	0/1451
1	AH	0.34	0/1059	0.54	0/1451
1	AI	0.34	0/1059	0.56	0/1451
1	AJ	0.33	0/1059	0.54	0/1451
1	AK	0.34	0/1059	0.54	0/1451
1	AL	0.34	0/1059	0.56	0/1451
1	AM	0.33	0/1059	0.53	0/1451
1	AN	0.34	0/1059	0.54	0/1451
1	AO	0.34	0/1059	0.55	0/1451
1	AP	0.33	0/1059	0.54	0/1451
1	AQ	0.34	0/1059	0.54	0/1451
1	AR	0.34	0/1059	0.55	0/1451
1	AS	0.33	0/1059	0.54	0/1451
1	AT	0.34	0/1059	0.54	0/1451
1	AU	0.34	0/1059	0.55	0/1451
1	AV	0.32	0/1059	0.54	0/1451
1	AW	0.34	0/1059	0.54	0/1451
1	AX	0.34	0/1059	0.56	0/1451
1	AY	0.33	0/1059	0.53	0/1451
1	AZ	0.34	0/1059	0.54	0/1451
1	BA	0.34	0/1059	0.55	0/1451
1	BB	0.33	0/1059	0.53	0/1451
1	BC	0.34	0/1059	0.54	0/1451
1	BD	0.34	0/1059	0.56	0/1451
1	BE	0.33	0/1059	0.53	0/1451
1	BF	0.34	0/1059	0.54	0/1451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	BG	0.34	0/1059	0.55	0/1451
1	BH	0.33	0/1059	0.54	0/1451
1	BI	0.34	0/1059	0.54	0/1451
1	BJ	0.34	0/1059	0.56	0/1451
1	BK	0.33	0/1059	0.53	0/1451
1	BL	0.34	0/1059	0.54	0/1451
1	BM	0.34	0/1059	0.55	0/1451
1	BN	0.33	0/1059	0.53	0/1451
1	BO	0.34	0/1059	0.54	0/1451
1	BP	0.34	0/1059	0.56	0/1451
1	BQ	0.33	0/1059	0.54	0/1451
1	BR	0.34	0/1059	0.54	0/1451
1	BS	0.34	0/1059	0.56	0/1451
1	BT	0.33	0/1059	0.53	0/1451
1	BU	0.34	0/1059	0.54	0/1451
1	BV	0.34	0/1059	0.56	0/1451
1	BW	0.33	0/1059	0.54	0/1451
1	BX	0.34	0/1059	0.54	0/1451
1	BY	0.34	0/1059	0.55	0/1451
1	BZ	0.33	0/1059	0.53	0/1451
1	CA	0.34	0/1059	0.54	0/1451
1	CB	0.34	0/1059	0.55	0/1451
1	CC	0.32	0/1059	0.53	0/1451
1	CD	0.34	0/1059	0.54	0/1451
1	CE	0.34	0/1059	0.55	0/1451
1	CF	0.32	0/1059	0.54	0/1451
1	CG	0.34	0/1059	0.54	0/1451
1	CH	0.34	0/1059	0.55	0/1451
All	All	0.34	0/63540	0.54	0/87060

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	1036	0	1040	31	0
1	AB	1036	0	1040	44	0
1	AC	1036	0	1040	20	0
1	AD	1036	0	1040	53	0
1	AE	1036	0	1040	41	0
1	AF	1036	0	1040	33	0
1	AG	1036	0	1040	22	0
1	AH	1036	0	1040	39	0
1	AI	1036	0	1040	32	0
1	AJ	1036	0	1040	33	0
1	AK	1036	0	1040	46	0
1	AL	1036	0	1040	29	0
1	AM	1036	0	1040	32	0
1	AN	1036	0	1040	41	0
1	AO	1036	0	1040	28	0
1	AP	1036	0	1040	32	0
1	AQ	1036	0	1040	58	0
1	AR	1036	0	1040	40	0
1	AS	1036	0	1040	32	0
1	AT	1036	0	1040	42	0
1	AU	1036	0	1040	29	0
1	AV	1036	0	1040	34	0
1	AW	1036	0	1040	31	0
1	AX	1036	0	1040	30	0
1	AY	1036	0	1040	39	0
1	AZ	1036	0	1040	33	0
1	BA	1036	0	1040	30	0
1	BB	1036	0	1040	25	0
1	BC	1036	0	1040	45	0
1	BD	1036	0	1040	30	0
1	BE	1036	0	1040	31	0
1	BF	1036	0	1040	45	0
1	BG	1036	0	1040	23	0
1	BH	1036	0	1040	46	0
1	BI	1036	0	1040	42	0
1	BJ	1036	0	1040	39	0
1	BK	1036	0	1040	41	0
1	BL	1036	0	1040	33	0
1	BM	1036	0	1040	29	0
1	BN	1036	0	1040	23	0
1	BO	1036	0	1040	43	0
1	BP	1036	0	1040	28	0
1	BQ	1036	0	1040	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	1036	0	1040	39	0
1	BS	1036	0	1040	31	0
1	BT	1036	0	1040	34	0
1	BU	1036	0	1040	32	0
1	BV	1036	0	1040	29	0
1	BW	1036	0	1040	35	0
1	BX	1036	0	1040	40	0
1	BY	1036	0	1040	30	0
1	BZ	1036	0	1040	34	0
1	CA	1036	0	1040	56	0
1	CB	1036	0	1040	34	0
1	CC	1036	0	1040	26	0
1	CD	1036	0	1040	40	0
1	CE	1036	0	1040	32	0
1	CF	1036	0	1040	33	0
1	CG	1036	0	1040	40	0
1	CH	1036	0	1040	29	0
2	AF	1	0	0	0	0
2	AG	1	0	0	0	0
2	AJ	1	0	0	0	0
2	AL	1	0	0	0	0
2	AO	1	0	0	0	0
2	AP	1	0	0	0	0
2	AU	1	0	0	0	0
2	AX	1	0	0	0	0
2	BA	1	0	0	0	0
2	BB	1	0	0	0	0
2	BD	1	0	0	0	0
2	BJ	1	0	0	0	0
2	BM	1	0	0	0	0
2	BN	1	0	0	0	0
2	BP	1	0	0	0	0
2	BV	1	0	0	0	0
2	BY	1	0	0	0	0
2	BZ	1	0	0	0	0
2	CC	1	0	0	0	0
2	CH	1	0	0	0	0
All	All	62180	0	62400	1676	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1676) 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:AD:79:THR:HB	1:AR:80:ALA:HA	1.19	1.16
1:BY:80:ALA:HA	1:CF:79:THR:HB	1.33	1.11
1:BE:79:THR:HB	1:CH:80:ALA:HA	1.31	1.10
1:BH:79:THR:HB	1:CB:80:ALA:HA	1.15	1.09
1:AY:79:THR:HB	1:BD:80:ALA:HA	1.37	1.07
1:AD:79:THR:CB	1:AR:80:ALA:HA	1.90	1.02
1:AA:79:THR:HB	1:AL:80:ALA:HA	1.46	0.98
1:BH:79:THR:CB	1:CB:80:ALA:HA	1.94	0.97
1:BS:80:ALA:HA	1:BT:79:THR:HB	1.48	0.95
1:AJ:79:THR:HB	1:AO:80:ALA:HA	1.48	0.94
1:AI:80:ALA:HA	1:BQ:79:THR:HB	1.52	0.92
1:AU:80:ALA:HA	1:AV:79:THR:HB	1.51	0.91
1:AF:80:ALA:HA	1:BW:79:THR:HB	1.49	0.91
1:BK:108:GLN:NE2	1:BO:10:GLY:O	2.03	0.91
1:BK:79:THR:HB	1:BP:80:ALA:HA	1.53	0.88
1:AQ:85:PRO:HA	1:BF:73:ALA:HB1	1.55	0.88
1:AY:108:GLN:NE2	1:BC:10:GLY:O	2.07	0.86
1:BH:79:THR:HB	1:CB:80:ALA:CA	2.05	0.86
1:AD:79:THR:HB	1:AR:80:ALA:CA	2.04	0.86
1:AB:10:GLY:O	1:BZ:108:GLN:NE2	2.10	0.84
1:AE:4:ASN:HB3	1:AE:21:PRO:HD3	1.60	0.84
1:AW:4:ASN:HB3	1:AW:21:PRO:HD3	1.60	0.84
1:BL:4:ASN:HB3	1:BL:21:PRO:HD3	1.60	0.84
1:CA:4:ASN:HB3	1:CA:21:PRO:HD3	1.60	0.84
1:AT:4:ASN:HB3	1:AT:21:PRO:HD3	1.60	0.83
1:BU:4:ASN:HB3	1:BU:21:PRO:HD3	1.60	0.83
1:AH:4:ASN:HB3	1:AH:21:PRO:HD3	1.60	0.83
1:BF:4:ASN:HB3	1:BF:21:PRO:HD3	1.60	0.83
1:AN:4:ASN:HB3	1:AN:21:PRO:HD3	1.60	0.83
1:BC:4:ASN:HB3	1:BC:21:PRO:HD3	1.60	0.82
1:BO:4:ASN:HB3	1:BO:21:PRO:HD3	1.60	0.82
1:AZ:4:ASN:HB3	1:AZ:21:PRO:HD3	1.60	0.82
1:CG:4:ASN:HB3	1:CG:21:PRO:HD3	1.60	0.82
1:BR:4:ASN:HB3	1:BR:21:PRO:HD3	1.60	0.82
1:AK:4:ASN:HB3	1:AK:21:PRO:HD3	1.60	0.82
1:AQ:4:ASN:HB3	1:AQ:21:PRO:HD3	1.60	0.82
1:AD:108:GLN:NE2	1:AQ:10:GLY:O	2.13	0.82
1:AB:4:ASN:HB3	1:AB:21:PRO:HD3	1.60	0.81
1:BX:4:ASN:HB3	1:BX:21:PRO:HD3	1.60	0.81
1:AY:31:PRO:HB3	1:AY:51:LEU:HB2	1.63	0.81
1:CD:4:ASN:HB3	1:CD:21:PRO:HD3	1.60	0.81
1:AA:31:PRO:HB3	1:AA:51:LEU:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BN:31:PRO:HB3	1:BN:51:LEU:HB2	1.63	0.81
1:CC:31:PRO:HB3	1:CC:51:LEU:HB2	1.63	0.81
1:BW:31:PRO:HB3	1:BW:51:LEU:HB2	1.63	0.81
1:AJ:31:PRO:HB3	1:AJ:51:LEU:HB2	1.63	0.80
1:AP:31:PRO:HB3	1:AP:51:LEU:HB2	1.63	0.80
1:BI:4:ASN:HB3	1:BI:21:PRO:HD3	1.60	0.80
1:AV:31:PRO:HB3	1:AV:51:LEU:HB2	1.63	0.80
1:AT:10:GLY:O	1:AV:108:GLN:NE2	2.15	0.80
1:BQ:31:PRO:HB3	1:BQ:51:LEU:HB2	1.63	0.80
1:AS:31:PRO:HB3	1:AS:51:LEU:HB2	1.63	0.80
1:BK:31:PRO:HB3	1:BK:51:LEU:HB2	1.63	0.80
1:BE:31:PRO:HB3	1:BE:51:LEU:HB2	1.63	0.80
1:AD:31:PRO:HB3	1:AD:51:LEU:HB2	1.63	0.79
1:BH:31:PRO:HB3	1:BH:51:LEU:HB2	1.63	0.79
1:BH:5:VAL:HG12	1:CA:125:THR:HG21	1.65	0.79
1:CF:31:PRO:HB3	1:CF:51:LEU:HB2	1.63	0.79
1:AG:31:PRO:HB3	1:AG:51:LEU:HB2	1.63	0.78
1:AM:31:PRO:HB3	1:AM:51:LEU:HB2	1.63	0.78
1:BT:31:PRO:HB3	1:BT:51:LEU:HB2	1.63	0.78
1:BZ:31:PRO:HB3	1:BZ:51:LEU:HB2	1.63	0.78
1:BB:31:PRO:HB3	1:BB:51:LEU:HB2	1.63	0.78
1:AK:79:THR:HG23	1:AK:81:SER:H	1.49	0.78
1:AQ:79:THR:HG23	1:AQ:81:SER:H	1.49	0.78
1:AT:79:THR:HG23	1:AT:81:SER:H	1.49	0.78
1:AW:79:THR:HG23	1:AW:81:SER:H	1.49	0.77
1:CG:79:THR:HG23	1:CG:81:SER:H	1.49	0.77
1:AN:79:THR:HG23	1:AN:81:SER:H	1.49	0.77
1:BO:79:THR:HG23	1:BO:81:SER:H	1.49	0.77
1:AQ:79:THR:HB	1:BF:77:PRO:CB	2.15	0.77
1:AJ:108:GLN:NE2	1:AN:10:GLY:O	2.17	0.77
1:BF:79:THR:HG23	1:BF:81:SER:H	1.49	0.77
1:AH:79:THR:HG23	1:AH:81:SER:H	1.49	0.76
1:AK:85:PRO:HA	1:AN:73:ALA:HB1	1.68	0.76
1:AZ:79:THR:HG23	1:AZ:81:SER:H	1.49	0.76
1:BU:79:THR:HG23	1:BU:81:SER:H	1.49	0.76
1:CD:79:THR:HG23	1:CD:81:SER:H	1.49	0.76
1:AI:52:VAL:HG22	1:AI:63:VAL:HG22	1.68	0.76
1:BD:52:VAL:HG22	1:BD:63:VAL:HG22	1.68	0.76
1:BI:79:THR:HG23	1:BI:81:SER:H	1.49	0.76
1:BL:79:THR:HG23	1:BL:81:SER:H	1.49	0.76
1:AC:80:ALA:HA	1:BZ:79:THR:HB	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:79:THR:HB	1:CE:80:ALA:HA	1.67	0.76
1:BV:52:VAL:HG22	1:BV:63:VAL:HG22	1.68	0.76
1:CB:52:VAL:HG22	1:CB:63:VAL:HG22	1.68	0.76
1:AE:79:THR:HG23	1:AE:81:SER:H	1.49	0.76
1:BC:79:THR:HG23	1:BC:81:SER:H	1.49	0.76
1:CA:79:THR:HG23	1:CA:81:SER:H	1.49	0.76
1:AR:52:VAL:HG22	1:AR:63:VAL:HG22	1.68	0.76
1:BJ:52:VAL:HG22	1:BJ:63:VAL:HG22	1.68	0.76
1:BR:79:THR:HG23	1:BR:81:SER:H	1.49	0.76
1:CH:52:VAL:HG22	1:CH:63:VAL:HG22	1.68	0.76
1:AC:52:VAL:HG22	1:AC:63:VAL:HG22	1.68	0.75
1:BP:52:VAL:HG22	1:BP:63:VAL:HG22	1.68	0.75
1:BX:79:THR:HG23	1:BX:81:SER:H	1.49	0.75
1:AB:79:THR:HG23	1:AB:81:SER:H	1.49	0.75
1:BA:52:VAL:HG22	1:BA:63:VAL:HG22	1.68	0.75
1:AX:52:VAL:HG22	1:AX:63:VAL:HG22	1.68	0.75
1:AF:52:VAL:HG22	1:AF:63:VAL:HG22	1.68	0.75
1:BM:52:VAL:HG22	1:BM:63:VAL:HG22	1.68	0.75
1:CE:52:VAL:HG22	1:CE:63:VAL:HG22	1.68	0.75
1:AO:52:VAL:HG22	1:AO:63:VAL:HG22	1.68	0.75
1:BY:52:VAL:HG22	1:BY:63:VAL:HG22	1.68	0.74
1:BG:52:VAL:HG22	1:BG:63:VAL:HG22	1.68	0.74
1:BS:52:VAL:HG22	1:BS:63:VAL:HG22	1.68	0.74
1:AD:6:VAL:HG22	1:AD:18:THR:HG22	1.70	0.74
1:AL:52:VAL:HG22	1:AL:63:VAL:HG22	1.68	0.74
1:AU:52:VAL:HG22	1:AU:63:VAL:HG22	1.68	0.74
1:BN:6:VAL:HG22	1:BN:18:THR:HG22	1.70	0.73
1:AP:6:VAL:HG22	1:AP:18:THR:HG22	1.70	0.73
1:CC:6:VAL:HG22	1:CC:18:THR:HG22	1.70	0.73
1:AG:6:VAL:HG22	1:AG:18:THR:HG22	1.70	0.73
1:AA:6:VAL:HG22	1:AA:18:THR:HG22	1.70	0.73
1:AS:6:VAL:HG22	1:AS:18:THR:HG22	1.70	0.73
1:AY:6:VAL:HG22	1:AY:18:THR:HG22	1.70	0.73
1:BQ:6:VAL:HG22	1:BQ:18:THR:HG22	1.70	0.73
1:BH:6:VAL:HG22	1:BH:18:THR:HG22	1.70	0.73
1:AJ:6:VAL:HG22	1:AJ:18:THR:HG22	1.70	0.73
1:BW:6:VAL:HG22	1:BW:18:THR:HG22	1.70	0.73
1:AM:6:VAL:HG22	1:AM:18:THR:HG22	1.70	0.72
1:BB:6:VAL:HG22	1:BB:18:THR:HG22	1.70	0.72
1:AX:80:ALA:HB2	1:BZ:80:ALA:HA	1.70	0.72
1:BX:10:GLY:O	1:CF:108:GLN:NE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BZ:6:VAL:HG22	1:BZ:18:THR:HG22	1.70	0.72
1:AV:6:VAL:HG22	1:AV:18:THR:HG22	1.70	0.72
1:BE:5:VAL:HG12	1:CG:125:THR:HG21	1.70	0.72
1:AM:5:VAL:HG12	1:BI:125:THR:HG21	1.71	0.72
1:BK:6:VAL:HG22	1:BK:18:THR:HG22	1.70	0.72
1:BY:80:ALA:HA	1:CF:79:THR:CB	2.17	0.72
1:AX:80:ALA:CB	1:BZ:80:ALA:HA	2.19	0.72
1:AU:80:ALA:CB	1:BW:80:ALA:HA	2.20	0.71
1:BT:6:VAL:HG22	1:BT:18:THR:HG22	1.70	0.71
1:BE:6:VAL:HG22	1:BE:18:THR:HG22	1.70	0.71
1:AS:5:VAL:HG12	1:CD:125:THR:HG21	1.72	0.71
1:AV:80:ALA:HA	1:CB:80:ALA:CB	2.21	0.71
1:BA:80:ALA:CB	1:CC:80:ALA:HA	2.21	0.71
1:CF:6:VAL:HG22	1:CF:18:THR:HG22	1.70	0.71
1:BH:108:GLN:NE2	1:CA:10:GLY:O	2.23	0.71
1:AV:80:ALA:HA	1:CB:80:ALA:HB2	1.71	0.70
1:BD:31:PRO:HB3	1:BD:51:LEU:HB2	1.74	0.70
1:AA:5:VAL:HG12	1:AK:125:THR:HG21	1.73	0.70
1:AI:31:PRO:HB3	1:AI:51:LEU:HB2	1.73	0.70
1:BE:79:THR:CB	1:CH:80:ALA:HA	2.18	0.70
1:BP:31:PRO:HB3	1:BP:51:LEU:HB2	1.73	0.70
1:BM:31:PRO:HB3	1:BM:51:LEU:HB2	1.73	0.70
1:AR:31:PRO:HB3	1:AR:51:LEU:HB2	1.73	0.70
1:AX:31:PRO:HB3	1:AX:51:LEU:HB2	1.74	0.70
1:AY:5:VAL:HG12	1:BC:125:THR:HG21	1.74	0.70
1:AC:31:PRO:HB3	1:AC:51:LEU:HB2	1.74	0.69
1:AF:31:PRO:HB3	1:AF:51:LEU:HB2	1.73	0.69
1:AU:73:ALA:HB2	1:AU:90:ALA:HB2	1.75	0.69
1:CC:73:ALA:HB2	1:CC:90:ALA:HB2	1.75	0.69
1:AI:80:ALA:CB	1:BK:80:ALA:HA	2.23	0.69
1:AD:73:ALA:HB2	1:AD:90:ALA:HB2	1.75	0.69
1:AF:73:ALA:HB2	1:AF:90:ALA:HB2	1.75	0.69
1:AL:31:PRO:HB3	1:AL:51:LEU:HB2	1.73	0.69
1:AM:73:ALA:HB2	1:AM:90:ALA:HB2	1.75	0.69
1:BT:73:ALA:HB2	1:BT:90:ALA:HB2	1.75	0.69
1:AG:73:ALA:HB2	1:AG:90:ALA:HB2	1.75	0.69
1:AV:73:ALA:HB2	1:AV:90:ALA:HB2	1.75	0.69
1:BD:73:ALA:HB2	1:BD:90:ALA:HB2	1.75	0.69
1:CE:31:PRO:HB3	1:CE:51:LEU:HB2	1.74	0.69
1:CH:31:PRO:HB3	1:CH:51:LEU:HB2	1.73	0.69
1:AH:125:THR:HG21	1:BQ:5:VAL:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:73:ALA:HB2	1:BB:90:ALA:HB2	1.75	0.69
1:BG:31:PRO:HB3	1:BG:51:LEU:HB2	1.73	0.69
1:BJ:31:PRO:HB3	1:BJ:51:LEU:HB2	1.73	0.69
1:BS:73:ALA:HB2	1:BS:90:ALA:HB2	1.75	0.69
1:AR:73:ALA:HB2	1:AR:90:ALA:HB2	1.75	0.69
1:BB:80:ALA:HA	1:CH:80:ALA:HB2	1.75	0.69
1:BH:73:ALA:HB2	1:BH:90:ALA:HB2	1.75	0.69
1:BM:73:ALA:HB2	1:BM:90:ALA:HB2	1.75	0.69
