Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 11:21 PM EDT

PDB ID	:	3K19
Title	:	OmpF porin
Authors	:	Kefala, G.; Ahn, C.; Krupa, M.; Maslennikov, I.; Kwiatkowski, W.; Choe, S.; Center for Structures of Membrane Proteins (CSMP)
Deposited on	:	2009-09-26
Resolution	:	3.79 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 (1)) were used in the production of this report:

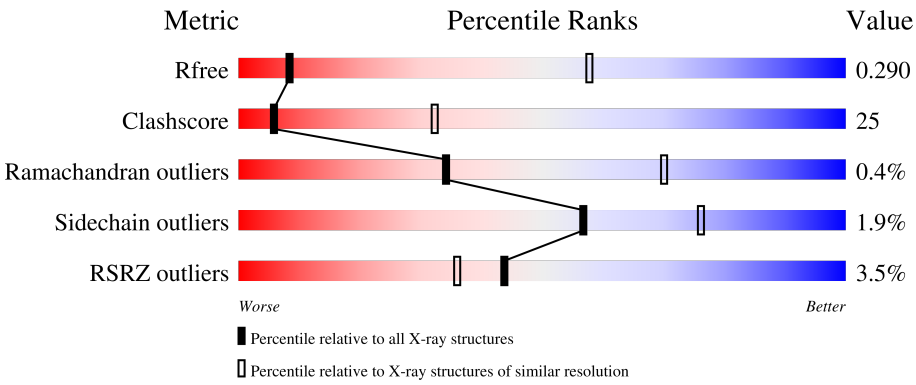
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.79 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	A	340	4% 64% 34% •
1	B	340	% 64% 35% •
1	C	340	2% 65% 34% •
1	D	340	% 64% 35% •
1	E	340	% 64% 35% •

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Mol	Chain	Length	Quality of chain
1	F	340	%, 63%, 35%
1	G	340	5%, 64%, 35%
1	H	340	5%, 64%, 35%
1	I	340	7%, 62%, 36%
1	J	340	4%, 64%, 34%
1	K	340	4%, 64%, 35%
1	L	340	7%, 63%, 36%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 31524 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 Outer membrane protein F.

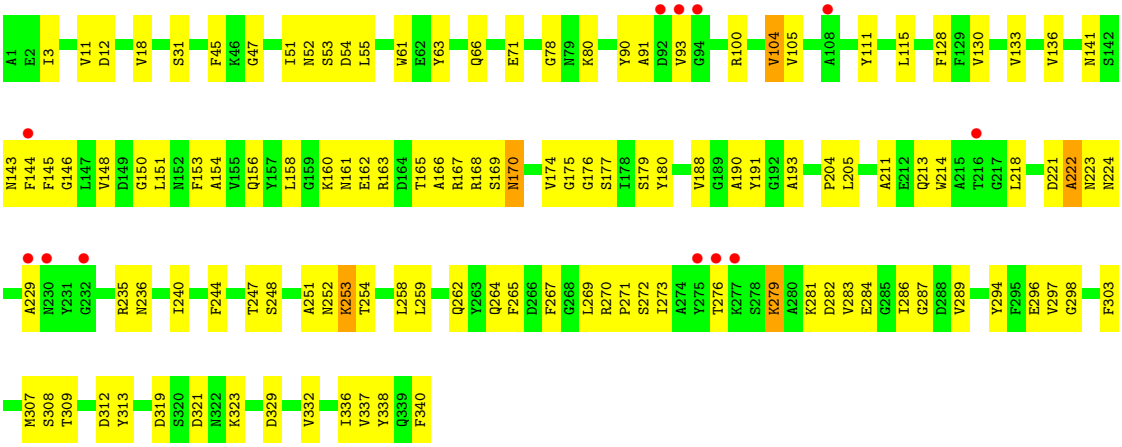
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2627	1654	438	532	3	8	0	0
1	B	340	2627	1654	438	532	3	0	0	0
1	C	340	2627	1654	438	532	3	0	0	0
1	D	340	2627	1654	438	532	3	8	0	0
1	E	340	2627	1654	438	532	3	0	0	0
1	F	340	2627	1654	438	532	3	0	0	0
1	G	340	2627	1654	438	532	3	8	0	0
1	H	340	2627	1654	438	532	3	0	0	0
1	I	340	2627	1654	438	532	3	0	0	0
1	J	340	2627	1654	438	532	3	8	0	0
1	K	340	2627	1654	438	532	3	0	0	0
1	L	340	2627	1654	438	532	3	0	0	0