1:BW:73:ALA:HB2	1:BW:90:ALA:HB2	1.75	0.69
1:CE:73:ALA:HB2	1:CE:90:ALA:HB2	1.75	0.69
1:CF:73:ALA:HB2	1:CF:90:ALA:HB2	1.75	0.69
1:AJ:73:ALA:HB2	1:AJ:90:ALA:HB2	1.75	0.69
1:AY:73:ALA:HB2	1:AY:90:ALA:HB2	1.75	0.69
1:BS:31:PRO:HB3	1:BS:51:LEU:HB2	1.73	0.69
1:BY:73:ALA:HB2	1:BY:90:ALA:HB2	1.75	0.69
1:CB:31:PRO:HB3	1:CB:51:LEU:HB2	1.74	0.69
1:BV:31:PRO:HB3	1:BV:51:LEU:HB2	1.73	0.69
1:AI:73:ALA:HB2	1:AI:90:ALA:HB2	1.75	0.68
1:AL:73:ALA:HB2	1:AL:90:ALA:HB2	1.75	0.68
1:BA:73:ALA:HB2	1:BA:90:ALA:HB2	1.75	0.68
1:BG:73:ALA:HB2	1:BG:90:ALA:HB2	1.75	0.68
1:BK:73:ALA:HB2	1:BK:90:ALA:HB2	1.75	0.68
1:AO:73:ALA:HB2	1:AO:90:ALA:HB2	1.75	0.68
1:BA:31:PRO:HB3	1:BA:51:LEU:HB2	1.73	0.68
1:BV:73:ALA:HB2	1:BV:90:ALA:HB2	1.75	0.68
1:CB:73:ALA:HB2	1:CB:90:ALA:HB2	1.75	0.68
1:AO:31:PRO:HB3	1:AO:51:LEU:HB2	1.73	0.68
1:BP:73:ALA:HB2	1:BP:90:ALA:HB2	1.75	0.68
1:BY:31:PRO:HB3	1:BY:51:LEU:HB2	1.74	0.68
1:AX:73:ALA:HB2	1:AX:90:ALA:HB2	1.75	0.68
1:BQ:73:ALA:HB2	1:BQ:90:ALA:HB2	1.75	0.68
1:AD:74:VAL:O	1:AR:83:ILE:HB	1.94	0.68
1:AM:79:THR:HB	1:BJ:80:ALA:HA	1.75	0.68
1:AU:31:PRO:HB3	1:AU:51:LEU:HB2	1.73	0.68
1:BE:73:ALA:HB2	1:BE:90:ALA:HB2	1.75	0.68
1:BF:31:PRO:HB3	1:BF:51:LEU:HB2	1.76	0.68
1:BR:73:ALA:HB1	1:BU:85:PRO:HA	1.75	0.68
1:AC:73:ALA:HB2	1:AC:90:ALA:HB2	1.75	0.67
1:AD:19:PHE:HB3	1:AD:34:TRP:HB3	1.77	0.67
1:AH:31:PRO:HB3	1:AH:51:LEU:HB2	1.76	0.67
1:CD:31:PRO:HB3	1:CD:51:LEU:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:73:ALA:HB2	1:CH:90:ALA:HB2	1.75	0.67
1:AS:80:ALA:HA	1:BY:80:ALA:CB	2.24	0.67
1:BX:125:THR:HG21	1:CF:5:VAL:HG12	1.75	0.67
1:CA:31:PRO:HB3	1:CA:51:LEU:HB2	1.77	0.67
1:AN:31:PRO:HB3	1:AN:51:LEU:HB2	1.77	0.67
1:AQ:31:PRO:HB3	1:AQ:51:LEU:HB2	1.77	0.67
1:AY:80:ALA:HA	1:CE:80:ALA:CB	2.25	0.67
1:BL:31:PRO:HB3	1:BL:51:LEU:HB2	1.77	0.67
1:AA:73:ALA:HB2	1:AA:90:ALA:HB2	1.75	0.67
1:AB:73:ALA:HB1	1:CA:85:PRO:HA	1.76	0.67
1:AH:10:GLY:O	1:BQ:108:GLN:NE2	2.27	0.67
1:AM:19:PHE:HB3	1:AM:34:TRP:HB3	1.77	0.67
1:BT:19:PHE:HB3	1:BT:34:TRP:HB3	1.77	0.67
1:BZ:73:ALA:HB2	1:BZ:90:ALA:HB2	1.75	0.67
1:AJ:19:PHE:HB3	1:AJ:34:TRP:HB3	1.77	0.67
1:AS:19:PHE:HB3	1:AS:34:TRP:HB3	1.77	0.67
1:BR:10:GLY:O	1:BT:108:GLN:NE2	2.27	0.67
1:AA:19:PHE:HB3	1:AA:34:TRP:HB3	1.77	0.67
1:AY:19:PHE:HB3	1:AY:34:TRP:HB3	1.77	0.67
1:BC:31:PRO:HB3	1:BC:51:LEU:HB2	1.77	0.67
1:AF:113:ILE:HG13	1:BJ:95:VAL:CG2	2.24	0.67
1:AK:31:PRO:HB3	1:AK:51:LEU:HB2	1.77	0.67
1:BB:19:PHE:HB3	1:BB:34:TRP:HB3	1.77	0.67
1:AT:31:PRO:HB3	1:AT:51:LEU:HB2	1.77	0.67
1:BJ:73:ALA:HB2	1:BJ:90:ALA:HB2	1.75	0.67
1:CF:19:PHE:HB3	1:CF:34:TRP:HB3	1.77	0.67
1:AB:31:PRO:HB3	1:AB:51:LEU:HB2	1.77	0.66
1:BO:31:PRO:HB3	1:BO:51:LEU:HB2	1.77	0.66
1:CC:19:PHE:HB3	1:CC:34:TRP:HB3	1.77	0.66
1:AT:85:PRO:HA	1:CD:73:ALA:HB1	1.77	0.66
1:AD:129:LEU:HD21	1:AQ:50:ALA:HB1	1.78	0.66
1:AP:73:ALA:HB2	1:AP:90:ALA:HB2	1.75	0.66
1:BN:73:ALA:HB2	1:BN:90:ALA:HB2	1.75	0.66
1:AE:31:PRO:HB3	1:AE:51:LEU:HB2	1.77	0.66
1:AV:19:PHE:HB3	1:AV:34:TRP:HB3	1.77	0.66
1:CG:31:PRO:HB3	1:CG:51:LEU:HB2	1.76	0.66
1:BK:19:PHE:HB3	1:BK:34:TRP:HB3	1.77	0.66
1:AS:73:ALA:HB2	1:AS:90:ALA:HB2	1.75	0.66
1:AZ:31:PRO:HB3	1:AZ:51:LEU:HB2	1.77	0.66
1:BQ:19:PHE:HB3	1:BQ:34:TRP:HB3	1.77	0.66
1:AE:125:THR:HG21	1:BW:5:VAL:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:80:ALA:HB3	1:BK:80:ALA:HA	1.76	0.66
1:AP:19:PHE:HB3	1:AP:34:TRP:HB3	1.77	0.66
1:BE:19:PHE:HB3	1:BE:34:TRP:HB3	1.77	0.66
1:AG:19:PHE:HB3	1:AG:34:TRP:HB3	1.77	0.66
1:BU:31:PRO:HB3	1:BU:51:LEU:HB2	1.77	0.66
1:BW:19:PHE:HB3	1:BW:34:TRP:HB3	1.77	0.66
1:CH:19:PHE:HB3	1:CH:34:TRP:HB3	1.78	0.66
1:BY:19:PHE:HB3	1:BY:34:TRP:HB3	1.78	0.65
1:BZ:19:PHE:HB3	1:BZ:34:TRP:HB3	1.77	0.65
1:AU:19:PHE:HB3	1:AU:34:TRP:HB3	1.78	0.65
1:AW:31:PRO:HB3	1:AW:51:LEU:HB2	1.77	0.65
1:BH:80:ALA:HB3	1:CB:81:SER:OG	1.96	0.65
1:AY:79:THR:CB	1:BD:80:ALA:HA	2.20	0.65
1:BI:31:PRO:HB3	1:BI:51:LEU:HB2	1.77	0.65
1:BK:5:VAL:HG12	1:BO:125:THR:HG21	1.78	0.65
1:BN:19:PHE:HB3	1:BN:34:TRP:HB3	1.77	0.65
1:BP:19:PHE:HB3	1:BP:34:TRP:HB3	1.78	0.65
1:CB:19:PHE:HB3	1:CB:34:TRP:HB3	1.78	0.65
1:AF:19:PHE:HB3	1:AF:34:TRP:HB3	1.78	0.65
1:AL:19:PHE:HB3	1:AL:34:TRP:HB3	1.78	0.65
1:AC:19:PHE:HB3	1:AC:34:TRP:HB3	1.78	0.65
1:AR:19:PHE:HB3	1:AR:34:TRP:HB3	1.78	0.65
1:BA:22:GLN:HG3	1:BA:35:TRP:CD2	2.32	0.65
1:BY:22:GLN:HG3	1:BY:35:TRP:CD2	2.32	0.65
1:AF:22:GLN:HG3	1:AF:35:TRP:CD2	2.32	0.65
1:AI:19:PHE:HB3	1:AI:34:TRP:HB3	1.78	0.65
1:AM:80:ALA:HA	1:BS:80:ALA:CB	2.27	0.65
1:AM:108:GLN:NE2	1:BI:10:GLY:O	2.30	0.65
1:BM:22:GLN:HG3	1:BM:35:TRP:CD2	2.32	0.65
1:BS:22:GLN:HG3	1:BS:35:TRP:CD2	2.32	0.65
1:AS:108:GLN:NE2	1:CD:10:GLY:O	2.30	0.65
1:BH:19:PHE:HB3	1:BH:34:TRP:HB3	1.77	0.65
1:BR:31:PRO:HB3	1:BR:51:LEU:HB2	1.77	0.65
1:BV:19:PHE:HB3	1:BV:34:TRP:HB3	1.78	0.65
1:BX:31:PRO:HB3	1:BX:51:LEU:HB2	1.77	0.65
1:CH:22:GLN:HG3	1:CH:35:TRP:CD2	2.32	0.65
1:AD:5:VAL:HG12	1:AQ:125:THR:HG21	1.78	0.65
1:AI:22:GLN:HG3	1:AI:35:TRP:CD2	2.32	0.65
1:AO:22:GLN:HG3	1:AO:35:TRP:CD2	2.32	0.65
1:AO:42:LEU:HA	1:AO:45:TYR:CD2	2.32	0.65
1:AR:42:LEU:HA	1:AR:45:TYR:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:80:ALA:HA	1:CH:80:ALA:CB	2.27	0.65
1:BG:19:PHE:HB3	1:BG:34:TRP:HB3	1.78	0.65
1:BS:42:LEU:HA	1:BS:45:TYR:CD2	2.32	0.65
1:BY:42:LEU:HA	1:BY:45:TYR:CD2	2.32	0.65
1:AL:42:LEU:HA	1:AL:45:TYR:CD2	2.32	0.65
1:AN:85:PRO:HA	1:BI:73:ALA:HB1	1.79	0.65
1:AO:19:PHE:HB3	1:AO:34:TRP:HB3	1.78	0.65
1:AR:22:GLN:HG3	1:AR:35:TRP:CD2	2.32	0.65
1:BM:42:LEU:HA	1:BM:45:TYR:CD2	2.32	0.64
1:AM:80:ALA:HA	1:BS:80:ALA:HB2	1.79	0.64
1:AX:22:GLN:HG3	1:AX:35:TRP:CD2	2.32	0.64
1:BG:22:GLN:HG3	1:BG:35:TRP:CD2	2.32	0.64
1:AC:22:GLN:HG3	1:AC:35:TRP:CD2	2.32	0.64
1:AI:42:LEU:HA	1:AI:45:TYR:CD2	2.32	0.64
1:BJ:22:GLN:HG3	1:BJ:35:TRP:CD2	2.32	0.64
1:CB:42:LEU:HA	1:CB:45:TYR:CD2	2.32	0.64
1:AX:19:PHE:HB3	1:AX:34:TRP:HB3	1.78	0.64
1:AX:42:LEU:HA	1:AX:45:TYR:CD2	2.32	0.64
1:BD:22:GLN:HG3	1:BD:35:TRP:CD2	2.32	0.64
1:BM:19:PHE:HB3	1:BM:34:TRP:HB3	1.78	0.64
1:BV:22:GLN:HG3	1:BV:35:TRP:CD2	2.32	0.64
1:BG:42:LEU:HA	1:BG:45:TYR:CD2	2.32	0.64
1:CE:19:PHE:HB3	1:CE:34:TRP:HB3	1.78	0.64
1:CE:42:LEU:HA	1:CE:45:TYR:CD2	2.32	0.64
1:AC:42:LEU:HA	1:AC:45:TYR:CD2	2.32	0.64
1:AF:42:LEU:HA	1:AF:45:TYR:CD2	2.32	0.64
1:AF:130:VAL:HG13	1:BJ:101:LEU:HD11	1.80	0.64
1:AI:76:ALA:HB2	1:BK:77:PRO:HB2	1.80	0.64
1:AU:42:LEU:HA	1:AU:45:TYR:CD2	2.32	0.64
1:BJ:42:LEU:HA	1:BJ:45:TYR:CD2	2.32	0.64
1:AQ:106:THR:HG22	1:AQ:108:GLN:H	1.63	0.64
1:AU:22:GLN:HG3	1:AU:35:TRP:CD2	2.32	0.64
1:AU:80:ALA:HB2	1:BW:80:ALA:HA	1.78	0.64
1:BU:106:THR:HG22	1:BU:108:GLN:H	1.63	0.64
1:BP:22:GLN:HG3	1:BP:35:TRP:CD2	2.32	0.64
1:CB:22:GLN:HG3	1:CB:35:TRP:CD2	2.32	0.64
1:CE:22:GLN:HG3	1:CE:35:TRP:CD2	2.32	0.64
1:AH:106:THR:HG22	1:AH:108:GLN:H	1.63	0.64
1:AZ:106:THR:HG22	1:AZ:108:GLN:H	1.63	0.64
1:BV:42:LEU:HA	1:BV:45:TYR:CD2	2.32	0.64
1:CF:62:LYS:HG2	1:CF:100:THR:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:62:LYS:HG2	1:BB:100:THR:HG22	1.80	0.64
1:BD:42:LEU:HA	1:BD:45:TYR:CD2	2.32	0.64
1:BP:42:LEU:HA	1:BP:45:TYR:CD2	2.32	0.64
1:AA:62:LYS:HG2	1:AA:100:THR:HG22	1.80	0.63
1:AB:125:THR:HG21	1:BZ:5:VAL:HG12	1.80	0.63
1:AR:80:ALA:HB2	1:BT:80:ALA:HA	1.80	0.63
1:AS:62:LYS:HG2	1:AS:100:THR:HG22	1.80	0.63
1:BA:19:PHE:HB3	1:BA:34:TRP:HB3	1.78	0.63
1:BA:42:LEU:HA	1:BA:45:TYR:CD2	2.32	0.63
1:BD:19:PHE:HB3	1:BD:34:TRP:HB3	1.78	0.63
1:BD:62:LYS:HG2	1:BD:100:THR:HG22	1.80	0.63
1:BN:62:LYS:HG2	1:BN:100:THR:HG22	1.80	0.63
1:BV:62:LYS:HG2	1:BV:100:THR:HG22	1.80	0.63
1:CH:42:LEU:HA	1:CH:45:TYR:CD2	2.32	0.63
1:AK:106:THR:HG22	1:AK:108:GLN:H	1.63	0.63
1:AL:22:GLN:HG3	1:AL:35:TRP:CD2	2.32	0.63
1:AL:62:LYS:HG2	1:AL:100:THR:HG22	1.80	0.63
1:AY:62:LYS:HG2	1:AY:100:THR:HG22	1.80	0.63
1:BR:106:THR:HG22	1:BR:108:GLN:H	1.63	0.63
1:CB:62:LYS:HG2	1:CB:100:THR:HG22	1.80	0.63
1:CG:106:THR:HG22	1:CG:108:GLN:H	1.63	0.63
1:AT:73:ALA:HB1	1:AW:85:PRO:HA	1.80	0.63
1:BJ:19:PHE:HB3	1:BJ:34:TRP:HB3	1.78	0.63
1:AN:106:THR:HG22	1:AN:108:GLN:H	1.63	0.63
1:BD:80:ALA:HB2	1:CF:80:ALA:HA	1.78	0.63
1:AB:106:THR:HG22	1:AB:108:GLN:H	1.63	0.63
1:BE:121:LEU:HD12	1:CG:121:LEU:HD12	1.80	0.63
1:BI:106:THR:HG22	1:BI:108:GLN:H	1.63	0.63
1:BJ:62:LYS:HG2	1:BJ:100:THR:HG22	1.80	0.63
1:AJ:62:LYS:HG2	1:AJ:100:THR:HG22	1.80	0.63
1:BK:62:LYS:HG2	1:BK:100:THR:HG22	1.80	0.63
1:BT:62:LYS:HG2	1:BT:100:THR:HG22	1.80	0.63
1:BW:62:LYS:HG2	1:BW:100:THR:HG22	1.80	0.63
1:AC:62:LYS:HG2	1:AC:100:THR:HG22	1.80	0.63
1:BX:106:THR:HG22	1:BX:108:GLN:H	1.63	0.63
1:AR:62:LYS:HG2	1:AR:100:THR:HG22	1.80	0.62
1:AS:80:ALA:HA	1:BY:80:ALA:HB2	1.80	0.62
1:BC:106:THR:HG22	1:BC:108:GLN:H	1.63	0.62
1:BF:106:THR:HG22	1:BF:108:GLN:H	1.63	0.62
1:BO:106:THR:HG22	1:BO:108:GLN:H	1.63	0.62
1:BS:19:PHE:HB3	1:BS:34:TRP:HB3	1.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BS:62:LYS:HG2	1:BS:100:THR:HG22	1.80	0.62
1:BZ:62:LYS:HG2	1:BZ:100:THR:HG22	1.80	0.62
1:CC:62:LYS:HG2	1:CC:100:THR:HG22	1.80	0.62
1:AD:62:LYS:HG2	1:AD:100:THR:HG22	1.80	0.62
1:AG:62:LYS:HG2	1:AG:100:THR:HG22	1.80	0.62
1:AP:62:LYS:HG2	1:AP:100:THR:HG22	1.80	0.62
1:AT:106:THR:HG22	1:AT:108:GLN:H	1.63	0.62
1:BA:62:LYS:HG2	1:BA:100:THR:HG22	1.80	0.62
1:AH:73:ALA:HB1	1:BR:85:PRO:HA	1.81	0.62
1:AO:62:LYS:HG2	1:AO:100:THR:HG22	1.80	0.62
1:AV:62:LYS:HG2	1:AV:100:THR:HG22	1.80	0.62
1:BL:106:THR:HG22	1:BL:108:GLN:H	1.63	0.62
1:AT:125:THR:HG21	1:AV:5:VAL:HG12	1.80	0.62
1:BE:62:LYS:HG2	1:BE:100:THR:HG22	1.80	0.62
1:BP:62:LYS:HG2	1:BP:100:THR:HG22	1.80	0.62
1:BQ:62:LYS:HG2	1:BQ:100:THR:HG22	1.80	0.62
1:CD:106:THR:HG22	1:CD:108:GLN:H	1.63	0.62
1:AQ:79:THR:HB	1:BF:77:PRO:HB2	1.81	0.62
1:AW:106:THR:HG22	1:AW:108:GLN:H	1.63	0.62
1:BM:62:LYS:HG2	1:BM:100:THR:HG22	1.80	0.62
1:AF:62:LYS:HG2	1:AF:100:THR:HG22	1.80	0.62
1:AM:62:LYS:HG2	1:AM:100:THR:HG22	1.80	0.62
1:BG:62:LYS:HG2	1:BG:100:THR:HG22	1.80	0.62
1:AI:62:LYS:HG2	1:AI:100:THR:HG22	1.80	0.62
1:BH:62:LYS:HG2	1:BH:100:THR:HG22	1.80	0.62
1:CA:106:THR:HG22	1:CA:108:GLN:H	1.63	0.62
1:CE:62:LYS:HG2	1:CE:100:THR:HG22	1.80	0.62
1:AE:106:THR:HG22	1:AE:108:GLN:H	1.63	0.62
1:AU:62:LYS:HG2	1:AU:100:THR:HG22	1.80	0.61
1:AX:62:LYS:HG2	1:AX:100:THR:HG22	1.80	0.61
1:BY:62:LYS:HG2	1:BY:100:THR:HG22	1.80	0.61
1:AI:95:VAL:CG2	1:BM:113:ILE:HG13	2.30	0.61
1:AL:80:ALA:HB2	1:BN:80:ALA:HA	1.81	0.61
1:CH:62:LYS:HG2	1:CH:100:THR:HG22	1.80	0.61
1:AF:116:TYR:HB3	1:BJ:67:ILE:HD13	1.83	0.60
1:BH:100:THR:OG1	1:CA:94:PRO:HD2	2.01	0.60
1:AK:6:VAL:HG22	1:AK:18:THR:HG22	1.85	0.59
1:AY:50:ALA:HB1	1:BC:129:LEU:HD21	1.83	0.59
1:BA:80:ALA:HB2	1:CC:80:ALA:HA	1.82	0.59
1:BH:121:LEU:HD12	1:CA:121:LEU:HD12	1.84	0.59
1:CA:26:ASN:HB2	1:CA:30:ASP:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BU:26:ASN:HB2	1:BU:30:ASP:HB2	1.85	0.59
1:AK:26:ASN:HB2	1:AK:30:ASP:HB2	1.85	0.59
1:AX:8:ALA:O	1:CB:119:ASN:ND2	2.35	0.59
1:BE:136:GLN:HG3	1:CG:34:TRP:HH2	1.66	0.59
1:BX:26:ASN:HB2	1:BX:30:ASP:HB2	1.85	0.59
1:AP:80:ALA:HA	1:BV:80:ALA:HB2	1.83	0.59
1:AQ:26:ASN:HB2	1:AQ:30:ASP:HB2	1.85	0.59
1:CD:26:ASN:HB2	1:CD:30:ASP:HB2	1.85	0.59
1:AB:26:ASN:HB2	1:AB:30:ASP:HB2	1.85	0.59
1:AJ:80:ALA:HA	1:BP:80:ALA:HB2	1.85	0.59
1:BL:26:ASN:HB2	1:BL:30:ASP:HB2	1.85	0.59
1:BO:26:ASN:HB2	1:BO:30:ASP:HB2	1.85	0.59
1:AH:6:VAL:HG22	1:AH:18:THR:HG22	1.85	0.59
1:AV:26:ASN:HB3	1:AW:26:ASN:HA	1.85	0.59
1:CD:6:VAL:HG22	1:CD:18:THR:HG22	1.85	0.59
1:AC:42:LEU:HA	1:AC:45:TYR:CE2	2.38	0.59
1:AT:26:ASN:HB2	1:AT:30:ASP:HB2	1.85	0.59
1:AY:80:ALA:HA	1:CE:80:ALA:HB2	1.83	0.59
1:BF:6:VAL:HG22	1:BF:18:THR:HG22	1.85	0.59
1:BF:26:ASN:HB2	1:BF:30:ASP:HB2	1.85	0.59
1:BV:42:LEU:HA	1:BV:45:TYR:CE2	2.38	0.59
1:AJ:82:GLY:O	1:BP:75:THR:HA	2.02	0.59
1:AU:119:ASN:ND2	1:BY:8:ALA:O	2.36	0.59
1:AZ:26:ASN:HB2	1:AZ:30:ASP:HB2	1.85	0.59
1:BI:6:VAL:HG22	1:BI:18:THR:HG22	1.85	0.59
1:BX:6:VAL:HG22	1:BX:18:THR:HG22	1.85	0.59
1:AJ:26:ASN:HB3	1:AK:26:ASN:HA	1.85	0.59
1:AL:80:ALA:CB	1:BN:80:ALA:HA	2.33	0.59
1:AN:6:VAL:HG22	1:AN:18:THR:HG22	1.85	0.59
1:AN:26:ASN:HB2	1:AN:30:ASP:HB2	1.85	0.59
1:AU:42:LEU:HA	1:AU:45:TYR:CE2	2.38	0.59
1:BE:26:ASN:HB3	1:BF:26:ASN:HA	1.85	0.59
1:BM:42:LEU:HA	1:BM:45:TYR:CE2	2.38	0.59
1:CC:26:ASN:HB3	1:CD:26:ASN:HA	1.85	0.59
1:CE:42:LEU:HA	1:CE:45:TYR:CE2	2.38	0.59
1:AF:42:LEU:HA	1:AF:45:TYR:CE2	2.38	0.58
1:AG:26:ASN:HB3	1:AH:26:ASN:HA	1.85	0.58
1:AH:26:ASN:HB2	1:AH:30:ASP:HB2	1.85	0.58
1:AL:42:LEU:HA	1:AL:45:TYR:CE2	2.38	0.58
1:BI:26:ASN:HB2	1:BI:30:ASP:HB2	1.85	0.58
1:BP:42:LEU:HA	1:BP:45:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BU:6:VAL:HG22	1:BU:18:THR:HG22	1.85	0.58
1:AB:6:VAL:HG22	1:AB:18:THR:HG22	1.85	0.58
1:AI:42:LEU:HA	1:AI:45:TYR:CE2	2.38	0.58
1:AS:26:ASN:HB3	1:AT:26:ASN:HA	1.85	0.58
1:BG:42:LEU:HA	1:BG:45:TYR:CE2	2.38	0.58
1:BW:26:ASN:HB3	1:BX:26:ASN:HA	1.85	0.58
1:CG:26:ASN:HB2	1:CG:30:ASP:HB2	1.85	0.58
1:AT:6:VAL:HG22	1:AT:18:THR:HG22	1.85	0.58
1:AW:26:ASN:HB2	1:AW:30:ASP:HB2	1.85	0.58
1:BR:26:ASN:HB2	1:BR:30:ASP:HB2	1.85	0.58
1:BS:42:LEU:HA	1:BS:45:TYR:CE2	2.38	0.58
1:BY:42:LEU:HA	1:BY:45:TYR:CE2	2.38	0.58
1:AB:85:PRO:HA	1:AK:73:ALA:HB1	1.86	0.58
1:AE:26:ASN:HB2	1:AE:30:ASP:HB2	1.85	0.58
1:AR:42:LEU:HA	1:AR:45:TYR:CE2	2.38	0.58
1:AX:42:LEU:HA	1:AX:45:TYR:CE2	2.38	0.58
1:BK:26:ASN:HB3	1:BL:26:ASN:HA	1.85	0.58
1:AE:10:GLY:O	1:BW:108:GLN:NE2	2.37	0.58
1:AL:35:TRP:HB3	1:AL:45:TYR:HD1	1.69	0.58
1:AO:42:LEU:HA	1:AO:45:TYR:CE2	2.38	0.58
1:AR:76:ALA:HB2	1:BT:77:PRO:HB2	1.86	0.58
1:BH:26:ASN:HB3	1:BI:26:ASN:HA	1.85	0.58
1:BK:50:ALA:HB1	1:BO:129:LEU:HD21	1.84	0.58
1:BY:35:TRP:HB3	1:BY:45:TYR:HD1	1.69	0.58
1:CG:6:VAL:HG22	1:CG:18:THR:HG22	1.85	0.58
1:CH:42:LEU:HA	1:CH:45:TYR:CE2	2.38	0.58
1:AC:35:TRP:HB3	1:AC:45:TYR:HD1	1.69	0.58
1:AM:26:ASN:HB3	1:AN:26:ASN:HA	1.85	0.58
1:BC:6:VAL:HG22	1:BC:18:THR:HG22	1.85	0.58
1:BD:42:LEU:HA	1:BD:45:TYR:CE2	2.38	0.58
1:BP:35:TRP:HB3	1:BP:45:TYR:HD1	1.69	0.58
1:CB:42:LEU:HA	1:CB:45:TYR:CE2	2.38	0.58
1:CE:35:TRP:HB3	1:CE:45:TYR:HD1	1.69	0.58
1:AE:6:VAL:HG22	1:AE:18:THR:HG22	1.85	0.58
1:AO:35:TRP:HB3	1:AO:45:TYR:HD1	1.69	0.58
1:AW:6:VAL:HG22	1:AW:18:THR:HG22	1.85	0.58
1:BB:26:ASN:HB3	1:BC:26:ASN:HA	1.85	0.58
1:BC:26:ASN:HB2	1:BC:30:ASP:HB2	1.85	0.58
1:AD:26:ASN:HB3	1:AE:26:ASN:HA	1.85	0.58
1:AU:8:ALA:O	1:BY:119:ASN:ND2	2.36	0.58
1:BA:42:LEU:HA	1:BA:45:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:35:TRP:HB3	1:BD:45:TYR:HD1	1.69	0.58
1:CB:35:TRP:HB3	1:CB:45:TYR:HD1	1.69	0.58
1:AZ:6:VAL:HG22	1:AZ:18:THR:HG22	1.85	0.58
1:BJ:42:LEU:HA	1:BJ:45:TYR:CE2	2.38	0.58
1:AO:80:ALA:HB2	1:BQ:80:ALA:HA	1.85	0.57
1:AU:35:TRP:HB3	1:AU:45:TYR:HD1	1.69	0.57
1:BA:80:ALA:HB3	1:CC:80:ALA:HA	1.84	0.57
1:BJ:35:TRP:HB3	1:BJ:45:TYR:HD1	1.69	0.57
1:BM:35:TRP:HB3	1:BM:45:TYR:HD1	1.69	0.57
1:BR:6:VAL:HG22	1:BR:18:THR:HG22	1.85	0.57
1:CH:35:TRP:HB3	1:CH:45:TYR:HD1	1.69	0.57
1:AY:26:ASN:HB3	1:AZ:26:ASN:HA	1.85	0.57
1:BD:80:ALA:CB	1:CF:80:ALA:HA	2.34	0.57
1:BL:35:TRP:HZ3	1:BO:133:THR:O	1.87	0.57
1:BL:85:PRO:HA	1:BO:73:ALA:HB1	1.85	0.57
1:AO:4:ASN:HB3	1:AO:20:GLU:HA	1.86	0.57
1:AV:77:PRO:HB2	1:CB:76:ALA:HB2	1.87	0.57
1:BA:76:ALA:HB2	1:CC:77:PRO:HB2	1.86	0.57
1:CA:6:VAL:HG22	1:CA:18:THR:HG22	1.85	0.57
1:AA:26:ASN:HB3	1:AB:26:ASN:HA	1.85	0.57
1:AQ:6:VAL:HG22	1:AQ:18:THR:HG22	1.85	0.57
1:BA:35:TRP:HB3	1:BA:45:TYR:HD1	1.69	0.57
1:BL:6:VAL:HG22	1:BL:18:THR:HG22	1.85	0.57
1:BS:35:TRP:HB3	1:BS:45:TYR:HD1	1.69	0.57
1:CB:4:ASN:HB3	1:CB:20:GLU:HA	1.86	0.57
1:BM:4:ASN:HB3	1:BM:20:GLU:HA	1.86	0.57
1:BQ:26:ASN:HB3	1:BR:26:ASN:HA	1.85	0.57
1:AI:35:TRP:HB3	1:AI:45:TYR:HD1	1.69	0.57
1:BA:4:ASN:HB3	1:BA:20:GLU:HA	1.86	0.57
1:BJ:4:ASN:HB3	1:BJ:20:GLU:HA	1.86	0.57
1:BN:26:ASN:HB3	1:BO:26:ASN:HA	1.85	0.57
1:AP:26:ASN:HB3	1:AQ:26:ASN:HA	1.85	0.57
1:BX:33:GLU:HG3	1:BX:49:THR:HG22	1.87	0.57
1:BT:26:ASN:HB3	1:BU:26:ASN:HA	1.85	0.57
1:BV:35:TRP:HB3	1:BV:45:TYR:HD1	1.69	0.57
1:CD:33:GLU:HG3	1:CD:49:THR:HG22	1.87	0.57
1:AB:33:GLU:HG3	1:AB:49:THR:HG22	1.87	0.57
1:AF:35:TRP:HB3	1:AF:45:TYR:HD1	1.69	0.57
1:AI:4:ASN:HB3	1:AI:20:GLU:HA	1.86	0.57
1:AL:4:ASN:HB3	1:AL:20:GLU:HA	1.86	0.57
1:BA:119:ASN:ND2	1:CE:8:ALA:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:4:ASN:HB3	1:BD:20:GLU:HA	1.86	0.57
1:BO:6:VAL:HG22	1:BO:18:THR:HG22	1.85	0.57
1:BZ:26:ASN:HB3	1:CA:26:ASN:HA	1.85	0.57
1:CF:26:ASN:HB3	1:CG:26:ASN:HA	1.85	0.57
1:AR:35:TRP:HB3	1:AR:45:TYR:HD1	1.69	0.57
1:AW:33:GLU:HG3	1:AW:49:THR:HG22	1.87	0.57
1:BC:33:GLU:HG3	1:BC:49:THR:HG22	1.87	0.57
1:BG:35:TRP:HB3	1:BG:45:TYR:HD1	1.69	0.57
1:AA:108:GLN:NE2	1:AK:10:GLY:O	2.38	0.56
1:AF:95:VAL:CG2	1:BJ:113:ILE:HG13	2.34	0.56
1:AH:33:GLU:HG3	1:AH:49:THR:HG22	1.87	0.56
1:AQ:33:GLU:HG3	1:AQ:49:THR:HG22	1.87	0.56
1:AX:35:TRP:HB3	1:AX:45:TYR:HD1	1.69	0.56
1:BG:4:ASN:HB3	1:BG:20:GLU:HA	1.86	0.56
1:BL:33:GLU:HG3	1:BL:49:THR:HG22	1.87	0.56
1:BO:33:GLU:HG3	1:BO:49:THR:HG22	1.87	0.56
1:CH:4:ASN:HB3	1:CH:20:GLU:HA	1.87	0.56
1:AR:4:ASN:HB3	1:AR:20:GLU:HA	1.86	0.56
1:BA:8:ALA:O	1:CE:119:ASN:ND2	2.37	0.56
1:BI:33:GLU:HG3	1:BI:49:THR:HG22	1.87	0.56
1:AI:113:ILE:HG13	1:BM:95:VAL:CG2	2.35	0.56
1:AO:8:ALA:O	1:BS:119:ASN:ND2	2.38	0.56
1:AO:119:ASN:ND2	1:BS:8:ALA:O	2.37	0.56
1:BF:33:GLU:HG3	1:BF:49:THR:HG22	1.87	0.56
1:BP:4:ASN:HB3	1:BP:20:GLU:HA	1.86	0.56
1:BS:4:ASN:HB3	1:BS:20:GLU:HA	1.86	0.56
1:CA:33:GLU:HG3	1:CA:49:THR:HG22	1.87	0.56
1:AD:80:ALA:HB3	1:AR:81:SER:OG	2.05	0.56
1:AP:108:GLN:NE2	1:BF:10:GLY:O	2.37	0.56
1:AX:119:ASN:ND2	1:CB:8:ALA:O	2.37	0.56
1:BY:4:ASN:HB3	1:BY:20:GLU:HA	1.86	0.56
1:CG:33:GLU:HG3	1:CG:49:THR:HG22	1.87	0.56
1:AX:4:ASN:HB3	1:AX:20:GLU:HA	1.86	0.56
1:AD:80:ALA:HA	1:BJ:80:ALA:CB	2.35	0.56
1:AF:4:ASN:HB3	1:AF:20:GLU:HA	1.87	0.56
1:AU:4:ASN:HB3	1:AU:20:GLU:HA	1.86	0.56
1:BV:4:ASN:HB3	1:BV:20:GLU:HA	1.86	0.56
1:AR:80:ALA:CB	1:BT:80:ALA:HA	2.36	0.56
1:AT:33:GLU:HG3	1:AT:49:THR:HG22	1.87	0.56
1:AU:80:ALA:HB3	1:BW:80:ALA:HA	1.87	0.56
1:BU:33:GLU:HG3	1:BU:49:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:5:VAL:HG12	1:BF:125:THR:HG21	1.88	0.56
1:CE:4:ASN:HB3	1:CE:20:GLU:HA	1.86	0.56
1:AC:4:ASN:HB3	1:AC:20:GLU:HA	1.86	0.55
1:AD:136:GLN:HG3	1:AQ:34:TRP:HH2	1.70	0.55
1:AF:113:ILE:HG13	1:BJ:95:VAL:HG23	1.86	0.55
1:AM:52:VAL:HB	1:BI:135:PRO:HB3	1.88	0.55
1:AK:33:GLU:HG3	1:AK:49:THR:HG22	1.87	0.55
1:AD:50:ALA:HB1	1:AQ:129:LEU:HD21	1.89	0.55
1:AP:113:ILE:HG13	1:BF:95:VAL:CG2	2.36	0.55
1:AR:39:SER:HB3	1:AR:44:GLY:HA3	1.89	0.55
1:AZ:33:GLU:HG3	1:AZ:49:THR:HG22	1.87	0.55
1:AT:52:VAL:HG22	1:AT:63:VAL:HG22	1.89	0.55
1:BR:8:ALA:HB1	1:BR:14:PRO:HB3	1.89	0.55
1:BR:33:GLU:HG3	1:BR:49:THR:HG22	1.87	0.55
1:AT:8:ALA:HB1	1:AT:14:PRO:HB3	1.89	0.55
1:BS:39:SER:HB3	1:BS:44:GLY:HA3	1.89	0.55
1:AM:8:ALA:O	1:BI:119:ASN:ND2	2.40	0.55
1:BF:8:ALA:HB1	1:BF:14:PRO:HB3	1.89	0.55
1:BI:52:VAL:HG22	1:BI:63:VAL:HG22	1.89	0.55
1:BL:52:VAL:HG22	1:BL:63:VAL:HG22	1.89	0.55
1:AD:106:THR:HG22	1:AD:108:GLN:H	1.72	0.55
1:AE:33:GLU:HG3	1:AE:49:THR:HG22	1.87	0.55
1:AN:52:VAL:HG22	1:AN:63:VAL:HG22	1.89	0.55
1:AP:106:THR:HG22	1:AP:108:GLN:H	1.72	0.55
1:BH:50:ALA:HB1	1:CA:129:LEU:HD21	1.89	0.55
1:BP:39:SER:HB3	1:BP:44:GLY:HA3	1.89	0.55
1:BQ:106:THR:HG22	1:BQ:108:GLN:H	1.72	0.55
1:AD:77:PRO:HB2	1:BJ:76:ALA:HB2	1.89	0.55
1:AN:8:ALA:HB1	1:AN:14:PRO:HB3	1.89	0.55
1:AQ:52:VAL:HG22	1:AQ:63:VAL:HG22	1.89	0.55
1:BN:106:THR:HG22	1:BN:108:GLN:H	1.72	0.55
1:CE:39:SER:HB3	1:CE:44:GLY:HA3	1.89	0.55
1:AH:52:VAL:HG22	1:AH:63:VAL:HG22	1.89	0.54
1:AN:33:GLU:HG3	1:AN:49:THR:HG22	1.87	0.54
1:AU:39:SER:HB3	1:AU:44:GLY:HA3	1.89	0.54
1:AX:76:ALA:HB2	1:BZ:77:PRO:HB2	1.89	0.54
1:BL:8:ALA:HB1	1:BL:14:PRO:HB3	1.89	0.54
1:BR:52:VAL:HG22	1:BR:63:VAL:HG22	1.89	0.54
1:CA:52:VAL:HG22	1:CA:63:VAL:HG22	1.89	0.54
1:CH:39:SER:HB3	1:CH:44:GLY:HA3	1.89	0.54
1:AY:106:THR:HG22	1:AY:108:GLN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BU:8:ALA:HB1	1:BU:14:PRO:HB3	1.89	0.54
1:AB:8:ALA:HB1	1:AB:14:PRO:HB3	1.89	0.54
1:AB:133:THR:O	1:CA:35:TRP:HZ3	1.90	0.54
1:AP:95:VAL:CG2	1:BF:113:ILE:HG13	2.38	0.54
1:AW:52:VAL:HG22	1:AW:63:VAL:HG22	1.89	0.54
1:BG:39:SER:HB3	1:BG:44:GLY:HA3	1.89	0.54
1:BH:106:THR:HG22	1:BH:108:GLN:H	1.72	0.54
1:AJ:106:THR:HG22	1:AJ:108:GLN:H	1.72	0.54
1:AL:39:SER:HB3	1:AL:44:GLY:HA3	1.89	0.54
1:AM:77:PRO:HB2	1:BS:76:ALA:HB2	1.89	0.54
1:AM:106:THR:HG22	1:AM:108:GLN:H	1.72	0.54
1:BB:106:THR:HG22	1:BB:108:GLN:H	1.72	0.54
1:BD:39:SER:HB3	1:BD:44:GLY:HA3	1.89	0.54
1:BO:52:VAL:HG22	1:BO:63:VAL:HG22	1.89	0.54
1:BZ:106:THR:HG22	1:BZ:108:GLN:H	1.72	0.54
1:CD:52:VAL:HG22	1:CD:63:VAL:HG22	1.89	0.54
1:AA:79:THR:CB	1:AL:80:ALA:HA	2.29	0.54
1:AD:79:THR:O	1:BJ:80:ALA:HB2	2.07	0.54
1:AE:8:ALA:HB1	1:AE:14:PRO:HB3	1.89	0.54
1:AX:39:SER:HB3	1:AX:44:GLY:HA3	1.89	0.54
1:BA:39:SER:HB3	1:BA:44:GLY:HA3	1.89	0.54
1:BC:8:ALA:HB1	1:BC:14:PRO:HB3	1.89	0.54
1:BX:52:VAL:HG22	1:BX:63:VAL:HG22	1.89	0.54
1:CC:106:THR:HG22	1:CC:108:GLN:H	1.72	0.54
1:AC:39:SER:HB3	1:AC:44:GLY:HA3	1.89	0.54
1:AE:52:VAL:HG22	1:AE:63:VAL:HG22	1.89	0.54
1:AO:39:SER:HB3	1:AO:44:GLY:HA3	1.89	0.54
1:BE:4:ASN:HB3	1:BE:21:PRO:HD3	1.90	0.54
1:BO:8:ALA:HB1	1:BO:14:PRO:HB3	1.89	0.54
1:AG:106:THR:HG22	1:AG:108:GLN:H	1.72	0.54
1:BI:8:ALA:HB1	1:BI:14:PRO:HB3	1.89	0.54
1:CB:39:SER:HB3	1:CB:44:GLY:HA3	1.89	0.54
1:AA:4:ASN:HB3	1:AA:21:PRO:HD3	1.90	0.54
1:AH:8:ALA:HB1	1:AH:14:PRO:HB3	1.89	0.54
1:AI:39:SER:HB3	1:AI:44:GLY:HA3	1.89	0.54
1:AQ:8:ALA:HB1	1:AQ:14:PRO:HB3	1.89	0.54
1:AR:119:ASN:ND2	1:BV:8:ALA:O	2.41	0.54
1:AV:4:ASN:HB3	1:AV:21:PRO:HD3	1.90	0.54
1:BC:52:VAL:HG22	1:BC:63:VAL:HG22	1.89	0.54
1:BE:106:THR:HG22	1:BE:108:GLN:H	1.72	0.54
1:BV:39:SER:HB3	1:BV:44:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:8:ALA:HB1	1:CA:14:PRO:HB3	1.89	0.54
1:AF:39:SER:HB3	1:AF:44:GLY:HA3	1.89	0.54
1:AG:4:ASN:HB3	1:AG:21:PRO:HD3	1.90	0.54
1:BJ:39:SER:HB3	1:BJ:44:GLY:HA3	1.89	0.54
1:CD:8:ALA:HB1	1:CD:14:PRO:HB3	1.89	0.54
1:AA:106:THR:HG22	1:AA:108:GLN:H	1.72	0.54
1:BY:39:SER:HB3	1:BY:44:GLY:HA3	1.89	0.54
1:AO:8:ALA:HB1	1:AO:14:PRO:HB3	1.90	0.53
1:AP:4:ASN:HB3	1:AP:21:PRO:HD3	1.90	0.53
1:AS:106:THR:HG22	1:AS:108:GLN:H	1.72	0.53
1:AV:106:THR:HG22	1:AV:108:GLN:H	1.72	0.53
1:AZ:52:VAL:HG22	1:AZ:63:VAL:HG22	1.89	0.53
1:BD:8:ALA:HB1	1:BD:14:PRO:HB3	1.90	0.53
1:BH:4:ASN:HB3	1:BH:21:PRO:HD3	1.90	0.53
1:BV:8:ALA:HB1	1:BV:14:PRO:HB3	1.90	0.53
1:BW:106:THR:HG22	1:BW:108:GLN:H	1.72	0.53
1:AA:136:GLN:HG3	1:AK:34:TRP:HH2	1.72	0.53
1:AO:80:ALA:CB	1:BQ:80:ALA:HA	2.38	0.53
1:AX:8:ALA:HB1	1:AX:14:PRO:HB3	1.90	0.53
1:AY:80:ALA:HA	1:CE:80:ALA:HB3	1.90	0.53
1:BE:125:THR:HG21	1:CG:5:VAL:HG12	1.90	0.53