3 Residue-property plots (i)

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

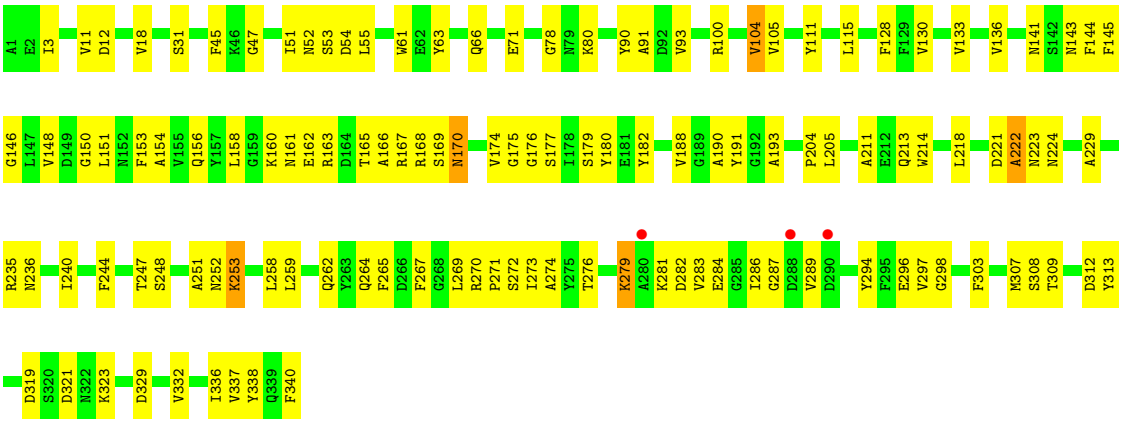
• Molecule 1: Outer membrane protein F

Chain A:



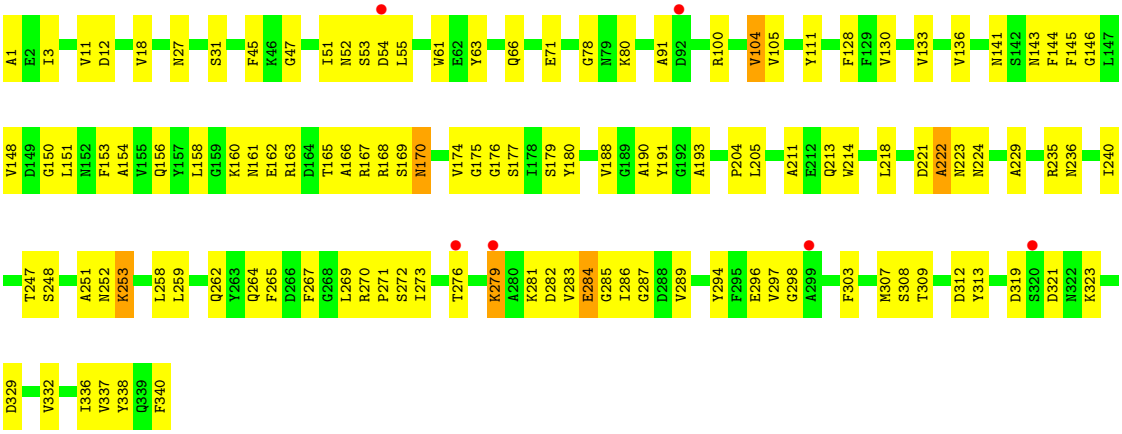
• Molecule 1: Outer membrane protein F

Chain B:



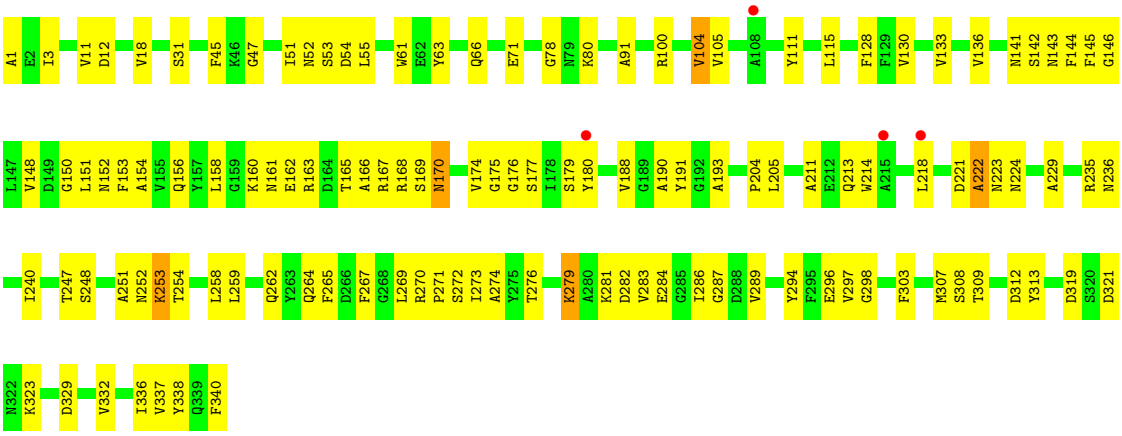
• Molecule 1: Outer membrane protein F

Chain C:



• Molecule 1: Outer membrane protein F

Chain D:

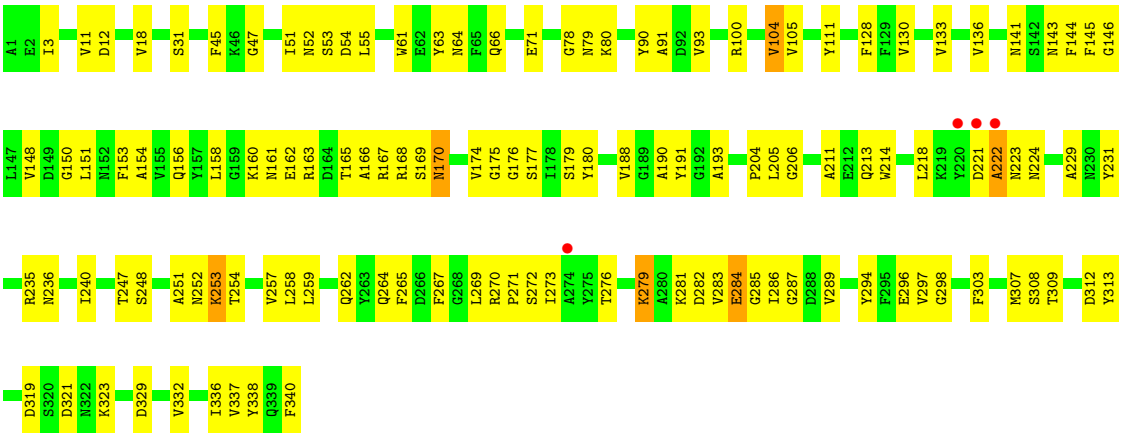


• Molecule 1: Outer membrane protein F

Chain E:

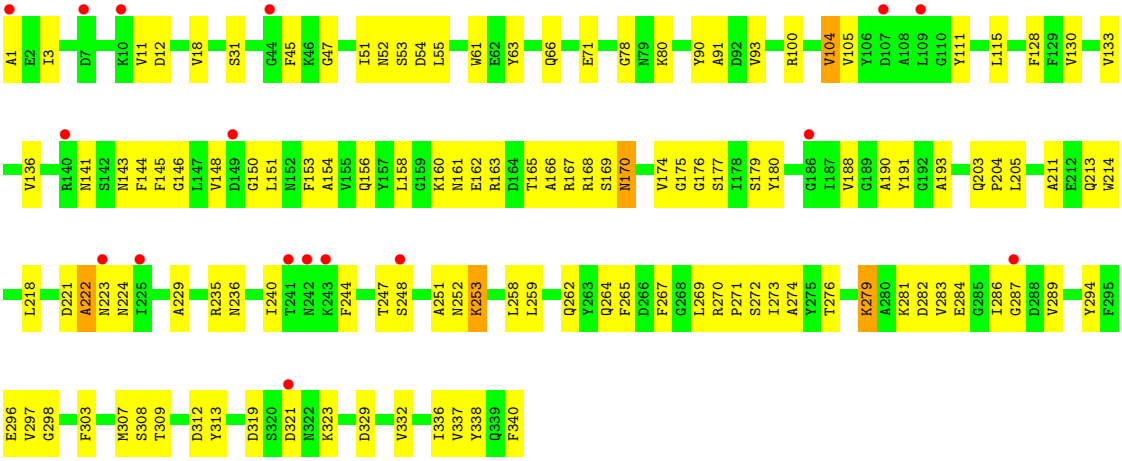
• Molecule 1: Outer membrane protein F

Chain F:



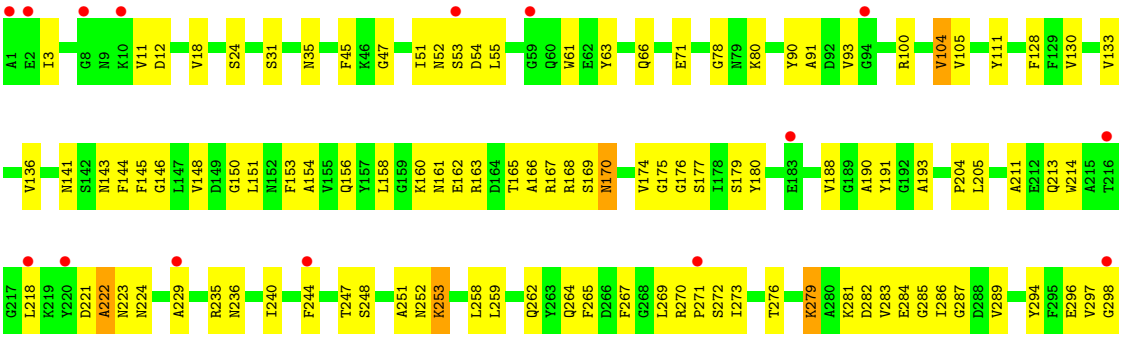
• Molecule 1: Outer membrane protein F

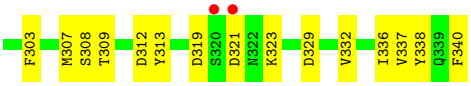
Chain G:



• Molecule 1: Outer membrane protein F

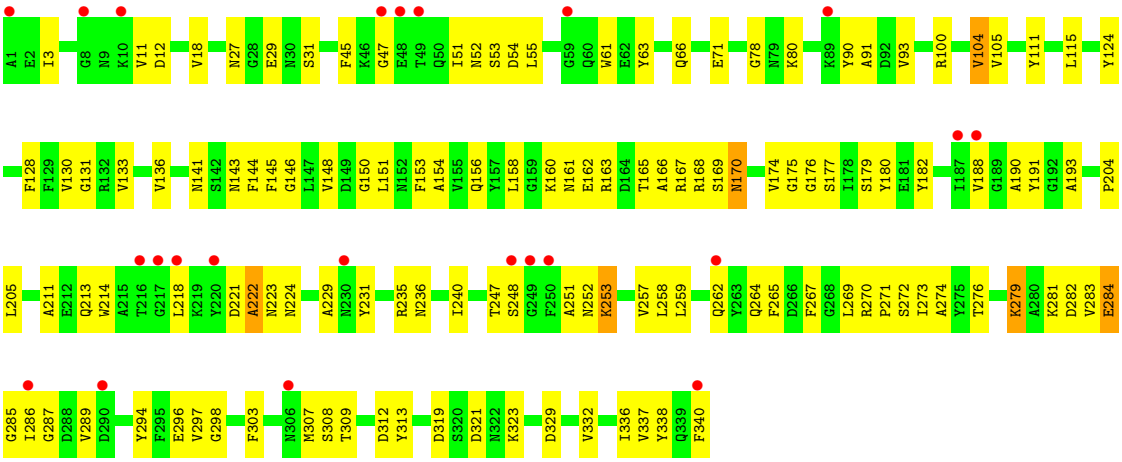
Chain H:





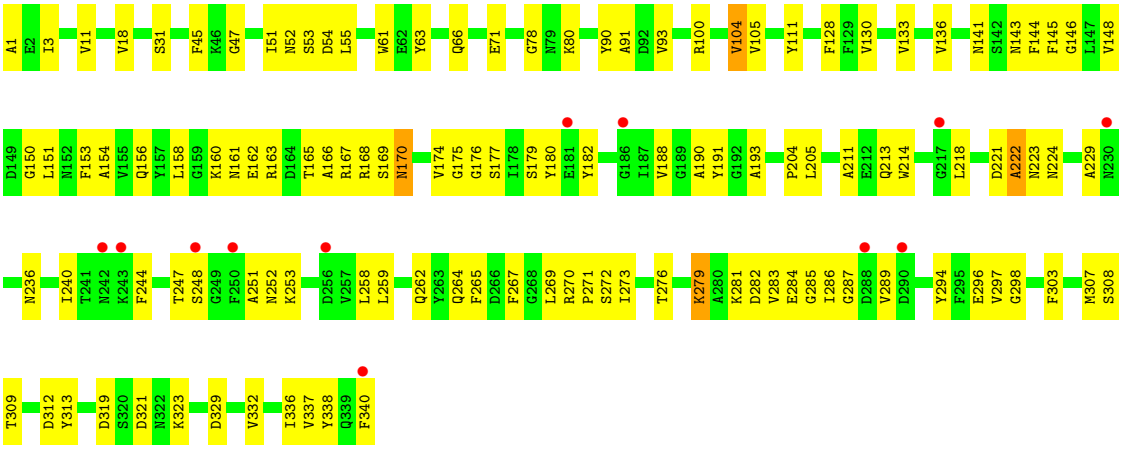
• Molecule 1: Outer membrane protein F

Chain I:



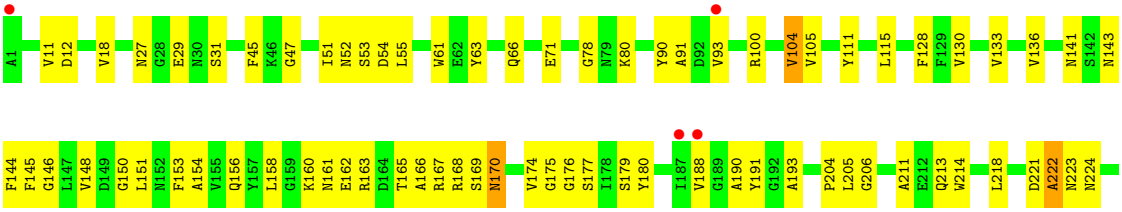
• Molecule 1: Outer membrane protein F

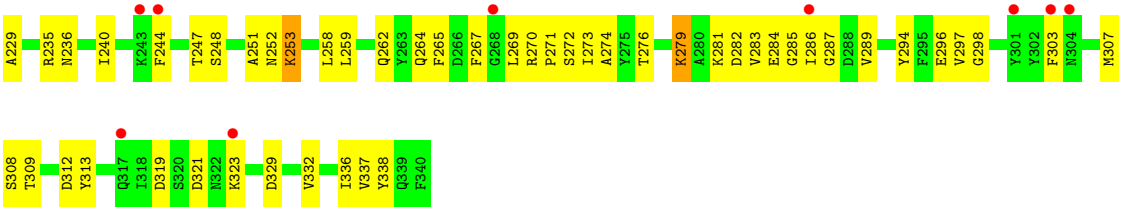
Chain J:



• Molecule 1: Outer membrane protein F

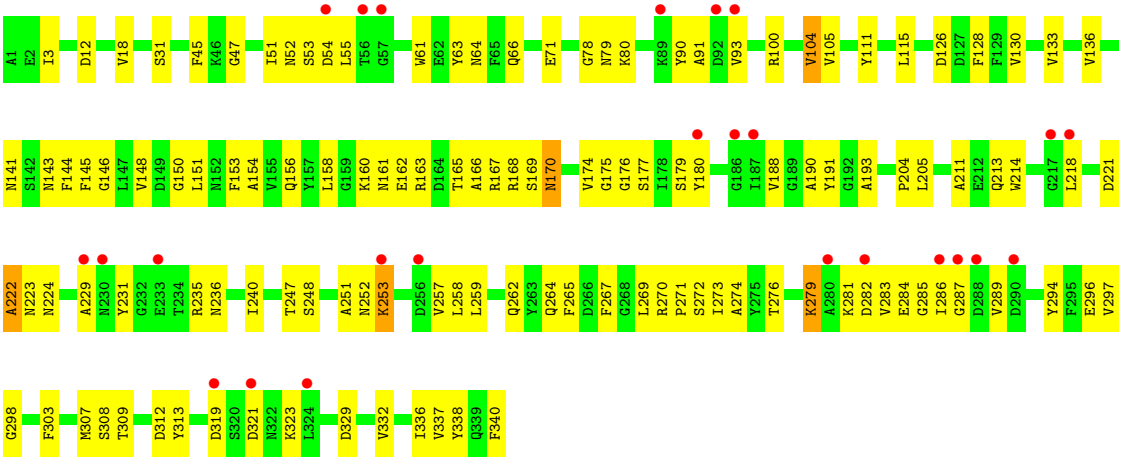
Chain K:





- Molecule 1: Outer membrane protein F

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.71Å 210.52Å 137.04Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	49.57 – 3.79 49.57 – 3.79	Depositor EDS
% Data completeness (in resolution range)	49.6 (49.57-3.79) 98.9 (49.57-3.79)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.280 , 0.288 0.280 , 0.290	Depositor DCC
R_{free} test set	3787 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	31524	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.29	0/2683	0.41	0/3628
1	B	0.27	0/2683	0.41	0/3628
1	C	0.28	0/2683	0.41	0/3628
1	D	0.29	0/2683	0.41	0/3628
1	E	0.28	0/2683	0.41	0/3628
1	F	0.28	0/2683	0.41	0/3628
1	G	0.27	0/2683	0.41	0/3628
1	H	0.27	0/2683	0.41	0/3628
1	I	0.27	0/2683	0.41	0/3628
1	J	0.27	0/2683	0.41	0/3628
1	K	0.27	0/2683	0.41	0/3628
1	L	0.27	0/2683	0.41	0/3628
All	All	0.28	0/32196	0.41	0/43536

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2444	142	0
1	B	2627	0	2444	149	0
1	C	2627	0	2444	143	0
1	D	2627	0	2444	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2627	0	2444	144	0
1	F	2627	0	2444	148	0
1	G	2627	0	2444	151	0
1	H	2627	0	2444	146	0
1	I	2627	0	2444	151	0
1	J	2627	0	2444	143	0
1	K	2627	0	2444	146	0
1	L	2627	0	2444	150	0
All	All	31524	0	29328	1531	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 25.