1:BK:106:THR:HG22	1:BK:108:GLN:H	1.72	0.53
1:BR:19:PHE:HB3	1:BR:34:TRP:HB3	1.91	0.53
1:BT:106:THR:HG22	1:BT:108:GLN:H	1.72	0.53
1:BW:4:ASN:HB3	1:BW:21:PRO:HD3	1.90	0.53
1:CG:52:VAL:HG22	1:CG:63:VAL:HG22	1.89	0.53
1:AD:4:ASN:HB3	1:AD:21:PRO:HD3	1.90	0.53
1:AK:8:ALA:HB1	1:AK:14:PRO:HB3	1.89	0.53
1:AW:8:ALA:HB1	1:AW:14:PRO:HB3	1.89	0.53
1:BF:52:VAL:HG22	1:BF:63:VAL:HG22	1.89	0.53
1:BL:37:LYS:HA	1:BL:45:TYR:CD1	2.44	0.53
1:BM:8:ALA:HB1	1:BM:14:PRO:HB3	1.90	0.53
1:BM:39:SER:HB3	1:BM:44:GLY:HA3	1.89	0.53
1:BO:19:PHE:HB3	1:BO:34:TRP:HB3	1.91	0.53
1:BY:8:ALA:HB1	1:BY:14:PRO:HB3	1.90	0.53
1:CB:8:ALA:HB1	1:CB:14:PRO:HB3	1.90	0.53
1:CC:4:ASN:HB3	1:CC:21:PRO:HD3	1.90	0.53
1:CF:106:THR:HG22	1:CF:108:GLN:H	1.72	0.53
1:CG:8:ALA:HB1	1:CG:14:PRO:HB3	1.89	0.53
1:AH:37:LYS:HA	1:AH:45:TYR:CD1	2.44	0.53
1:AP:79:THR:HB	1:BG:80:ALA:HA	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AW:37:LYS:HA	1:AW:45:TYR:CD1	2.44	0.53
1:BE:137:TYR:CE1	1:CG:1:GLN:HA	2.44	0.53
1:BF:19:PHE:HB3	1:BF:34:TRP:HB3	1.91	0.53
1:BI:19:PHE:HB3	1:BI:34:TRP:HB3	1.91	0.53
1:BL:19:PHE:HB3	1:BL:34:TRP:HB3	1.91	0.53
1:BZ:4:ASN:HB3	1:BZ:21:PRO:HD3	1.90	0.53
1:AE:37:LYS:HA	1:AE:45:TYR:CD1	2.44	0.53
1:AH:19:PHE:HB3	1:AH:34:TRP:HB3	1.91	0.53
1:AM:4:ASN:HB3	1:AM:21:PRO:HD3	1.90	0.53
1:AT:19:PHE:HB3	1:AT:34:TRP:HB3	1.91	0.53
1:BF:37:LYS:HA	1:BF:45:TYR:CD1	2.44	0.53
1:BK:4:ASN:HB3	1:BK:21:PRO:HD3	1.90	0.53
1:BQ:4:ASN:HB3	1:BQ:21:PRO:HD3	1.90	0.53
1:CE:8:ALA:HB1	1:CE:14:PRO:HB3	1.90	0.53
1:CG:19:PHE:HB3	1:CG:34:TRP:HB3	1.91	0.53
1:CG:37:LYS:HA	1:CG:45:TYR:CD1	2.44	0.53
1:AQ:37:LYS:HA	1:AQ:45:TYR:CD1	2.44	0.53
1:AZ:8:ALA:HB1	1:AZ:14:PRO:HB3	1.89	0.53
1:AZ:19:PHE:HB3	1:AZ:34:TRP:HB3	1.91	0.53
1:BA:8:ALA:HB1	1:BA:14:PRO:HB3	1.90	0.53
1:BX:8:ALA:HB1	1:BX:14:PRO:HB3	1.89	0.53
1:CF:4:ASN:HB3	1:CF:21:PRO:HD3	1.90	0.53
1:AU:8:ALA:HB1	1:AU:14:PRO:HB3	1.90	0.53
1:BR:37:LYS:HA	1:BR:45:TYR:CD1	2.44	0.53
1:BX:37:LYS:HA	1:BX:45:TYR:CD1	2.44	0.53
1:AB:129:LEU:HD21	1:BZ:50:ALA:HB1	1.90	0.53
1:AK:52:VAL:HG22	1:AK:63:VAL:HG22	1.89	0.53
1:AY:77:PRO:HB2	1:CE:76:ALA:HB2	1.89	0.53
1:BU:52:VAL:HG22	1:BU:63:VAL:HG22	1.89	0.53
1:CA:37:LYS:HA	1:CA:45:TYR:CD1	2.44	0.53
1:AD:80:ALA:HA	1:BJ:80:ALA:HB3	1.89	0.53
1:AJ:113:ILE:HG13	1:AN:95:VAL:CG2	2.39	0.53
1:BI:37:LYS:HA	1:BI:45:TYR:CD1	2.44	0.53
1:CA:19:PHE:HB3	1:CA:34:TRP:HB3	1.91	0.53
1:CH:8:ALA:HB1	1:CH:14:PRO:HB3	1.90	0.53
1:AF:8:ALA:HB1	1:AF:14:PRO:HB3	1.90	0.53
1:AJ:4:ASN:HB3	1:AJ:21:PRO:HD3	1.90	0.53
1:AJ:132:ASN:O	1:AO:37:LYS:HE2	2.09	0.53
1:BC:37:LYS:HA	1:BC:45:TYR:CD1	2.44	0.53
1:BN:4:ASN:HB3	1:BN:21:PRO:HD3	1.90	0.53
1:BU:37:LYS:HA	1:BU:45:TYR:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:19:PHE:HB3	1:BX:34:TRP:HB3	1.91	0.53
1:AB:52:VAL:HG22	1:AB:63:VAL:HG22	1.89	0.52
1:AQ:19:PHE:HB3	1:AQ:34:TRP:HB3	1.91	0.52
1:AW:19:PHE:HB3	1:AW:34:TRP:HB3	1.91	0.52
1:AE:1:GLN:HA	1:BW:137:TYR:CE1	2.44	0.52
1:AK:37:LYS:HA	1:AK:45:TYR:CD1	2.44	0.52
1:AY:4:ASN:HB3	1:AY:21:PRO:HD3	1.90	0.52
1:AZ:37:LYS:HA	1:AZ:45:TYR:CD1	2.44	0.52
1:BB:4:ASN:HB3	1:BB:21:PRO:HD3	1.90	0.52
1:AB:37:LYS:HA	1:AB:45:TYR:CD1	2.44	0.52
1:AN:37:LYS:HA	1:AN:45:TYR:CD1	2.44	0.52
1:AR:75:THR:HA	1:BT:82:GLY:O	2.09	0.52
1:BD:76:ALA:HB2	1:CF:77:PRO:HB2	1.92	0.52
1:BG:8:ALA:HB1	1:BG:14:PRO:HB3	1.90	0.52
1:AI:8:ALA:HB1	1:AI:14:PRO:HB3	1.90	0.52
1:AL:76:ALA:HB2	1:BN:77:PRO:HB2	1.90	0.52
1:AS:4:ASN:HB3	1:AS:21:PRO:HD3	1.90	0.52
1:AT:37:LYS:HA	1:AT:45:TYR:CD1	2.44	0.52
1:BO:37:LYS:HA	1:BO:45:TYR:CD1	2.44	0.52
1:BP:8:ALA:HB1	1:BP:14:PRO:HB3	1.90	0.52
1:AB:19:PHE:HB3	1:AB:34:TRP:HB3	1.91	0.52
1:AE:19:PHE:HB3	1:AE:34:TRP:HB3	1.91	0.52
1:AO:46:ARG:HG2	1:AO:69:ASP:HA	1.92	0.52
1:AS:80:ALA:HA	1:BY:80:ALA:HB3	1.92	0.52
1:AX:46:ARG:HG2	1:AX:69:ASP:HA	1.92	0.52
1:BC:19:PHE:HB3	1:BC:34:TRP:HB3	1.91	0.52
1:BM:46:ARG:HG2	1:BM:69:ASP:HA	1.92	0.52
1:BS:8:ALA:HB1	1:BS:14:PRO:HB3	1.90	0.52
1:BU:19:PHE:HB3	1:BU:34:TRP:HB3	1.91	0.52
1:AL:46:ARG:HG2	1:AL:69:ASP:HA	1.92	0.52
1:BG:46:ARG:HG2	1:BG:69:ASP:HA	1.92	0.52
1:BH:137:TYR:CE1	1:CA:1:GLN:HA	2.44	0.52
1:BK:4:ASN:HB3	1:BK:20:GLU:HA	1.92	0.52
1:BW:4:ASN:HB3	1:BW:20:GLU:HA	1.92	0.52
1:CB:46:ARG:HG2	1:CB:69:ASP:HA	1.92	0.52
1:AC:46:ARG:HG2	1:AC:69:ASP:HA	1.92	0.52
1:AD:97:ILE:HA	1:AQ:96:PHE:O	2.10	0.52
1:AL:8:ALA:HB1	1:AL:14:PRO:HB3	1.90	0.52
1:AN:19:PHE:HB3	1:AN:34:TRP:HB3	1.91	0.52
1:BE:136:GLN:HG3	1:CG:34:TRP:CH2	2.44	0.52
1:CD:37:LYS:HA	1:CD:45:TYR:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:46:ARG:HG2	1:CE:69:ASP:HA	1.92	0.52
1:CH:46:ARG:HG2	1:CH:69:ASP:HA	1.92	0.52
1:AD:4:ASN:HB3	1:AD:20:GLU:HA	1.92	0.52
1:AG:4:ASN:HB3	1:AG:20:GLU:HA	1.92	0.52
1:AR:8:ALA:HB1	1:AR:14:PRO:HB3	1.90	0.52
1:AT:79:THR:HB	1:CD:77:PRO:CB	2.39	0.52
1:BZ:4:ASN:HB3	1:BZ:20:GLU:HA	1.92	0.52
1:AC:8:ALA:HB1	1:AC:14:PRO:HB3	1.90	0.52
1:AM:4:ASN:HB3	1:AM:20:GLU:HA	1.92	0.52
1:AS:8:ALA:O	1:CD:119:ASN:ND2	2.43	0.52
1:BE:4:ASN:HB3	1:BE:20:GLU:HA	1.92	0.52
1:AK:19:PHE:HB3	1:AK:34:TRP:HB3	1.91	0.52
1:AK:85:PRO:HB3	1:AN:74:VAL:O	2.10	0.52
1:BR:125:THR:HG21	1:BT:5:VAL:HG12	1.91	0.52
1:AF:46:ARG:HG2	1:AF:69:ASP:HA	1.92	0.51
1:AQ:79:THR:HB	1:BF:77:PRO:HB3	1.90	0.51
1:AS:52:VAL:HB	1:CD:135:PRO:HB3	1.92	0.51
1:BB:4:ASN:HB3	1:BB:20:GLU:HA	1.92	0.51
1:BK:25:GLN:O	1:BO:137:TYR:HA	2.10	0.51
1:BY:46:ARG:HG2	1:BY:69:ASP:HA	1.92	0.51
1:CD:19:PHE:HB3	1:CD:34:TRP:HB3	1.91	0.51
1:AD:121:LEU:HD11	1:AQ:97:ILE:HD13	1.91	0.51
1:AF:105:CYS:HA	1:BJ:91:PHE:CZ	2.46	0.51
1:AJ:80:ALA:HA	1:BP:80:ALA:CB	2.40	0.51
1:BJ:8:ALA:HB1	1:BJ:14:PRO:HB3	1.91	0.51
1:AH:119:ASN:ND2	1:BQ:8:ALA:O	2.44	0.51
1:AL:75:THR:HA	1:BN:82:GLY:O	2.10	0.51
1:BJ:46:ARG:HG2	1:BJ:69:ASP:HA	1.92	0.51
1:BV:46:ARG:HG2	1:BV:69:ASP:HA	1.92	0.51
1:AE:121:LEU:HD12	1:BW:121:LEU:HD12	1.92	0.51
1:AA:121:LEU:HD12	1:AK:121:LEU:HD12	1.91	0.51
1:BP:46:ARG:HG2	1:BP:69:ASP:HA	1.92	0.51
1:BT:4:ASN:HB3	1:BT:21:PRO:HD3	1.90	0.51
1:AC:106:THR:HG22	1:AC:108:GLN:H	1.76	0.51
1:AE:135:PRO:HB3	1:BW:52:VAL:HB	1.92	0.51
1:AL:106:THR:HG22	1:AL:108:GLN:H	1.76	0.51
1:BS:46:ARG:HG2	1:BS:69:ASP:HA	1.92	0.51
1:BV:106:THR:HG22	1:BV:108:GLN:H	1.76	0.51
1:AS:4:ASN:HB3	1:AS:20:GLU:HA	1.92	0.51
1:AU:76:ALA:HB2	1:BW:77:PRO:HB2	1.91	0.51
1:CB:106:THR:HG22	1:CB:108:GLN:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:137:TYR:HD1	1:AR:2:ILE:HG23	1.75	0.51
1:AP:80:ALA:HA	1:BV:80:ALA:CB	2.40	0.51
1:BD:46:ARG:HG2	1:BD:69:ASP:HA	1.92	0.51
1:BS:84:GLN:HG3	1:BS:85:PRO:HD2	1.93	0.51
1:AO:106:THR:HG22	1:AO:108:GLN:H	1.76	0.51
1:AP:4:ASN:HB3	1:AP:20:GLU:HA	1.92	0.51
1:AR:46:ARG:HG2	1:AR:69:ASP:HA	1.92	0.51
1:AU:46:ARG:HG2	1:AU:69:ASP:HA	1.92	0.51
1:AV:4:ASN:HB3	1:AV:20:GLU:HA	1.92	0.51
1:CE:106:THR:HG22	1:CE:108:GLN:H	1.76	0.51
1:CH:106:THR:HG22	1:CH:108:GLN:H	1.76	0.51
1:AF:106:THR:HG22	1:AF:108:GLN:H	1.76	0.51
1:AI:106:THR:HG22	1:AI:108:GLN:H	1.76	0.51
1:AJ:4:ASN:HB3	1:AJ:20:GLU:HA	1.92	0.51
1:AO:84:GLN:HG3	1:AO:85:PRO:HD2	1.93	0.51
1:AX:80:ALA:HB3	1:BZ:80:ALA:HA	1.92	0.51
1:BA:46:ARG:HG2	1:BA:69:ASP:HA	1.92	0.51
1:BB:77:PRO:HB2	1:CH:76:ALA:HB2	1.91	0.51
1:BD:106:THR:HG22	1:BD:108:GLN:H	1.76	0.51
1:BJ:106:THR:HG22	1:BJ:108:GLN:H	1.76	0.51
1:CF:4:ASN:HB3	1:CF:20:GLU:HA	1.92	0.51
1:AI:46:ARG:HG2	1:AI:69:ASP:HA	1.92	0.50
1:AN:79:THR:HB	1:BI:77:PRO:CB	2.41	0.50
1:AX:106:THR:HG22	1:AX:108:GLN:H	1.76	0.50
1:AI:84:GLN:HG3	1:AI:85:PRO:HD2	1.93	0.50
1:AJ:74:VAL:HB	1:AO:84:GLN:HB3	1.92	0.50
1:BJ:84:GLN:HG3	1:BJ:85:PRO:HD2	1.93	0.50
1:BS:106:THR:HG22	1:BS:108:GLN:H	1.76	0.50
1:BT:4:ASN:HB3	1:BT:20:GLU:HA	1.92	0.50
1:BT:9:ASP:O	1:BT:14:PRO:HB3	2.12	0.50
1:BY:84:GLN:HG3	1:BY:85:PRO:HD2	1.93	0.50
1:AF:84:GLN:HG3	1:AF:85:PRO:HD2	1.93	0.50
1:AX:84:GLN:HG3	1:AX:85:PRO:HD2	1.93	0.50
1:BM:84:GLN:HG3	1:BM:85:PRO:HD2	1.93	0.50
1:BY:106:THR:HG22	1:BY:108:GLN:H	1.76	0.50
1:CC:4:ASN:HB3	1:CC:20:GLU:HA	1.92	0.50
1:CF:9:ASP:O	1:CF:14:PRO:HB3	2.12	0.50
1:AA:4:ASN:HB3	1:AA:20:GLU:HA	1.92	0.50
1:AJ:9:ASP:O	1:AJ:14:PRO:HB3	2.12	0.50
1:AY:4:ASN:HB3	1:AY:20:GLU:HA	1.92	0.50
1:BB:9:ASP:O	1:BB:14:PRO:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:9:ASP:O	1:BH:14:PRO:HB3	2.12	0.50
1:BN:4:ASN:HB3	1:BN:20:GLU:HA	1.92	0.50
1:BQ:9:ASP:O	1:BQ:14:PRO:HB3	2.12	0.50
1:BV:84:GLN:HG3	1:BV:85:PRO:HD2	1.93	0.50
1:AI:80:ALA:HB2	1:BK:80:ALA:HA	1.94	0.50
1:AM:9:ASP:O	1:AM:14:PRO:HB3	2.12	0.50
1:AR:84:GLN:HG3	1:AR:85:PRO:HD2	1.93	0.50
1:AV:9:ASP:O	1:AV:14:PRO:HB3	2.12	0.50
1:BD:119:ASN:ND2	1:CH:8:ALA:O	2.45	0.50
1:BH:4:ASN:HB3	1:BH:20:GLU:HA	1.92	0.50
1:BM:106:THR:HG22	1:BM:108:GLN:H	1.76	0.50
1:AS:9:ASP:O	1:AS:14:PRO:HB3	2.12	0.50
1:AW:42:LEU:HD23	1:AW:45:TYR:CE2	2.47	0.50
1:AJ:5:VAL:HG12	1:AN:125:THR:HG21	1.94	0.50
1:AU:106:THR:HG22	1:AU:108:GLN:H	1.76	0.50
1:BQ:4:ASN:HB3	1:BQ:20:GLU:HA	1.92	0.50
1:AC:84:GLN:HG3	1:AC:85:PRO:HD2	1.93	0.50
1:AE:42:LEU:HD23	1:AE:45:TYR:CE2	2.47	0.50
1:BA:106:THR:HG22	1:BA:108:GLN:H	1.76	0.50
1:BC:42:LEU:HD23	1:BC:45:TYR:CE2	2.47	0.50
1:BF:42:LEU:HD23	1:BF:45:TYR:CE2	2.47	0.50
1:BG:106:THR:HG22	1:BG:108:GLN:H	1.76	0.50
1:CD:42:LEU:HD23	1:CD:45:TYR:CE2	2.47	0.50
1:AY:9:ASP:O	1:AY:14:PRO:HB3	2.12	0.50
1:BG:84:GLN:HG3	1:BG:85:PRO:HD2	1.93	0.50
1:BI:42:LEU:HD23	1:BI:45:TYR:CE2	2.47	0.50
1:BU:42:LEU:HD23	1:BU:45:TYR:CE2	2.47	0.50
1:CC:9:ASP:O	1:CC:14:PRO:HB3	2.12	0.50
1:AB:135:PRO:HB3	1:BZ:52:VAL:HB	1.94	0.49
1:AK:42:LEU:HD23	1:AK:45:TYR:CE2	2.47	0.49
1:AN:42:LEU:HD23	1:AN:45:TYR:CE2	2.47	0.49
1:AP:9:ASP:O	1:AP:14:PRO:HB3	2.12	0.49
1:BE:9:ASP:O	1:BE:14:PRO:HB3	2.12	0.49
1:BP:84:GLN:HG3	1:BP:85:PRO:HD2	1.93	0.49
1:BZ:9:ASP:O	1:BZ:14:PRO:HB3	2.12	0.49
1:AE:73:ALA:HB1	1:BX:85:PRO:HA	1.94	0.49
1:AK:22:GLN:HG2	1:AK:35:TRP:CD2	2.48	0.49
1:AP:64:LYS:HG2	1:AP:98:GLU:HG2	1.95	0.49
1:AZ:42:LEU:HD23	1:AZ:45:TYR:CE2	2.47	0.49
1:BE:8:ALA:O	1:CG:119:ASN:ND2	2.44	0.49
1:BK:9:ASP:O	1:BK:14:PRO:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP:106:THR:HG22	1:BP:108:GLN:H	1.76	0.49
1:AA:64:LYS:HG2	1:AA:98:GLU:HG2	1.95	0.49
1:AD:9:ASP:O	1:AD:14:PRO:HB3	2.12	0.49
1:AG:9:ASP:O	1:AG:14:PRO:HB3	2.12	0.49
1:AR:106:THR:HG22	1:AR:108:GLN:H	1.76	0.49
1:BH:8:ALA:O	1:CA:119:ASN:ND2	2.45	0.49
1:BL:42:LEU:HD23	1:BL:45:TYR:CE2	2.47	0.49
1:BN:9:ASP:O	1:BN:14:PRO:HB3	2.12	0.49
1:BN:64:LYS:HG2	1:BN:98:GLU:HG2	1.95	0.49
1:BO:42:LEU:HD23	1:BO:45:TYR:CE2	2.47	0.49
1:BW:9:ASP:O	1:BW:14:PRO:HB3	2.12	0.49
1:CH:84:GLN:HG3	1:CH:85:PRO:HD2	1.93	0.49
1:AH:22:GLN:HG2	1:AH:35:TRP:CD2	2.48	0.49
1:AZ:35:TRP:HZ3	1:BC:133:THR:O	1.95	0.49
1:BD:84:GLN:HG3	1:BD:85:PRO:HD2	1.93	0.49
1:BO:22:GLN:HG2	1:BO:35:TRP:CD2	2.48	0.49
1:BR:22:GLN:HG2	1:BR:35:TRP:CD2	2.48	0.49
1:CE:84:GLN:HG3	1:CE:85:PRO:HD2	1.93	0.49
1:CG:42:LEU:HD23	1:CG:45:TYR:CE2	2.47	0.49
1:BL:22:GLN:HG2	1:BL:35:TRP:CD2	2.48	0.49
1:BZ:64:LYS:HG2	1:BZ:98:GLU:HG2	1.95	0.49
1:CG:22:GLN:HG2	1:CG:35:TRP:CD2	2.48	0.49
1:AE:85:PRO:HB3	1:AQ:74:VAL:O	2.13	0.49
1:AH:42:LEU:HD23	1:AH:45:TYR:CE2	2.47	0.49
1:AM:64:LYS:HG2	1:AM:98:GLU:HG2	1.95	0.49
1:AQ:22:GLN:HG2	1:AQ:35:TRP:CD2	2.48	0.49
1:CA:42:LEU:HD23	1:CA:45:TYR:CE2	2.47	0.49
1:AT:74:VAL:O	1:AW:85:PRO:HB3	2.13	0.49
1:AU:84:GLN:HG3	1:AU:85:PRO:HD2	1.93	0.49
1:BA:84:GLN:HG3	1:BA:85:PRO:HD2	1.93	0.49
1:BH:136:GLN:HG3	1:CA:34:TRP:HH2	1.78	0.49
1:AT:22:GLN:HG2	1:AT:35:TRP:CD2	2.48	0.49
1:AW:22:GLN:HG2	1:AW:35:TRP:CD2	2.48	0.49
1:BH:64:LYS:HG2	1:BH:98:GLU:HG2	1.94	0.49
1:BI:22:GLN:HG2	1:BI:35:TRP:CD2	2.48	0.49
1:BX:42:LEU:HD23	1:BX:45:TYR:CE2	2.47	0.49
1:CB:84:GLN:HG3	1:CB:85:PRO:HD2	1.93	0.49
1:AD:64:LYS:HG2	1:AD:98:GLU:HG2	1.95	0.49
1:AQ:42:LEU:HD23	1:AQ:45:TYR:CE2	2.47	0.49
1:BF:22:GLN:HG2	1:BF:35:TRP:CD2	2.48	0.49
1:BK:52:VAL:HB	1:BO:135:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:64:LYS:HG2	1:BK:98:GLU:HG2	1.95	0.49
1:BR:42:LEU:HD23	1:BR:45:TYR:CE2	2.47	0.49
1:BX:121:LEU:HD12	1:CF:121:LEU:HD12	1.95	0.49
1:CF:64:LYS:HG2	1:CF:98:GLU:HG2	1.94	0.49
1:AB:22:GLN:HG2	1:AB:35:TRP:CD2	2.48	0.49
1:CA:22:GLN:HG2	1:CA:35:TRP:CD2	2.48	0.49
1:AL:84:GLN:HG3	1:AL:85:PRO:HD2	1.93	0.48
1:AR:129:LEU:HD21	1:BV:50:ALA:HB1	1.93	0.48
1:BO:54:ARG:NH2	1:BO:103:ASP:OD2	2.46	0.48
1:AJ:77:PRO:HB2	1:BP:76:ALA:HB2	1.94	0.48
1:BB:64:LYS:HG2	1:BB:98:GLU:HG2	1.95	0.48
1:CD:22:GLN:HG2	1:CD:35:TRP:CD2	2.48	0.48
1:AB:42:LEU:HD23	1:AB:45:TYR:CE2	2.47	0.48
1:AY:136:GLN:HG3	1:BC:34:TRP:HH2	1.77	0.48
1:BK:26:ASN:OD1	1:BO:137:TYR:HB2	2.12	0.48
1:BU:22:GLN:HG2	1:BU:35:TRP:CD2	2.48	0.48
1:BX:22:GLN:HG2	1:BX:35:TRP:CD2	2.48	0.48
1:AE:22:GLN:HG2	1:AE:35:TRP:CD2	2.48	0.48
1:AN:22:GLN:HG2	1:AN:35:TRP:CD2	2.48	0.48
1:AS:64:LYS:HG2	1:AS:98:GLU:HG2	1.95	0.48
1:AY:64:LYS:HG2	1:AY:98:GLU:HG2	1.95	0.48
1:BC:22:GLN:HG2	1:BC:35:TRP:CD2	2.48	0.48
1:BW:64:LYS:HG2	1:BW:98:GLU:HG2	1.95	0.48
1:BC:54:ARG:NH2	1:BC:103:ASP:OD2	2.46	0.48
1:BF:54:ARG:NH2	1:BF:103:ASP:OD2	2.46	0.48
1:BQ:64:LYS:HG2	1:BQ:98:GLU:HG2	1.94	0.48
1:AA:9:ASP:O	1:AA:14:PRO:HB3	2.12	0.48
1:AV:64:LYS:HG2	1:AV:98:GLU:HG2	1.94	0.48
1:CC:64:LYS:HG2	1:CC:98:GLU:HG2	1.94	0.48
1:AT:42:LEU:HD23	1:AT:45:TYR:CE2	2.47	0.48
1:AT:79:THR:HB	1:CD:77:PRO:HB2	1.95	0.48
1:AY:8:ALA:O	1:BC:119:ASN:ND2	2.46	0.48
1:AI:101:LEU:HD11	1:BM:130:VAL:HG13	1.94	0.48
1:AJ:64:LYS:HG2	1:AJ:98:GLU:HG2	1.94	0.48
1:AS:77:PRO:HB2	1:BY:76:ALA:HB2	1.96	0.48
1:BV:137:TYR:N	1:BV:137:TYR:CD2	2.82	0.48
1:BO:64:LYS:HG2	1:BO:98:GLU:HG2	1.96	0.48
1:BR:64:LYS:HG2	1:BR:98:GLU:HG2	1.96	0.48
1:BT:64:LYS:HG2	1:BT:98:GLU:HG2	1.95	0.48
1:BU:64:LYS:HG2	1:BU:98:GLU:HG2	1.96	0.48
1:BY:137:TYR:N	1:BY:137:TYR:CD2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:74:VAL:O	1:AR:83:ILE:CB	2.61	0.47
1:AD:94:PRO:HD2	1:AQ:100:THR:OG1	2.13	0.47
1:BC:64:LYS:HG2	1:BC:98:GLU:HG2	1.96	0.47
1:BH:34:TRP:CH2	1:CA:136:GLN:HG3	2.49	0.47
1:CA:64:LYS:HG2	1:CA:98:GLU:HG2	1.96	0.47
1:AD:8:ALA:HB3	1:AQ:119:ASN:ND2	2.29	0.47
1:AI:137:TYR:CD2	1:AI:137:TYR:N	2.82	0.47
1:AZ:121:LEU:HA	1:AZ:121:LEU:HD23	1.73	0.47
1:BL:64:LYS:HG2	1:BL:98:GLU:HG2	1.96	0.47
1:AD:130:VAL:CG2	1:AQ:63:VAL:HG11	2.44	0.47
1:AF:137:TYR:N	1:AF:137:TYR:CD2	2.82	0.47
1:AI:91:PHE:CZ	1:BM:105:CYS:HA	2.50	0.47
1:AW:64:LYS:HG2	1:AW:98:GLU:HG2	1.96	0.47
1:AX:137:TYR:CD2	1:AX:137:TYR:N	2.82	0.47
1:AZ:22:GLN:HG2	1:AZ:35:TRP:CD2	2.48	0.47
1:BA:137:TYR:CD2	1:BA:137:TYR:N	2.82	0.47
1:AE:64:LYS:HG2	1:AE:98:GLU:HG2	1.96	0.47
1:AG:64:LYS:HG2	1:AG:98:GLU:HG2	1.95	0.47
1:AT:54:ARG:NH2	1:AT:103:ASP:OD2	2.46	0.47
1:AT:64:LYS:HG2	1:AT:98:GLU:HG2	1.96	0.47
1:BI:54:ARG:NH2	1:BI:103:ASP:OD2	2.46	0.47
1:BO:82:GLY:O	1:BO:84:GLN:HG3	2.15	0.47
1:BP:137:TYR:N	1:BP:137:TYR:CD2	2.82	0.47
1:BQ:78:SER:HB2	1:BQ:83:ILE:H	1.80	0.47
1:BR:54:ARG:NH2	1:BR:103:ASP:OD2	2.46	0.47
1:BR:95:VAL:CG2	1:BT:113:ILE:HG13	2.44	0.47
1:CA:121:LEU:HD23	1:CA:121:LEU:HA	1.73	0.47
1:AB:54:ARG:NH2	1:AB:103:ASP:OD2	2.46	0.47
1:AR:120:PHE:CE2	1:BV:65:VAL:HG11	2.49	0.47
1:AT:82:GLY:O	1:AT:84:GLN:HG3	2.15	0.47
1:BE:64:LYS:HG2	1:BE:98:GLU:HG2	1.95	0.47
1:BE:78:SER:HB2	1:BE:83:ILE:H	1.80	0.47
1:BZ:78:SER:HB2	1:BZ:83:ILE:H	1.80	0.47
1:AB:119:ASN:ND2	1:BZ:8:ALA:O	2.47	0.47
1:AC:137:TYR:N	1:AC:137:TYR:CD2	2.82	0.47
1:AD:130:VAL:HG23	1:AQ:63:VAL:HG11	1.95	0.47
1:AN:82:GLY:O	1:AN:84:GLN:HG3	2.15	0.47
1:AP:78:SER:HB2	1:AP:83:ILE:H	1.80	0.47
1:AQ:64:LYS:HG2	1:AQ:98:GLU:HG2	1.96	0.47
1:BK:137:TYR:HD1	1:BP:2:ILE:HG23	1.79	0.47
1:BL:82:GLY:O	1:BL:84:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BS:137:TYR:N	1:BS:137:TYR:CD2	2.82	0.47
1:BW:78:SER:HB2	1:BW:83:ILE:H	1.80	0.47
1:AA:78:SER:HB2	1:AA:83:ILE:H	1.80	0.47
1:AB:64:LYS:HG2	1:AB:98:GLU:HG2	1.96	0.47
1:AD:78:SER:HB2	1:AD:83:ILE:H	1.80	0.47
1:AE:82:GLY:O	1:AE:84:GLN:HG3	2.15	0.47
1:AL:137:TYR:N	1:AL:137:TYR:CD2	2.82	0.47
1:AW:82:GLY:O	1:AW:84:GLN:HG3	2.15	0.47
1:AZ:82:GLY:O	1:AZ:84:GLN:HG3	2.15	0.47
1:BD:75:THR:HA	1:CF:82:GLY:O	2.15	0.47
1:BF:82:GLY:O	1:BF:84:GLN:HG3	2.15	0.47
1:BI:82:GLY:O	1:BI:84:GLN:HG3	2.15	0.47
1:BI:121:LEU:HD23	1:BI:121:LEU:HA	1.73	0.47
1:BT:78:SER:HB2	1:BT:83:ILE:H	1.80	0.47
1:BY:121:LEU:HD23	1:BY:121:LEU:HA	1.75	0.47
1:CB:137:TYR:N	1:CB:137:TYR:CD2	2.82	0.47
1:CE:137:TYR:CD2	1:CE:137:TYR:N	2.82	0.47
1:CF:78:SER:HB2	1:CF:83:ILE:H	1.80	0.47
1:CG:54:ARG:NH2	1:CG:103:ASP:OD2	2.46	0.47
1:AB:113:ILE:HG13	1:BZ:95:VAL:CG2	2.44	0.47
1:AS:78:SER:HB2	1:AS:83:ILE:H	1.80	0.47
1:BI:64:LYS:HG2	1:BI:98:GLU:HG2	1.96	0.47
1:BX:82:GLY:O	1:BX:84:GLN:HG3	2.15	0.47
1:CG:121:LEU:HD23	1:CG:121:LEU:HA	1.73	0.47
1:AG:78:SER:HB2	1:AG:83:ILE:H	1.80	0.47
1:AI:95:VAL:HG23	1:BM:113:ILE:HG13	1.97	0.47
1:AI:121:LEU:HD23	1:AI:121:LEU:HA	1.75	0.47
1:AJ:74:VAL:HG11	1:AO:84:GLN:OE1	2.15	0.47
1:AK:54:ARG:NH2	1:AK:103:ASP:OD2	2.46	0.47
1:AU:137:TYR:CD2	1:AU:137:TYR:N	2.82	0.47
1:BD:137:TYR:CD2	1:BD:137:TYR:N	2.82	0.47
1:BH:74:VAL:O	1:CB:83:ILE:HB	2.14	0.47
1:BJ:137:TYR:CD2	1:BJ:137:TYR:N	2.82	0.47
1:BK:8:ALA:O	1:BO:119:ASN:ND2	2.48	0.47
1:BN:78:SER:HB2	1:BN:83:ILE:H	1.80	0.47
1:CC:78:SER:HB2	1:CC:83:ILE:H	1.80	0.47
1:CG:82:GLY:O	1:CG:84:GLN:HG3	2.15	0.47
1:AH:64:LYS:HG2	1:AH:98:GLU:HG2	1.96	0.47
1:AJ:95:VAL:CG2	1:AN:113:ILE:HG13	2.45	0.47
1:AN:54:ARG:NH2	1:AN:103:ASP:OD2	2.46	0.47
1:AN:64:LYS:HG2	1:AN:98:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:54:ARG:NH2	1:AQ:103:ASP:OD2	2.46	0.47
1:BG:137:TYR:CD2	1:BG:137:TYR:N	2.82	0.47
1:BH:102:PRO:HG2	1:CA:91:PHE:CD2	2.50	0.47
1:BL:54:ARG:NH2	1:BL:103:ASP:OD2	2.46	0.47
1:AC:37:LYS:HE2	1:BZ:132:ASN:O	2.15	0.46
1:AD:137:TYR:CD1	1:AR:2:ILE:HG23	2.49	0.46
1:AG:37:LYS:HA	1:AG:45:TYR:CE1	2.51	0.46
1:AZ:64:LYS:HG2	1:AZ:98:GLU:HG2	1.96	0.46
1:BC:22:GLN:HG2	1:BC:35:TRP:CG	2.51	0.46
1:BF:64:LYS:HG2	1:BF:98:GLU:HG2	1.96	0.46
1:BR:82:GLY:O	1:BR:84:GLN:HG3	2.15	0.46
1:BU:22:GLN:HG2	1:BU:35:TRP:CG	2.51	0.46
1:CD:64:LYS:HG2	1:CD:98:GLU:HG2	1.96	0.46
1:CH:137:TYR:CD2	1:CH:137:TYR:N	2.82	0.46
1:AA:37:LYS:HA	1:AA:45:TYR:CE1	2.51	0.46
1:AB:120:PHE:CE2	1:BZ:65:VAL:HG11	2.50	0.46
1:AD:102:PRO:HG2	1:AQ:91:PHE:HB2	1.97	0.46
1:AH:22:GLN:HG2	1:AH:35:TRP:CG	2.51	0.46
1:AP:37:LYS:HA	1:AP:45:TYR:CE1	2.51	0.46
1:AP:74:VAL:HG11	1:BG:84:GLN:OE1	2.14	0.46
1:AP:132:ASN:O	1:BG:37:LYS:HE2	2.15	0.46
1:BD:8:ALA:O	1:CH:119:ASN:ND2	2.48	0.46
1:BI:22:GLN:HG2	1:BI:35:TRP:CG	2.51	0.46
1:BK:37:LYS:HA	1:BK:45:TYR:CE1	2.51	0.46
1:BN:37:LYS:HA	1:BN:45:TYR:CE1	2.51	0.46
1:BS:84:GLN:HB3	1:BT:74:VAL:HB	1.97	0.46
1:BT:37:LYS:HA	1:BT:45:TYR:CE1	2.51	0.46
1:CD:22:GLN:HG2	1:CD:35:TRP:CG	2.51	0.46
1:AP:52:VAL:HB	1:BF:135:PRO:HB3	1.97	0.46
1:AY:78:SER:HB2	1:AY:83:ILE:H	1.80	0.46
1:AY:100:THR:OG1	1:BC:94:PRO:HD2	2.16	0.46
1:BB:37:LYS:HA	1:BB:45:TYR:CE1	2.51	0.46
1:BX:54:ARG:NH2	1:BX:103:ASP:OD2	2.46	0.46
1:BX:73:ALA:HB1	1:CG:85:PRO:HA	1.97	0.46
1:CA:82:GLY:O	1:CA:84:GLN:HG3	2.15	0.46
1:CD:54:ARG:NH2	1:CD:103:ASP:OD2	2.46	0.46
1:CG:22:GLN:HG2	1:CG:35:TRP:CG	2.51	0.46
1:AB:79:THR:HB	1:AK:77:PRO:CB	2.45	0.46
1:AB:82:GLY:O	1:AB:84:GLN:HG3	2.15	0.46
1:AE:22:GLN:HG2	1:AE:35:TRP:CG	2.51	0.46
1:AJ:37:LYS:HA	1:AJ:45:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:64:LYS:HG2	1:AK:98:GLU:HG2	1.96	0.46
1:AM:37:LYS:HA	1:AM:45:TYR:CE1	2.51	0.46
1:AQ:22:GLN:HG2	1:AQ:35:TRP:CG	2.51	0.46
1:AS:37:LYS:HA	1:AS:45:TYR:CE1	2.51	0.46
1:BH:78:SER:HB2	1:BH:83:ILE:H	1.80	0.46
1:AO:137:TYR:N	1:AO:137:TYR:CD2	2.82	0.46
1:AZ:85:PRO:HA	1:BC:73:ALA:HB1	1.98	0.46
1:BB:78:SER:HB2	1:BB:83:ILE:H	1.80	0.46
1:BE:80:ALA:HB3	1:CH:81:SER:OG	2.16	0.46
1:BL:22:GLN:HG2	1:BL:35:TRP:CG	2.51	0.46
1:BO:22:GLN:HG2	1:BO:35:TRP:CG	2.51	0.46
1:BR:22:GLN:HG2	1:BR:35:TRP:CG	2.51	0.46
1:AD:37:LYS:HA	1:AD:45:TYR:CE1	2.51	0.46
1:AF:101:LEU:HD11	1:BJ:130:VAL:HG13	1.97	0.46
1:AR:137:TYR:CD2	1:AR:137:TYR:N	2.82	0.46
1:BA:50:ALA:HB1	1:CE:129:LEU:HD21	1.98	0.46
1:BH:37:LYS:HA	1:BH:45:TYR:CE1	2.51	0.46
1:BU:82:GLY:O	1:BU:84:GLN:HG3	2.15	0.46
1:CD:82:GLY:O	1:CD:84:GLN:HG3	2.15	0.46
1:CF:37:LYS:HA	1:CF:45:TYR:CE1	2.51	0.46
1:AK:82:GLY:O	1:AK:84:GLN:HG3	2.15	0.46
1:AQ:82:GLY:O	1:AQ:84:GLN:HG3	2.15	0.46
1:BE:108:GLN:NE2	1:CG:10:GLY:O	2.49	0.46
1:BM:137:TYR:N	1:BM:137:TYR:CD2	2.82	0.46
1:BX:34:TRP:HH2	1:CF:136:GLN:HG3	1.81	0.46
1:AH:77:PRO:CB	1:BR:79:THR:HB	2.46	0.46
1:AH:79:THR:HG22	1:AH:84:GLN:HG2	1.98	0.46
1:AO:50:ALA:HB1	1:BS:129:LEU:HD21	1.98	0.46
1:AW:22:GLN:HG2	1:AW:35:TRP:CG	2.51	0.46
1:BF:79:THR:HG22	1:BF:84:GLN:HG2	1.98	0.46
1:BG:121:LEU:HD23	1:BG:121:LEU:HA	1.75	0.46
1:BO:121:LEU:HD23	1:BO:121:LEU:HA	1.73	0.46
1:BR:135:PRO:HB3	1:BT:52:VAL:HB	1.98	0.46
1:CA:22:GLN:HG2	1:CA:35:TRP:CG	2.51	0.46
1:CD:79:THR:HG22	1:CD:84:GLN:HG2	1.98	0.46
1:CG:64:LYS:HG2	1:CG:98:GLU:HG2	1.96	0.46
1:AH:34:TRP:HH2	1:BQ:136:GLN:HG3	1.81	0.46
1:AM:50:ALA:HB1	1:BI:129:LEU:HD21	1.97	0.46
1:AM:65:VAL:HG11	1:BI:120:PHE:CE2	2.50	0.46
1:AN:22:GLN:HG2	1:AN:35:TRP:CG	2.51	0.46
1:BC:82:GLY:O	1:BC:84:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BZ:37:LYS:HA	1:BZ:45:TYR:CE1	2.51	0.46
1:CC:37:LYS:HA	1:CC:45:TYR:CE1	2.51	0.46
1:AA:8:ALA:O	1:AK:119:ASN:ND2	2.49	0.46
1:AB:22:GLN:HG2	1:AB:35:TRP:CG	2.51	0.46
1:AD:120:PHE:CE2	1:AQ:65:VAL:HG11	2.51	0.46
1:AE:54:ARG:NH2	1:AE:103:ASP:OD2	2.46	0.46
1:AK:79:THR:HG22	1:AK:84:GLN:HG2	1.98	0.46
1:AM:80:ALA:HA	1:BS:80:ALA:HB3	1.97	0.46
1:AT:22:GLN:HG2	1:AT:35:TRP:CG	2.51	0.46
1:AV:78:SER:HB2	1:AV:83:ILE:H	1.80	0.46
1:AV:121:LEU:HA	1:AV:121:LEU:HD23	1.78	0.46
1:BE:37:LYS:HA	1:BE:45:TYR:CE1	2.51	0.46
1:BF:121:LEU:HD23	1:BF:121:LEU:HA	1.73	0.46
1:BK:78:SER:HB2	1:BK:83:ILE:H	1.80	0.46
1:BX:64:LYS:HG2	1:BX:98:GLU:HG2	1.96	0.46
1:CC:121:LEU:HD23	1:CC:121:LEU:HA	1.78	0.46
1:AD:136:GLN:HG3	1:AQ:34:TRP:CH2	2.51	0.45
1:AH:82:GLY:O	1:AH:84:GLN:HG3	2.15	0.45
1:AH:129:LEU:HD21	1:BQ:50:ALA:HB1	1.97	0.45
1:AJ:78:SER:HB2	1:AJ:83:ILE:H	1.80	0.45
1:AK:79:THR:HB	1:AN:77:PRO:HB2	1.98	0.45
1:AM:78:SER:HB2	1:AM:83:ILE:H	1.80	0.45
1:AQ:79:THR:HG22	1:AQ:84:GLN:HG2	1.98	0.45
1:AT:129:LEU:HD21	1:AV:50:ALA:HB1	1.99	0.45
1:BX:79:THR:HG22	1:BX:84:GLN:HG2	1.98	0.45
1:AT:79:THR:HG22	1:AT:84:GLN:HG2	1.98	0.45
1:AV:37:LYS:HA	1:AV:45:TYR:CE1	2.51	0.45
1:AY:37:LYS:HA	1:AY:45:TYR:CE1	2.51	0.45
1:BA:129:LEU:HD21	1:CE:50:ALA:HB1	1.98	0.45
1:AK:121:LEU:HD23	1:AK:121:LEU:HA	1.73	0.45
1:AO:129:LEU:HD21	1:BS:50:ALA:HB1	1.98	0.45
1:AY:129:LEU:HD21	1:BC:50:ALA:HB1	1.97	0.45
1:AZ:22:GLN:HG2	1:AZ:35:TRP:CG	2.51	0.45
1:AH:54:ARG:NH2	1:AH:103:ASP:OD2	2.46	0.45
1:AK:22:GLN:HG2	1:AK:35:TRP:CG	2.50	0.45
1:BC:79:THR:HG22	1:BC:84:GLN:HG2	1.98	0.45
1:BK:129:LEU:HD21	1:BO:50:ALA:HB1	1.98	0.45
1:CA:54:ARG:NH2	1:CA:103:ASP:OD2	2.46	0.45
1:AH:121:LEU:HD12	1:BQ:121:LEU:HD12	1.98	0.45
1:AM:121:LEU:HD12	1:BI:121:LEU:HD12	1.98	0.45