All (1531) 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:E:321:ASP:OD1	1:K:287:GLY:HA2	1.18	1.35
1:E:287:GLY:CA	1:I:321:ASP:OD1	1.76	1.33
1:I:287:GLY:CA	1:K:321:ASP:OD1	1.75	1.32
1:B:287:GLY:CA	1:L:321:ASP:OD1	1.76	1.32
1:C:287:GLY:HA2	1:G:321:ASP:OD1	1.17	1.31
1:H:321:ASP:OD1	1:L:287:GLY:CA	1.78	1.29
1:B:321:ASP:OD1	1:H:287:GLY:HA2	1.22	1.28
1:C:287:GLY:CA	1:G:321:ASP:OD1	1.83	1.27
1:C:321:ASP:OD1	1:D:287:GLY:HA2	1.11	1.27
1:A:321:ASP:OD1	1:J:287:GLY:CA	1.82	1.25
1:D:321:ASP:OD1	1:G:287:GLY:CA	1.83	1.25
1:A:287:GLY:HA2	1:F:321:ASP:OD1	1.10	1.25
1:F:287:GLY:CA	1:J:321:ASP:OD1	1.82	1.25
1:E:321:ASP:OD1	1:K:287:GLY:CA	1.84	1.24
1:F:287:GLY:HA2	1:J:321:ASP:OD1	1.11	1.23
1:C:321:ASP:OD1	1:D:287:GLY:CA	1.85	1.21
1:D:321:ASP:OD1	1:G:287:GLY:HA2	1.06	1.19
1:A:287:GLY:CA	1:F:321:ASP:OD1	1.90	1.18
1:E:287:GLY:HA2	1:I:321:ASP:OD1	1.02	1.17
1:B:287:GLY:HA2	1:L:321:ASP:OD1	1.02	1.17
1:I:287:GLY:HA2	1:K:321:ASP:OD1	1.00	1.15
1:A:321:ASP:OD1	1:J:287:GLY:HA2	0.98	1.15
1:B:321:ASP:OD1	1:H:287:GLY:CA	1.94	1.15
1:H:321:ASP:OD1	1:L:287:GLY:HA2	0.98	1.13
1:G:71:GLU:HB3	1:H:80:LYS:HD2	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:GLU:HB3	1:E:80:LYS:HD2	1.36	1.07
1:L:313:TYR:CD1	1:L:332:VAL:HG22	1.92	1.04
1:A:80:LYS:HD2	1:C:71:GLU:HB3	1.37	1.04
1:I:313:TYR:CD1	1:I:332:VAL:HG22	1.92	1.04
1:K:313:TYR:CD1	1:K:332:VAL:HG22	1.93	1.03
1:C:313:TYR:CD1	1:C:332:VAL:HG22	1.94	1.03
1:J:313:TYR:CD1	1:J:332:VAL:HG22	1.93	1.03
1:H:313:TYR:CD1	1:H:332:VAL:HG22	1.92	1.03
1:A:313:TYR:CD1	1:A:332:VAL:HG22	1.94	1.02
1:G:80:LYS:HD2	1:I:71:GLU:HB3	1.40	1.02
1:F:313:TYR:CD1	1:F:332:VAL:HG22	1.94	1.02
1:G:313:TYR:CD1	1:G:332:VAL:HG22	1.93	1.02
1:J:71:GLU:HB3	1:K:80:LYS:HD2	1.41	1.02
1:B:313:TYR:CD1	1:B:332:VAL:HG22	1.93	1.02
1:H:71:GLU:HB3	1:I:80:LYS:HD2	1.40	1.01
1:D:313:TYR:CD1	1:D:332:VAL:HG22	1.96	1.00
1:E:313:TYR:CD1	1:E:332:VAL:HG22	1.94	1.00
1:K:71:GLU:HB3	1:L:80:LYS:HD2	1.43	1.00
1:D:80:LYS:HD2	1:F:71:GLU:HB3	1.44	1.00
1:A:71:GLU:HB3	1:B:80:LYS:HD2	1.39	1.00
1:B:71:GLU:HB3	1:C:80:LYS:HD2	1.40	0.99
1:J:80:LYS:HD2	1:L:71:GLU:HB3	1.41	0.99
1:E:71:GLU:HB3	1:F:80:LYS:HD2	1.41	0.98
1:E:165:THR:HG22	1:E:167:ARG:H	1.30	0.97
1:D:165:THR:HG22	1:D:167:ARG:H	1.29	0.96
1:C:165:THR:HG22	1:C:167:ARG:H	1.30	0.96