1:AR:8:ALA:O	1:BV:119:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BQ:37:LYS:HA	1:BQ:45:TYR:CE1	2.51	0.45
1:BV:121:LEU:HD23	1:BV:121:LEU:HA	1.75	0.45
1:CH:121:LEU:HD23	1:CH:121:LEU:HA	1.75	0.45
1:AD:100:THR:OG1	1:AQ:94:PRO:HD2	2.17	0.45
1:AE:121:LEU:HD23	1:AE:121:LEU:HA	1.73	0.45
1:BK:79:THR:CG2	1:BQ:79:THR:HG21	2.47	0.45
1:AB:121:LEU:HD23	1:AB:121:LEU:HA	1.73	0.45
1:AH:77:PRO:HB2	1:BR:79:THR:HB	1.98	0.45
1:AI:80:ALA:HB2	1:BK:79:THR:O	2.17	0.45
1:AR:10:GLY:H	1:BV:112:ASP:HA	1.82	0.45
1:AW:79:THR:HG22	1:AW:84:GLN:HG2	1.98	0.45
1:AZ:54:ARG:NH2	1:AZ:103:ASP:OD2	2.46	0.45
1:BF:32:ALA:O	1:BF:49:THR:HA	2.17	0.45
1:BI:32:ALA:O	1:BI:49:THR:HA	2.17	0.45
1:BW:37:LYS:HA	1:BW:45:TYR:CE1	2.51	0.45
1:AP:8:ALA:O	1:BF:119:ASN:ND2	2.49	0.45
1:AA:113:ILE:HD12	1:AA:113:ILE:HA	1.88	0.45
1:AB:79:THR:HG22	1:AB:84:GLN:HG2	1.98	0.45
1:AQ:32:ALA:O	1:AQ:49:THR:HA	2.17	0.45
1:AS:136:GLN:HG3	1:CD:34:TRP:HH2	1.82	0.45
1:BB:121:LEU:HD23	1:BB:121:LEU:HA	1.78	0.45
1:BO:79:THR:HG22	1:BO:84:GLN:HG2	1.98	0.45
1:BU:79:THR:HG22	1:BU:84:GLN:HG2	1.98	0.45
1:BX:22:GLN:HG2	1:BX:35:TRP:CG	2.51	0.45
1:CA:79:THR:HG22	1:CA:84:GLN:HG2	1.98	0.45
1:CG:32:ALA:O	1:CG:49:THR:HA	2.17	0.45
1:AN:79:THR:HB	1:BI:77:PRO:HB2	1.99	0.45
1:AN:79:THR:HG22	1:AN:84:GLN:HG2	1.98	0.45
1:BB:113:ILE:HD12	1:BB:113:ILE:HA	1.88	0.45
1:BX:129:LEU:HD21	1:CF:50:ALA:HB1	1.99	0.45
1:AH:32:ALA:O	1:AH:49:THR:HA	2.17	0.44
1:AH:121:LEU:HD23	1:AH:121:LEU:HA	1.73	0.44
1:AR:8:ALA:HB3	1:BV:119:ASN:ND2	2.32	0.44
1:AR:74:VAL:HB	1:BT:84:GLN:HB3	1.98	0.44
1:AW:32:ALA:O	1:AW:49:THR:HA	2.17	0.44
1:BI:85:PRO:HB3	1:CA:74:VAL:O	2.17	0.44
1:CA:32:ALA:O	1:CA:49:THR:HA	2.17	0.44
1:AE:79:THR:HG22	1:AE:84:GLN:HG2	1.98	0.44
1:AF:99:PHE:CD1	1:BJ:95:VAL:HG22	2.52	0.44
1:AN:46:ARG:HG2	1:AN:69:ASP:HA	2.00	0.44
1:BE:22:GLN:HG3	1:BE:35:TRP:CE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:22:GLN:HG2	1:BF:35:TRP:CG	2.51	0.44
1:BI:79:THR:HG22	1:BI:84:GLN:HG2	1.98	0.44
1:BL:85:PRO:HB3	1:BO:74:VAL:O	2.16	0.44
1:AE:32:ALA:O	1:AE:49:THR:HA	2.17	0.44
1:AG:80:ALA:HA	1:BM:80:ALA:CB	2.47	0.44
1:AK:79:THR:HB	1:AN:77:PRO:CB	2.47	0.44
1:AV:22:GLN:HG3	1:AV:35:TRP:CE3	2.53	0.44
1:BA:80:ALA:HB2	1:CC:79:THR:O	2.16	0.44
1:BH:136:GLN:HG3	1:CA:34:TRP:CH2	2.52	0.44
1:BK:65:VAL:HG11	1:BO:120:PHE:CE2	2.52	0.44
1:BW:22:GLN:HG3	1:BW:35:TRP:CE3	2.53	0.44
1:BX:32:ALA:O	1:BX:49:THR:HA	2.17	0.44
1:CA:46:ARG:HG2	1:CA:69:ASP:HA	2.00	0.44
1:CF:22:GLN:HG3	1:CF:35:TRP:CE3	2.53	0.44
1:AB:74:VAL:O	1:CA:85:PRO:HB3	2.17	0.44
1:AB:79:THR:HB	1:AK:77:PRO:HB2	2.00	0.44
1:BC:32:ALA:O	1:BC:49:THR:HA	2.17	0.44
1:BL:79:THR:HG22	1:BL:84:GLN:HG2	1.98	0.44
1:BR:79:THR:HG22	1:BR:84:GLN:HG2	1.98	0.44
1:BT:22:GLN:HG3	1:BT:35:TRP:CE3	2.53	0.44
1:BX:94:PRO:HD2	1:CF:100:THR:OG1	2.17	0.44
1:AA:22:GLN:HG3	1:AA:35:TRP:CE3	2.53	0.44
1:AE:46:ARG:HG2	1:AE:69:ASP:HA	2.00	0.44
1:AO:76:ALA:HB2	1:BQ:77:PRO:HB2	1.99	0.44
1:AS:113:ILE:HD12	1:AS:113:ILE:HA	1.88	0.44
1:AZ:79:THR:HG22	1:AZ:84:GLN:HG2	1.98	0.44
1:BR:77:PRO:CB	1:BU:79:THR:HB	2.48	0.44
1:BU:46:ARG:HG2	1:BU:69:ASP:HA	2.00	0.44
1:BZ:22:GLN:HG3	1:BZ:35:TRP:CE3	2.53	0.44
1:CG:79:THR:HG22	1:CG:84:GLN:HG2	1.98	0.44
1:AD:22:GLN:HG3	1:AD:35:TRP:CE3	2.53	0.44
1:AG:22:GLN:HG3	1:AG:35:TRP:CE3	2.53	0.44
1:AK:32:ALA:O	1:AK:49:THR:HA	2.17	0.44
1:AK:46:ARG:HG2	1:AK:69:ASP:HA	2.00	0.44
1:AM:136:GLN:HG3	1:BI:34:TRP:HH2	1.82	0.44
1:AS:50:ALA:HB1	1:CD:129:LEU:HD21	2.00	0.44
1:BL:46:ARG:HG2	1:BL:69:ASP:HA	2.00	0.44
1:BN:22:GLN:HG3	1:BN:35:TRP:CE3	2.53	0.44
1:BR:121:LEU:HD23	1:BR:121:LEU:HA	1.73	0.44
1:AD:8:ALA:O	1:AQ:119:ASN:ND2	2.50	0.44
1:AN:32:ALA:O	1:AN:49:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:22:GLN:HG3	1:AS:35:TRP:CE3	2.53	0.44
1:AX:50:ALA:HB1	1:CB:129:LEU:HD21	1.99	0.44
1:AY:65:VAL:HG11	1:BC:120:PHE:CE2	2.52	0.44
1:AZ:32:ALA:O	1:AZ:49:THR:HA	2.17	0.44
1:BK:22:GLN:HG3	1:BK:35:TRP:CE3	2.53	0.44
1:BU:32:ALA:O	1:BU:49:THR:HA	2.17	0.44
1:BU:54:ARG:NH2	1:BU:103:ASP:OD2	2.46	0.44
1:CD:121:LEU:HA	1:CD:121:LEU:HD23	1.73	0.44
1:CG:46:ARG:HG2	1:CG:69:ASP:HA	2.00	0.44
1:BQ:22:GLN:HG3	1:BQ:35:TRP:CE3	2.53	0.44
1:CB:121:LEU:HD23	1:CB:121:LEU:HA	1.75	0.44
1:AH:46:ARG:HG2	1:AH:69:ASP:HA	2.00	0.44
1:AP:22:GLN:HG3	1:AP:35:TRP:CE3	2.53	0.44
1:AS:121:LEU:HD12	1:CD:121:LEU:HD12	1.98	0.44
1:AB:32:ALA:O	1:AB:49:THR:HA	2.17	0.43
1:AB:46:ARG:HG2	1:AB:69:ASP:HA	2.00	0.43
1:AJ:5:VAL:HG21	1:AJ:48:LEU:CD2	2.48	0.43
1:AY:22:GLN:HG3	1:AY:35:TRP:CE3	2.53	0.43
1:BE:5:VAL:HG21	1:BE:48:LEU:CD2	2.49	0.43
1:BW:5:VAL:HG21	1:BW:48:LEU:CD2	2.48	0.43
1:BY:81:SER:OG	1:CF:80:ALA:HB3	2.17	0.43
1:AB:77:PRO:HB2	1:CA:79:THR:HB	2.00	0.43
1:AD:79:THR:OG1	1:AR:80:ALA:HA	2.15	0.43
1:AL:101:LEU:HD11	1:BP:130:VAL:HG13	2.00	0.43
1:AM:5:VAL:HG21	1:AM:48:LEU:CD2	2.48	0.43
1:AP:5:VAL:HG21	1:AP:48:LEU:CD2	2.48	0.43
1:AT:32:ALA:O	1:AT:49:THR:HA	2.17	0.43
1:AW:54:ARG:NH2	1:AW:103:ASP:OD2	2.46	0.43
1:AY:5:VAL:HG21	1:AY:48:LEU:CD2	2.48	0.43
1:AZ:46:ARG:HG2	1:AZ:69:ASP:HA	2.00	0.43
1:BR:46:ARG:HG2	1:BR:69:ASP:HA	2.00	0.43
1:BX:119:ASN:ND2	1:CF:8:ALA:O	2.51	0.43
1:AQ:79:THR:CB	1:BF:77:PRO:HB2	2.48	0.43
1:AY:34:TRP:HH2	1:BC:136:GLN:HG3	1.84	0.43
1:BB:5:VAL:HG21	1:BB:48:LEU:CD2	2.48	0.43
1:AF:10:GLY:O	1:BJ:108:GLN:OE1	2.36	0.43
1:AP:71:THR:HG21	1:BF:109:ASN:ND2	2.34	0.43
1:AU:114:LEU:HD21	1:BY:127:THR:HA	2.00	0.43
1:BA:95:VAL:CG2	1:CE:113:ILE:HG13	2.49	0.43
1:BH:22:GLN:HG3	1:BH:35:TRP:CE3	2.53	0.43
1:BI:74:VAL:CG1	1:BI:85:PRO:HG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:74:VAL:CG1	1:BL:85:PRO:HG2	2.49	0.43
1:BO:46:ARG:HG2	1:BO:69:ASP:HA	2.00	0.43
1:BR:32:ALA:O	1:BR:49:THR:HA	2.17	0.43
1:BT:5:VAL:HG21	1:BT:48:LEU:CD2	2.49	0.43
1:CC:5:VAL:HG21	1:CC:48:LEU:CD2	2.48	0.43
1:CC:22:GLN:HG3	1:CC:35:TRP:CE3	2.53	0.43
1:CD:32:ALA:O	1:CD:49:THR:HA	2.17	0.43
1:AG:5:VAL:HG21	1:AG:48:LEU:CD2	2.48	0.43
1:AK:74:VAL:CG1	1:AK:85:PRO:HG2	2.49	0.43
1:AX:121:LEU:HD23	1:AX:121:LEU:HA	1.75	0.43
1:BO:32:ALA:O	1:BO:49:THR:HA	2.17	0.43
1:CF:5:VAL:HG21	1:CF:48:LEU:CD2	2.48	0.43
1:AA:121:LEU:HD23	1:AA:121:LEU:HA	1.78	0.43
1:AD:5:VAL:HG21	1:AD:48:LEU:CD2	2.48	0.43
1:AH:74:VAL:O	1:BR:85:PRO:HB3	2.18	0.43
1:AJ:22:GLN:HG3	1:AJ:35:TRP:CE3	2.53	0.43
1:AT:74:VAL:CG1	1:AT:85:PRO:HG2	2.49	0.43
1:AY:121:LEU:HA	1:AY:121:LEU:HD23	1.78	0.43
1:BI:39:SER:OG	1:BI:40:PRO:HD2	2.19	0.43
1:BL:32:ALA:O	1:BL:49:THR:HA	2.17	0.43
1:BN:121:LEU:HD23	1:BN:121:LEU:HA	1.78	0.43
1:BQ:5:VAL:HG21	1:BQ:48:LEU:CD2	2.49	0.43
1:BU:39:SER:OG	1:BU:40:PRO:HD2	2.19	0.43
1:BZ:113:ILE:HD12	1:BZ:113:ILE:HA	1.88	0.43
1:CA:74:VAL:CG1	1:CA:85:PRO:HG2	2.49	0.43
1:CD:46:ARG:HG2	1:CD:69:ASP:HA	2.00	0.43
1:AB:74:VAL:CG1	1:AB:85:PRO:HG2	2.49	0.43
1:AM:22:GLN:HG3	1:AM:35:TRP:CE3	2.53	0.43
1:AT:46:ARG:HG2	1:AT:69:ASP:HA	2.00	0.43
1:AY:52:VAL:HB	1:BC:135:PRO:HB3	2.01	0.43
1:BA:91:PHE:CZ	1:CE:105:CYS:HA	2.54	0.43
1:BS:37:LYS:HE2	1:BT:132:ASN:O	2.18	0.43
1:BT:32:ALA:O	1:BT:49:THR:HA	2.19	0.43
1:BX:39:SER:OG	1:BX:40:PRO:HD2	2.19	0.43
1:AD:121:LEU:HD12	1:AQ:121:LEU:HD12	2.00	0.43
1:AL:113:ILE:HD12	1:AL:113:ILE:HA	1.90	0.43
1:AN:74:VAL:CG1	1:AN:85:PRO:HG2	2.49	0.43
1:AQ:39:SER:OG	1:AQ:40:PRO:HD2	2.19	0.43
1:AS:5:VAL:HG21	1:AS:48:LEU:CD2	2.48	0.43
1:BC:39:SER:OG	1:BC:40:PRO:HD2	2.19	0.43
1:BC:46:ARG:HG2	1:BC:69:ASP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:32:ALA:O	1:BK:49:THR:HA	2.19	0.43
1:BW:32:ALA:O	1:BW:49:THR:HA	2.19	0.43
1:AE:74:VAL:CG1	1:AE:85:PRO:HG2	2.49	0.43
1:AJ:32:ALA:O	1:AJ:49:THR:HA	2.19	0.43
1:AQ:74:VAL:CG1	1:AQ:85:PRO:HG2	2.49	0.43
1:AV:5:VAL:HG21	1:AV:48:LEU:CD2	2.49	0.43
1:BC:74:VAL:CG1	1:BC:85:PRO:HG2	2.49	0.43
1:CD:39:SER:OG	1:CD:40:PRO:HD2	2.19	0.43
1:AD:7:LEU:HD13	1:AQ:116:TYR:O	2.19	0.43
1:AD:32:ALA:O	1:AD:49:THR:HA	2.19	0.43
1:AJ:84:GLN:HB3	1:BP:74:VAL:HB	2.00	0.43
1:AL:95:VAL:CG2	1:BP:113:ILE:HG13	2.49	0.43
1:AM:32:ALA:O	1:AM:49:THR:HA	2.19	0.43
1:AQ:46:ARG:HG2	1:AQ:69:ASP:HA	2.00	0.43
1:AV:32:ALA:O	1:AV:49:THR:HA	2.19	0.43
1:AW:39:SER:OG	1:AW:40:PRO:HD2	2.19	0.43
1:AZ:85:PRO:HB3	1:BC:74:VAL:O	2.18	0.43
1:BB:22:GLN:HG3	1:BB:35:TRP:CE3	2.53	0.43
1:BE:32:ALA:O	1:BE:49:THR:HA	2.19	0.43
1:BE:137:TYR:CZ	1:CG:1:GLN:HA	2.53	0.43
1:BF:39:SER:OG	1:BF:40:PRO:HD2	2.19	0.43
1:BO:39:SER:OG	1:BO:40:PRO:HD2	2.19	0.43
1:BO:74:VAL:CG1	1:BO:85:PRO:HG2	2.49	0.43
1:BQ:32:ALA:O	1:BQ:49:THR:HA	2.19	0.43
1:BR:39:SER:OG	1:BR:40:PRO:HD2	2.19	0.43
1:BZ:32:ALA:O	1:BZ:49:THR:HA	2.19	0.43
1:CD:74:VAL:CG1	1:CD:85:PRO:HG2	2.49	0.43
1:CE:113:ILE:HD12	1:CE:113:ILE:HA	1.90	0.43
1:AB:39:SER:OG	1:AB:40:PRO:HD2	2.19	0.42
1:AD:7:LEU:CD1	1:AQ:120:PHE:HB2	2.49	0.42
1:AX:114:LEU:HD21	1:CB:127:THR:HA	2.00	0.42
1:AY:121:LEU:HD12	1:BC:121:LEU:HD12	2.01	0.42
1:BF:46:ARG:HG2	1:BF:69:ASP:HA	2.00	0.42
1:BH:137:TYR:CZ	1:CA:1:GLN:HA	2.54	0.42
1:BI:46:ARG:HG2	1:BI:69:ASP:HA	2.00	0.42
1:BM:121:LEU:HD23	1:BM:121:LEU:HA	1.75	0.42
1:BN:5:VAL:HG21	1:BN:48:LEU:CD2	2.48	0.42
1:BZ:5:VAL:HG21	1:BZ:48:LEU:CD2	2.49	0.42
1:AB:95:VAL:CG2	1:BZ:113:ILE:HG13	2.49	0.42
1:AD:46:ARG:NE	1:AD:69:ASP:OD1	2.53	0.42
1:AD:135:PRO:HB3	1:AQ:25:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:32:ALA:O	1:AS:49:THR:HA	2.19	0.42
1:AU:127:THR:HA	1:BY:114:LEU:HD21	2.01	0.42
1:AW:74:VAL:CG1	1:AW:85:PRO:HG2	2.49	0.42
1:AZ:74:VAL:CG1	1:AZ:85:PRO:HG2	2.49	0.42
1:BU:74:VAL:CG1	1:BU:85:PRO:HG2	2.49	0.42
1:BW:113:ILE:HD12	1:BW:113:ILE:HA	1.88	0.42
1:AF:95:VAL:HG23	1:BJ:113:ILE:HG13	2.01	0.42
1:AH:39:SER:OG	1:AH:40:PRO:HD2	2.19	0.42
1:AH:74:VAL:CG1	1:AH:85:PRO:HG2	2.49	0.42
1:AL:114:LEU:CD2	1:BP:127:THR:HA	2.49	0.42
1:BR:74:VAL:CG1	1:BR:85:PRO:HG2	2.49	0.42
1:CG:39:SER:OG	1:CG:40:PRO:HD2	2.19	0.42
1:AA:46:ARG:NE	1:AA:69:ASP:OD1	2.53	0.42
1:AE:85:PRO:HA	1:AQ:73:ALA:HB1	2.01	0.42
1:AF:50:ALA:HB1	1:BJ:129:LEU:HD21	2.01	0.42
1:AK:39:SER:OG	1:AK:40:PRO:HD2	2.19	0.42
1:AN:39:SER:OG	1:AN:40:PRO:HD2	2.19	0.42
1:AP:113:ILE:HG13	1:BF:95:VAL:HG22	2.01	0.42
1:AV:80:ALA:HA	1:CB:80:ALA:HB3	1.96	0.42
1:BU:121:LEU:HA	1:BU:121:LEU:HD23	1.73	0.42
1:BZ:46:ARG:NE	1:BZ:69:ASP:OD1	2.53	0.42
1:AD:120:PHE:CE1	1:AQ:48:LEU:HD21	2.54	0.42
1:AH:135:PRO:HB3	1:BQ:52:VAL:HB	2.01	0.42
1:AR:121:LEU:HA	1:AR:121:LEU:HD23	1.75	0.42
1:AX:36:GLU:HB3	1:AX:46:ARG:H	1.85	0.42
1:BH:5:VAL:HG21	1:BH:48:LEU:CD2	2.48	0.42
1:BH:34:TRP:HH2	1:CA:136:GLN:HG3	1.85	0.42
1:BH:112:ASP:HA	1:CA:10:GLY:H	1.84	0.42
1:BM:36:GLU:HB3	1:BM:46:ARG:H	1.85	0.42
1:BQ:121:LEU:HD23	1:BQ:121:LEU:HA	1.78	0.42
1:CA:39:SER:OG	1:CA:40:PRO:HD2	2.19	0.42
1:AE:34:TRP:HH2	1:BW:136:GLN:HG3	1.84	0.42
1:AE:121:LEU:HD13	1:BW:117:ALA:HB1	2.02	0.42
1:AK:76:ALA:HB3	1:AN:76:ALA:HA	2.02	0.42
1:AL:36:GLU:HB3	1:AL:46:ARG:H	1.85	0.42
1:AW:46:ARG:HG2	1:AW:69:ASP:HA	2.00	0.42
1:BK:136:GLN:HG3	1:BO:34:TRP:HH2	1.84	0.42
1:BN:32:ALA:O	1:BN:49:THR:HA	2.19	0.42
1:BV:36:GLU:HB3	1:BV:46:ARG:H	1.85	0.42
1:CF:121:LEU:HA	1:CF:121:LEU:HD23	1.78	0.42
1:AC:36:GLU:HB3	1:AC:46:ARG:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:121:LEU:HD23	1:AG:121:LEU:HA	1.78	0.42
1:AP:32:ALA:O	1:AP:49:THR:HA	2.19	0.42
1:AR:36:GLU:HB3	1:AR:46:ARG:H	1.85	0.42
1:BF:74:VAL:CG1	1:BF:85:PRO:HG2	2.49	0.42
1:BH:102:PRO:HG2	1:CA:91:PHE:HB2	2.02	0.42
1:BK:5:VAL:HG21	1:BK:48:LEU:CD2	2.49	0.42
1:BW:46:ARG:NE	1:BW:69:ASP:OD1	2.53	0.42
1:BX:74:VAL:CG1	1:BX:85:PRO:HG2	2.49	0.42
1:CC:32:ALA:O	1:CC:49:THR:HA	2.19	0.42
1:CD:5:VAL:HG21	1:CD:48:LEU:CD2	2.50	0.42
1:AA:32:ALA:O	1:AA:49:THR:HA	2.19	0.42
1:AA:52:VAL:HB	1:AK:135:PRO:HB3	2.01	0.42
1:AA:120:PHE:CE2	1:AK:65:VAL:HG11	2.54	0.42
1:AB:77:PRO:CB	1:CA:79:THR:HB	2.50	0.42
1:AE:5:VAL:HG21	1:AE:48:LEU:CD2	2.50	0.42
1:AE:119:ASN:ND2	1:BW:8:ALA:O	2.52	0.42
1:AK:47:ARG:HB2	1:AK:68:TYR:HB2	2.02	0.42
1:AQ:5:VAL:HG21	1:AQ:48:LEU:CD2	2.50	0.42
1:AY:32:ALA:O	1:AY:49:THR:HA	2.19	0.42
1:AZ:47:ARG:HB2	1:AZ:68:TYR:HB2	2.02	0.42
1:BH:97:ILE:HA	1:CA:96:PHE:O	2.19	0.42
1:BJ:36:GLU:HB3	1:BJ:46:ARG:H	1.85	0.42
1:BX:46:ARG:HG2	1:BX:69:ASP:HA	2.00	0.42
1:CF:32:ALA:O	1:CF:49:THR:HA	2.19	0.42
1:CG:5:VAL:HG21	1:CG:48:LEU:CD2	2.50	0.42
1:AA:5:VAL:HG21	1:AA:48:LEU:CD2	2.48	0.42
1:AE:39:SER:OG	1:AE:40:PRO:HD2	2.19	0.42
1:AG:32:ALA:O	1:AG:49:THR:HA	2.19	0.42
1:AN:49:THR:O	1:AN:65:VAL:HA	2.20	0.42
1:AT:5:VAL:HG21	1:AT:48:LEU:CD2	2.50	0.42
1:AT:39:SER:OG	1:AT:40:PRO:HD2	2.19	0.42
1:AT:95:VAL:CG2	1:AV:113:ILE:HG13	2.50	0.42
1:AU:36:GLU:HB3	1:AU:46:ARG:H	1.85	0.42
1:AX:121:LEU:HD12	1:CB:121:LEU:HD12	2.02	0.42
1:BP:36:GLU:HB3	1:BP:46:ARG:H	1.85	0.42
1:CG:74:VAL:CG1	1:CG:85:PRO:HG2	2.49	0.42
1:AA:129:LEU:HD21	1:AK:50:ALA:HB1	2.01	0.42
1:AS:46:ARG:NE	1:AS:69:ASP:OD1	2.53	0.42
1:AT:49:THR:O	1:AT:65:VAL:HA	2.20	0.42
1:AZ:49:THR:O	1:AZ:65:VAL:HA	2.20	0.42
1:BB:46:ARG:NE	1:BB:69:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:5:VAL:HG21	1:BC:48:LEU:CD2	2.50	0.42
1:BH:125:THR:HG21	1:CA:5:VAL:HG12	2.00	0.42
1:BI:47:ARG:HB2	1:BI:68:TYR:HB2	2.02	0.42
1:BJ:121:LEU:HA	1:BJ:121:LEU:HD23	1.75	0.42
1:BL:49:THR:O	1:BL:65:VAL:HA	2.20	0.42
1:BL:79:THR:HB	1:BO:77:PRO:HB2	2.02	0.42
1:BO:5:VAL:HG21	1:BO:48:LEU:CD2	2.50	0.42
1:BO:47:ARG:HB2	1:BO:68:TYR:HB2	2.02	0.42
1:BO:49:THR:O	1:BO:65:VAL:HA	2.20	0.42
1:CG:47:ARG:HB2	1:CG:68:TYR:HB2	2.02	0.42
1:AA:5:VAL:HG21	1:AA:48:LEU:HD23	2.02	0.41
1:AE:49:THR:O	1:AE:65:VAL:HA	2.20	0.41
1:AJ:1:GLN:O	1:AN:136:GLN:NE2	2.53	0.41
1:AK:8:ALA:HB1	1:AK:14:PRO:CB	2.50	0.41
1:AO:36:GLU:HB3	1:AO:46:ARG:H	1.85	0.41
1:AW:49:THR:O	1:AW:65:VAL:HA	2.20	0.41
1:BA:36:GLU:HB3	1:BA:46:ARG:H	1.85	0.41
1:BB:5:VAL:HG21	1:BB:48:LEU:HD23	2.02	0.41
1:BC:47:ARG:HB2	1:BC:68:TYR:HB2	2.02	0.41
1:BD:36:GLU:HB3	1:BD:46:ARG:H	1.85	0.41
1:BD:127:THR:HA	1:CH:114:LEU:CD2	2.49	0.41
1:BI:8:ALA:HB1	1:BI:14:PRO:CB	2.50	0.41
1:BK:79:THR:HG23	1:BQ:79:THR:HG21	2.02	0.41
1:AH:47:ARG:HB2	1:AH:68:TYR:HB2	2.02	0.41
1:AI:36:GLU:HB3	1:AI:46:ARG:H	1.85	0.41
1:AI:130:VAL:HG13	1:BM:101:LEU:HD11	2.01	0.41
1:AN:8:ALA:HB1	1:AN:14:PRO:CB	2.50	0.41
1:AT:47:ARG:HB2	1:AT:68:TYR:HB2	2.02	0.41
1:AX:127:THR:HA	1:CB:114:LEU:HD21	2.02	0.41
1:AZ:5:VAL:HG21	1:AZ:48:LEU:CD2	2.50	0.41
1:AZ:39:SER:OG	1:AZ:40:PRO:HD2	2.19	0.41
1:BB:32:ALA:O	1:BB:49:THR:HA	2.19	0.41
1:BD:127:THR:HA	1:CH:114:LEU:HD21	2.01	0.41
1:BG:36:GLU:HB3	1:BG:46:ARG:H	1.85	0.41
1:BI:49:THR:O	1:BI:65:VAL:HA	2.20	0.41
1:BK:34:TRP:HH2	1:BO:136:GLN:HG3	1.85	0.41
1:BL:39:SER:OG	1:BL:40:PRO:HD2	2.19	0.41
1:BQ:5:VAL:HG21	1:BQ:48:LEU:HD23	2.03	0.41
1:AF:129:LEU:HD21	1:BJ:50:ALA:HB1	2.01	0.41
1:AJ:5:VAL:HG21	1:AJ:48:LEU:HD23	2.03	0.41
1:AN:5:VAL:HG21	1:AN:48:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:127:THR:HA	1:BV:114:LEU:CD2	2.50	0.41
1:AV:46:ARG:NE	1:AV:69:ASP:OD1	2.53	0.41
1:BF:8:ALA:HB1	1:BF:14:PRO:CB	2.51	0.41
1:BS:121:LEU:HD23	1:BS:121:LEU:HA	1.75	0.41
1:BW:121:LEU:HD23	1:BW:121:LEU:HA	1.78	0.41
1:BY:36:GLU:HB3	1:BY:46:ARG:H	1.85	0.41
1:CA:8:ALA:HB1	1:CA:14:PRO:CB	2.50	0.41
1:CG:49:THR:O	1:CG:65:VAL:HA	2.20	0.41
1:AE:8:ALA:HB1	1:AE:14:PRO:CB	2.50	0.41
1:AT:119:ASN:ND2	1:AV:8:ALA:O	2.54	0.41
1:AT:135:PRO:HB3	1:AV:52:VAL:HB	2.01	0.41
1:AW:5:VAL:HG21	1:AW:48:LEU:CD2	2.50	0.41
1:AW:54:ARG:HD2	1:AX:35:TRP:HH2	1.86	0.41
1:BF:47:ARG:HB2	1:BF:68:TYR:HB2	2.02	0.41
1:BF:49:THR:O	1:BF:65:VAL:HA	2.20	0.41
1:BH:5:VAL:HG21	1:BH:48:LEU:HD23	2.02	0.41
1:BH:32:ALA:O	1:BH:49:THR:HA	2.19	0.41
1:BK:46:ARG:NE	1:BK:69:ASP:OD1	2.53	0.41
1:BN:5:VAL:HG21	1:BN:48:LEU:HD23	2.02	0.41
1:BW:5:VAL:HG21	1:BW:48:LEU:HD23	2.02	0.41
1:BX:49:THR:O	1:BX:65:VAL:HA	2.20	0.41
1:AF:99:PHE:CE1	1:BJ:95:VAL:HG22	2.54	0.41
1:AM:79:THR:CG2	1:BT:79:THR:HG21	2.51	0.41
1:AQ:47:ARG:HB2	1:AQ:68:TYR:HB2	2.02	0.41
1:AU:121:LEU:HD23	1:AU:121:LEU:HA	1.75	0.41
1:AW:47:ARG:HB2	1:AW:68:TYR:HB2	2.02	0.41
1:AY:5:VAL:HG21	1:AY:48:LEU:HD23	2.02	0.41
1:BF:5:VAL:HG21	1:BF:48:LEU:CD2	2.50	0.41
1:BK:5:VAL:HG21	1:BK:48:LEU:HD23	2.03	0.41
1:BR:5:VAL:HG21	1:BR:48:LEU:CD2	2.50	0.41
1:BR:54:ARG:HD2	1:BS:35:TRP:HH2	1.86	0.41
1:BT:5:VAL:HG21	1:BT:48:LEU:HD23	2.03	0.41
1:BV:113:ILE:HD12	1:BV:113:ILE:HA	1.90	0.41
1:BX:8:ALA:HB1	1:BX:14:PRO:CB	2.50	0.41
1:CC:46:ARG:NE	1:CC:69:ASP:OD1	2.53	0.41
1:AA:136:GLN:HG3	1:AK:34:TRP:CH2	2.55	0.41
1:AB:5:VAL:HG21	1:AB:48:LEU:CD2	2.50	0.41
1:AE:54:ARG:HD2	1:AF:35:TRP:HH2	1.86	0.41
1:AI:67:ILE:HD13	1:BM:116:TYR:HB3	2.03	0.41
1:AJ:46:ARG:NE	1:AJ:69:ASP:OD1	2.53	0.41
1:AT:94:PRO:HD2	1:AV:100:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:5:VAL:HG21	1:BE:48:LEU:HD23	2.02	0.41
1:BE:121:LEU:HA	1:BE:121:LEU:HD23	1.78	0.41
1:BH:46:ARG:NE	1:BH:69:ASP:OD1	2.53	0.41
1:BK:113:ILE:HD12	1:BK:113:ILE:HA	1.88	0.41
1:BL:8:ALA:HB1	1:BL:14:PRO:CB	2.50	0.41
1:BR:49:THR:O	1:BR:65:VAL:HA	2.20	0.41
1:BX:54:ARG:HD2	1:BY:35:TRP:HH2	1.86	0.41
1:CA:5:VAL:HG21	1:CA:48:LEU:CD2	2.50	0.41
1:CA:49:THR:O	1:CA:65:VAL:HA	2.20	0.41
1:CD:8:ALA:HB1	1:CD:14:PRO:CB	2.50	0.41
1:CE:36:GLU:HB3	1:CE:46:ARG:H	1.85	0.41
1:AB:8:ALA:HB1	1:AB:14:PRO:CB	2.50	0.41
1:AC:25:GLN:NE2	1:AC:52:VAL:O	2.52	0.41
1:AH:54:ARG:HD2	1:AI:35:TRP:HH2	1.86	0.41
1:AK:5:VAL:HG21	1:AK:48:LEU:CD2	2.50	0.41
1:AT:8:ALA:HB1	1:AT:14:PRO:CB	2.50	0.41
1:BA:113:ILE:HG13	1:CE:95:VAL:CG2	2.50	0.41
1:BC:8:ALA:HB1	1:BC:14:PRO:CB	2.51	0.41
1:BM:113:ILE:HD12	1:BM:113:ILE:HA	1.90	0.41
1:BX:47:ARG:HB2	1:BX:68:TYR:HB2	2.02	0.41
1:CF:46:ARG:NE	1:CF:69:ASP:OD1	2.53	0.41
1:CH:36:GLU:HB3	1:CH:46:ARG:H	1.85	0.41
1:AH:5:VAL:HG21	1:AH:48:LEU:CD2	2.50	0.41
1:AQ:54:ARG:HD2	1:AR:35:TRP:HH2	1.86	0.41
1:AU:37:LYS:HE2	1:AV:132:ASN:O	2.21	0.41
1:BU:47:ARG:HB2	1:BU:68:TYR:HB2	2.02	0.41
1:AB:49:THR:O	1:AB:65:VAL:HA	2.20	0.41
1:AK:49:THR:O	1:AK:65:VAL:HA	2.20	0.41
1:AQ:8:ALA:HB1	1:AQ:14:PRO:CB	2.50	0.41
1:AQ:49:THR:O	1:AQ:65:VAL:HA	2.20	0.41
1:AZ:8:ALA:HB1	1:AZ:14:PRO:CB	2.50	0.41
1:AZ:54:ARG:HD2	1:BA:35:TRP:HH2	1.86	0.41
1:BD:129:LEU:HD21	1:CH:50:ALA:HB1	2.01	0.41
1:BH:7:LEU:CD1	1:CA:120:PHE:HB2	2.51	0.41
1:BI:5:VAL:HG21	1:BI:48:LEU:CD2	2.50	0.41
1:BK:132:ASN:O	1:BP:37:LYS:HE2	2.20	0.41
1:BL:47:ARG:HB2	1:BL:68:TYR:HB2	2.02	0.41
1:BR:34:TRP:HH2	1:BT:136:GLN:HG3	1.86	0.41
1:BR:47:ARG:HB2	1:BR:68:TYR:HB2	2.02	0.41
1:BS:84:GLN:OE1	1:BT:74:VAL:HG11	2.20	0.41
1:BT:46:ARG:NE	1:BT:69:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BT:105:CYS:HB3	1:BU:42:LEU:HD12	2.03	0.41
1:BU:5:VAL:HG21	1:BU:48:LEU:CD2	2.50	0.41
1:BU:49:THR:O	1:BU:65:VAL:HA	2.20	0.41
1:BX:5:VAL:HG21	1:BX:48:LEU:CD2	2.50	0.41
1:BZ:105:CYS:HB3	1:CA:42:LEU:HD12	2.03	0.41
1:CD:54:ARG:HD2	1:CE:35:TRP:HH2	1.86	0.41
1:AD:80:ALA:HA	1:BJ:80:ALA:HB2	2.02	0.41
1:AF:67:ILE:HD13	1:BJ:116:TYR:HB3	2.02	0.41
1:AP:5:VAL:HG21	1:AP:48:LEU:HD23	2.02	0.41
1:AT:54:ARG:HD2	1:AU:35:TRP:HH2	1.86	0.41
1:AX:129:LEU:HD21	1:CB:50:ALA:HB1	2.03	0.41
1:AY:25:GLN:O	1:BC:137:TYR:HA	2.21	0.41
1:AY:26:ASN:OD1	1:BC:137:TYR:HB2	2.20	0.41
1:BH:65:VAL:HG11	1:CA:120:PHE:CE2	2.56	0.41
1:BO:8:ALA:HB1	1:BO:14:PRO:CB	2.50	0.41
1:BS:36:GLU:HB3	1:BS:46:ARG:H	1.85	0.41
1:CA:47:ARG:HB2	1:CA:68:TYR:HB2	2.02	0.41
1:CC:113:ILE:HD12	1:CC:113:ILE:HA	1.88	0.41
1:CD:47:ARG:HB2	1:CD:68:TYR:HB2	2.02	0.41
1:AF:134:ALA:HA	1:BH:22:GLN:NE2	2.35	0.40
1:AP:116:TYR:HB3	1:BF:67:ILE:HD13	2.03	0.40
1:AS:5:VAL:HG21	1:AS:48:LEU:HD23	2.02	0.40
1:AW:113:ILE:HD12	1:AW:113:ILE:HA	1.96	0.40
1:BF:5:VAL:HG21	1:BF:48:LEU:HD23	2.04	0.40
1:BL:54:ARG:HD2	1:BM:35:TRP:HH2	1.86	0.40
1:BX:74:VAL:O	1:CG:85:PRO:HB3	2.20	0.40
1:BX:121:LEU:HD23	1:BX:121:LEU:HA	1.73	0.40
1:BZ:5:VAL:HG21	1:BZ:48:LEU:HD23	2.03	0.40
1:CD:49:THR:O	1:CD:65:VAL:HA	2.20	0.40
1:CF:105:CYS:HB3	1:CG:42:LEU:HD12	2.03	0.40
1:AG:80:ALA:HA	1:BM:80:ALA:HB2	2.03	0.40
1:AM:105:CYS:HB3	1:AN:42:LEU:HD12	2.03	0.40
1:AP:105:CYS:HB3	1:AQ:42:LEU:HD12	2.03	0.40
1:AQ:121:LEU:HD23	1:AQ:121:LEU:HA	1.73	0.40
1:AS:105:CYS:HB3	1:AT:42:LEU:HD12	2.03	0.40
1:AV:105:CYS:HB3	1:AW:42:LEU:HD12	2.03	0.40
1:AY:79:THR:O	1:CE:80:ALA:HB2	2.22	0.40
1:BB:39:SER:OG	1:BB:40:PRO:HD2	2.22	0.40
1:BC:54:ARG:HD2	1:BD:35:TRP:HH2	1.86	0.40
1:BD:25:GLN:NE2	1:BD:52:VAL:O	2.52	0.40
1:BF:54:ARG:HD2	1:BG:35:TRP:HH2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:85:PRO:HA	1:CG:73:ALA:HB1	2.02	0.40
1:BG:25:GLN:NE2	1:BG:52:VAL:O	2.52	0.40
1:BH:113:ILE:HD12	1:BH:113:ILE:HA	1.88	0.40
1:CA:54:ARG:HD2	1:CB:35:TRP:HH2	1.86	0.40
1:AB:47:ARG:HB2	1:AB:68:TYR:HB2	2.02	0.40
1:AG:5:VAL:HG21	1:AG:48:LEU:HD23	2.02	0.40
1:AJ:121:LEU:HA	1:AJ:121:LEU:HD23	1.78	0.40
1:AM:95:VAL:CG2	1:BI:113:ILE:HG13	2.52	0.40
1:AV:39:SER:OG	1:AV:40:PRO:HD2	2.22	0.40
1:AY:105:CYS:HB3	1:AZ:42:LEU:HD12	2.03	0.40
1:BB:105:CYS:HB3	1:BC:42:LEU:HD12	2.03	0.40
1:BE:46:ARG:NE	1:BE:69:ASP:OD1	2.53	0.40
1:BH:39:SER:OG	1:BH:40:PRO:HD2	2.22	0.40
1:BI:54:ARG:HD2	1:BJ:35:TRP:HH2	1.86	0.40
1:BU:5:VAL:HG21	1:BU:48:LEU:HD23	2.04	0.40
1:BU:54:ARG:HD2	1:BV:35:TRP:HH2	1.86	0.40
1:AD:5:VAL:HG21	1:AD:48:LEU:HD23	2.02	0.40
1:AE:5:VAL:HG12	1:BW:125:THR:HG21	2.03	0.40
1:AG:39:SER:OG	1:AG:40:PRO:HD2	2.22	0.40
1:AH:49:THR:O	1:AH:65:VAL:HA	2.20	0.40
1:AL:25:GLN:NE2	1:AL:52:VAL:O	2.52	0.40
1:AV:5:VAL:HG21	1:AV:48:LEU:HD23	2.03	0.40
1:BK:105:CYS:HB3	1:BL:42:LEU:HD12	2.03	0.40
1:BL:5:VAL:HG21	1:BL:48:LEU:CD2	2.50	0.40
1:BN:46:ARG:NE	1:BN:69:ASP:OD1	2.53	0.40
1:BW:105:CYS:HB3	1:BX:42:LEU:HD12	2.03	0.40
1:CC:105:CYS:HB3	1:CD:42:LEU:HD12	2.03	0.40
1:AE:47:ARG:HB2	1:AE:68:TYR:HB2	2.02	0.40
1:AG:36:GLU:OE2	1:AG:38:SER:HB3	2.22	0.40
1:AK:54:ARG:HD2	1:AL:35:TRP:HH2	1.86	0.40
1:AN:121:LEU:HA	1:AN:121:LEU:HD23	1.73	0.40
1:AT:5:VAL:HG21	1:AT:48:LEU:HD23	2.03	0.40
1:BC:49:THR:O	1:BC:65:VAL:HA	2.20	0.40
1:BH:97:ILE:HD13	1:CA:121:LEU:HD11	2.03	0.40
1:CC:5:VAL:HG21	1:CC:48:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AB	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AC	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AD	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AE	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AF	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AG	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AH	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AI	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AJ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AK	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AL	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AM	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AN	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AO	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AP	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AQ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AR	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AS	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AT	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AU	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AV	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AW	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AX	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AY	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AZ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BA	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BB	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BC	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BD	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BE	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BF	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BG	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BH	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BI	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BJ	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BK	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BL	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BM	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BN	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BO	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BP	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BQ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BR	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BS	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BT	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BU	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BV	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BW	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BX	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BY	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BZ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CA	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CB	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	CC	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CD	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	CF	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CG	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CH	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
All	All	8100/8220 (98%)	7940 (98%)	160 (2%)	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	111/111 (100%)	111 (100%)	0	100	100
1	AB	111/111 (100%)	111 (100%)	0	100	100
1	AC	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AD	111/111 (100%)	111 (100%)	0	100	100
1	AE	111/111 (100%)	111 (100%)	0	100	100
1	AF	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AG	111/111 (100%)	111 (100%)	0	100	100
1	AH	111/111 (100%)	111 (100%)	0	100	100
1	AI	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AJ	111/111 (100%)	111 (100%)	0	100	100
1	AK	111/111 (100%)	111 (100%)	0	100	100
1	AL	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AM	111/111 (100%)	111 (100%)	0	100	100
1	AN	111/111 (100%)	111 (100%)	0	100	100
1	AO	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AP	111/111 (100%)	111 (100%)	0	100	100
1	AQ	111/111 (100%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AR	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AS	111/111 (100%)	111 (100%)	0	100	100
1	AT	111/111 (100%)	111 (100%)	0	100	100
1	AU	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AV	111/111 (100%)	111 (100%)	0	100	100
1	AW	111/111 (100%)	111 (100%)	0	100	100
1	AX	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AY	111/111 (100%)	111 (100%)	0	100	100
1	AZ	111/111 (100%)	111 (100%)	0	100	100
1	BA	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BB	111/111 (100%)	111 (100%)	0	100	100
1	BC	111/111 (100%)	111 (100%)	0	100	100
1	BD	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BE	111/111 (100%)	111 (100%)	0	100	100
1	BF	111/111 (100%)	111 (100%)	0	100	100
1	BG	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BH	111/111 (100%)	111 (100%)	0	100	100
1	BI	111/111 (100%)	111 (100%)	0	100	100
1	BJ	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BK	111/111 (100%)	111 (100%)	0	100	100
1	BL	111/111 (100%)	111 (100%)	0	100	100
1	BM	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BN	111/111 (100%)	111 (100%)	0	100	100
1	BO	111/111 (100%)	111 (100%)	0	100	100
1	BP	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BQ	111/111 (100%)	111 (100%)	0	100	100
1	BR	111/111 (100%)	111 (100%)	0	100	100
1	BS	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BT	111/111 (100%)	111 (100%)	0	100	100
1	BU	111/111 (100%)	111 (100%)	0	100	100
1	BV	111/111 (100%)	110 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BW	111/111 (100%)	111 (100%)	0	100	100
1	BX	111/111 (100%)	111 (100%)	0	100	100
1	BY	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BZ	111/111 (100%)	111 (100%)	0	100	100
1	CA	111/111 (100%)	111 (100%)	0	100	100
1	CB	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	CC	111/111 (100%)	111 (100%)	0	100	100
1	CD	111/111 (100%)	111 (100%)	0	100	100
1	CE	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	CF	111/111 (100%)	111 (100%)	0	100	100
1	CG	111/111 (100%)	111 (100%)	0	100	100
1	CH	111/111 (100%)	110 (99%)	1 (1%)	78	88
All	All	6660/6660 (100%)	6640 (100%)	20 (0%)	92	96

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AC	137	TYR
1	AF	137	TYR
1	AI	137	TYR
1	AL	137	TYR
1	AO	137	TYR
1	AR	137	TYR
1	AU	137	TYR
1	AX	137	TYR
1	BA	137	TYR
1	BD	137	TYR
1	BG	137	TYR
1	BJ	137	TYR
1	BM	137	TYR
1	BP	137	TYR
1	BS	137	TYR
1	BV	137	TYR
1	BY	137	TYR
1	CB	137	TYR
1	CE	137	TYR
1	CH	137	TYR

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

Mol	Chain	Res	Type
1	AA	1	GLN
1	AB	136	GLN
1	AD	1	GLN
1	AE	55	ASN
1	AF	119	ASN
1	AG	1	GLN
1	AH	55	ASN
1	AH	136	GLN
1	AJ	1	GLN
1	AK	136	GLN
1	AM	1	GLN
1	AN	136	GLN
1	AP	1	GLN
1	AQ	136	GLN
1	AS	1	GLN
1	AT	55	ASN
1	AT	136	GLN
1	AV	1	GLN
1	AY	1	GLN
1	BB	1	GLN
1	BC	55	ASN
1	BC	136	GLN
1	BE	1	GLN
1	BE	108	GLN
1	BF	136	GLN
1	BH	1	GLN
1	BH	108	GLN
1	BI	136	GLN
1	BJ	119	ASN
1	BK	1	GLN
1	BL	55	ASN
1	BN	1	GLN
1	BO	55	ASN
1	BO	136	GLN
1	BQ	1	GLN
1	BR	136	GLN
1	BT	1	GLN
1	BW	1	GLN
1	BW	108	GLN
1	BX	136	GLN
1	BZ	1	GLN

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Mol	Chain	Res	Type
1	CA	136	GLN
1	CC	1	GLN
1	CD	55	ASN
1	CD	136	GLN
1	CF	1	GLN
1	CG	136	GLN

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)

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	137/137 (100%)	-0.60	0	100	100	58, 84, 108, 123	0
1	AB	137/137 (100%)	-0.58	0	100	100	57, 83, 104, 118	0
1	AC	137/137 (100%)	-0.39	0	100	100	56, 85, 114, 137	0
1	AD	137/137 (100%)	-0.56	0	100	100	58, 84, 108, 123	0
1	AE	137/137 (100%)	-0.55	0	100	100	57, 83, 104, 118	0
1	AF	137/137 (100%)	-0.47	0	100	100	56, 85, 114, 137	0
1	AG	137/137 (100%)	-0.58	0	100	100	58, 84, 108, 123	0
1	AH	137/137 (100%)	-0.59	0	100	100	57, 83, 104, 118	0
1	AI	137/137 (100%)	-0.55	0	100	100	56, 85, 114, 137	0
1	AJ	137/137 (100%)	-0.60	0	100	100	58, 84, 108, 123	0
1	AK	137/137 (100%)	-0.58	0	100	100	57, 83, 104, 118	0
1	AL	137/137 (100%)	-0.60	0	100	100	56, 85, 114, 137	0
1	AM	137/137 (100%)	-0.63	0	100	100	58, 84, 108, 123	0
1	AN	137/137 (100%)	-0.62	0	100	100	57, 83, 104, 118	0
1	AO	137/137 (100%)	-0.53	0	100	100	56, 85, 114, 137	0
1	AP	137/137 (100%)	-0.69	0	100	100	58, 84, 108, 123	0
1	AQ	137/137 (100%)	-0.62	0	100	100	57, 83, 104, 118	0
1	AR	137/137 (100%)	-0.44	0	100	100	56, 85, 114, 137	0
1	AS	137/137 (100%)	-0.63	0	100	100	58, 84, 108, 123	0
1	AT	137/137 (100%)	-0.62	0	100	100	57, 83, 104, 118	0
1	AU	137/137 (100%)	-0.61	0	100	100	56, 85, 114, 137	0
1	AV	137/137 (100%)	-0.62	0	100	100	58, 84, 108, 123	0
1	AW	137/137 (100%)	-0.53	0	100	100	57, 83, 104, 118	0
1	AX	137/137 (100%)	-0.57	0	100	100	56, 85, 114, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AY	137/137 (100%)	-0.64	0	100	100	58, 84, 108, 123	0
1	AZ	137/137 (100%)	-0.56	0	100	100	57, 83, 104, 118	0
1	BA	137/137 (100%)	-0.45	0	100	100	56, 85, 114, 137	0
1	BB	137/137 (100%)	-0.63	0	100	100	58, 84, 108, 123	0
1	BC	137/137 (100%)	-0.59	0	100	100	57, 83, 104, 118	0
1	BD	137/137 (100%)	-0.54	0	100	100	56, 85, 114, 137	0
1	BE	137/137 (100%)	-0.61	0	100	100	58, 84, 108, 123	0
1	BF	137/137 (100%)	-0.63	0	100	100	57, 83, 104, 118	0
1	BG	137/137 (100%)	-0.64	0	100	100	56, 85, 114, 137	0
1	BH	137/137 (100%)	-0.61	0	100	100	58, 84, 108, 123	0
1	BI	137/137 (100%)	-0.66	0	100	100	57, 83, 104, 118	0
1	BJ	137/137 (100%)	-0.49	0	100	100	56, 85, 114, 137	0
1	BK	137/137 (100%)	-0.57	1 (0%)	87	81	58, 84, 108, 123	0
1	BL	137/137 (100%)	-0.68	0	100	100	57, 83, 104, 118	0
1	BM	137/137 (100%)	-0.57	1 (0%)	87	81	56, 85, 114, 137	0
1	BN	137/137 (100%)	-0.54	0	100	100	58, 84, 108, 123	0
1	BO	137/137 (100%)	-0.60	0	100	100	57, 83, 104, 118	0
1	BP	137/137 (100%)	-0.55	0	100	100	56, 85, 114, 137	0
1	BQ	137/137 (100%)	-0.59	0	100	100	58, 84, 108, 123	0
1	BR	137/137 (100%)	-0.69	0	100	100	57, 83, 104, 118	0
1	BS	137/137 (100%)	-0.57	0	100	100	56, 85, 114, 137	0
1	BT	137/137 (100%)	-0.58	0	100	100	58, 84, 108, 123	0
1	BU	137/137 (100%)	-0.63	0	100	100	57, 83, 104, 118	0
1	BV	137/137 (100%)	-0.56	0	100	100	56, 85, 114, 137	0
1	BW	137/137 (100%)	-0.70	0	100	100	58, 84, 108, 123	0
1	BX	137/137 (100%)	-0.62	0	100	100	57, 83, 104, 118	0
1	BY	137/137 (100%)	-0.53	0	100	100	56, 85, 114, 137	0
1	BZ	137/137 (100%)	-0.57	0	100	100	58, 84, 108, 123	0
1	CA	137/137 (100%)	-0.67	0	100	100	57, 83, 104, 118	0
1	CB	137/137 (100%)	-0.55	0	100	100	56, 85, 114, 137	0
1	CC	137/137 (100%)	-0.56	0	100	100	58, 84, 108, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	CD	137/137 (100%)	-0.64	0	100	100	57, 83, 104, 118	0
1	CE	137/137 (100%)	-0.59	0	100	100	56, 85, 114, 137	0
1	CF	137/137 (100%)	-0.53	0	100	100	58, 84, 108, 123	0
1	CG	137/137 (100%)	-0.60	0	100	100	57, 83, 104, 118	0
1	CH	137/137 (100%)	-0.57	0	100	100	56, 85, 114, 137	0
All	All	8220/8220 (100%)	-0.58	2 (0%)	100	100	56, 84, 108, 137	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BK	12	ALA	2.5
1	BM	77	PRO	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	BP	201	1/1	0.82	0.21	51,51,51,51	0
2	CA	AG	201	1/1	0.87	0.14	51,51,51,51	0
2	CA	BV	201	1/1	0.90	0.14	51,51,51,51	0
2	CA	BB	201	1/1	0.92	0.12	51,51,51,51	0
2	CA	AP	201	1/1	0.93	0.26	51,51,51,51	0
2	CA	BY	201	1/1	0.94	0.26	51,51,51,51	0
2	CA	AL	201	1/1	0.95	0.24	51,51,51,51	0
2	CA	BZ	201	1/1	0.95	0.17	51,51,51,51	0
2	CA	BD	201	1/1	0.96	0.29	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	CA	BN	201	1/1	0.96	0.20	51,51,51,51	0
2	CA	CC	201	1/1	0.96	0.25	51,51,51,51	0
2	CA	AU	201	1/1	0.97	0.20	51,51,51,51	0
2	CA	BJ	201	1/1	0.97	0.18	51,51,51,51	0
2	CA	AJ	201	1/1	0.98	0.24	51,51,51,51	0
2	CA	AO	201	1/1	0.98	0.17	51,51,51,51	0
2	CA	AX	201	1/1	0.98	0.24	51,51,51,51	0
2	CA	BM	201	1/1	0.98	0.15	51,51,51,51	0
2	CA	BA	201	1/1	0.98	0.18	51,51,51,51	0
2	CA	CH	201	1/1	0.98	0.19	51,51,51,51	0
2	CA	AF	201	1/1	0.99	0.26	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.