1:B:165:THR:HG22	1:B:167:ARG:H	1.29	0.95
1:J:165:THR:HG22	1:J:167:ARG:H	1.30	0.95
1:F:165:THR:HG22	1:F:167:ARG:H	1.30	0.95
1:K:165:THR:HG22	1:K:167:ARG:H	1.28	0.94
1:A:165:THR:HG22	1:A:167:ARG:H	1.30	0.94
1:L:165:THR:HG22	1:L:167:ARG:H	1.27	0.94
1:I:165:THR:HG22	1:I:167:ARG:H	1.29	0.94
1:G:165:THR:HG22	1:G:167:ARG:H	1.31	0.92
1:H:165:THR:HG22	1:H:167:ARG:H	1.31	0.92
1:A:321:ASP:CG	1:J:287:GLY:HA2	1.91	0.91
1:B:287:GLY:CA	1:L:321:ASP:CG	2.39	0.91
1:I:27:ASN:HD22	1:I:29:GLU:HB2	1.36	0.90
1:A:321:ASP:CG	1:J:287:GLY:CA	2.41	0.89
1:L:165:THR:HG22	1:L:167:ARG:N	1.87	0.89
1:A:165:THR:HG22	1:A:167:ARG:N	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:287:GLY:CA	1:K:321:ASP:CG	2.42	0.88
1:F:165:THR:HG22	1:F:167:ARG:N	1.89	0.88
1:K:165:THR:HG22	1:K:167:ARG:N	1.88	0.88
1:B:279:LYS:HE3	1:B:281:LYS:HZ2	1.39	0.87
1:E:165:THR:HG22	1:E:167:ARG:N	1.89	0.87
1:A:309:THR:HG22	1:A:336:ILE:HA	1.57	0.87
1:C:165:THR:HG22	1:C:167:ARG:N	1.89	0.87
1:D:165:THR:HG22	1:D:167:ARG:N	1.89	0.87
1:E:287:GLY:CA	1:I:321:ASP:CG	2.42	0.87
1:C:313:TYR:HD1	1:C:332:VAL:HG22	1.40	0.86
1:J:165:THR:HG22	1:J:167:ARG:N	1.89	0.86
1:B:165:THR:HG22	1:B:167:ARG:N	1.89	0.86
1:G:165:THR:HG22	1:G:167:ARG:N	1.90	0.86
1:H:165:THR:HG22	1:H:167:ARG:N	1.90	0.85
1:H:279:LYS:HE3	1:H:281:LYS:HZ2	1.38	0.85
1:H:321:ASP:CG	1:L:287:GLY:CA	2.44	0.85
1:I:165:THR:HG22	1:I:167:ARG:N	1.88	0.85
1:J:309:THR:HG22	1:J:336:ILE:HA	1.58	0.85
1:I:279:LYS:HE3	1:I:281:LYS:HZ2	1.40	0.85
1:G:313:TYR:HD1	1:G:332:VAL:HG22	1.40	0.85
1:K:313:TYR:HD1	1:K:332:VAL:HG22	1.40	0.85
1:F:309:THR:HG22	1:F:336:ILE:HA	1.59	0.85
1:K:279:LYS:HE3	1:K:281:LYS:HZ2	1.42	0.85
1:C:309:THR:HG22	1:C:336:ILE:HA	1.59	0.84
1:D:309:THR:HG22	1:D:336:ILE:HA	1.57	0.84
1:G:309:THR:HG22	1:G:336:ILE:HA	1.58	0.84
1:K:71:GLU:HG3	1:L:100:ARG:NH2	1.91	0.84
1:J:313:TYR:HD1	1:J:332:VAL:HG22	1.39	0.84
1:L:286:ILE:HG21	1:L:289:VAL:HG21	1.58	0.84
1:A:313:TYR:HD1	1:A:332:VAL:HG22	1.40	0.84
1:B:309:THR:HG22	1:B:336:ILE:HA	1.58	0.84
1:E:279:LYS:HE3	1:E:281:LYS:HZ2	1.42	0.84
1:E:286:ILE:HG21	1:E:289:VAL:HG21	1.60	0.84
1:F:286:ILE:HG21	1:F:289:VAL:HG21	1.60	0.83
1:L:279:LYS:HE3	1:L:281:LYS:HZ2	1.41	0.83
1:E:313:TYR:HD1	1:E:332:VAL:HG22	1.41	0.83
1:F:279:LYS:HE3	1:F:281:LYS:HZ2	1.41	0.83
1:F:313:TYR:HD1	1:F:332:VAL:HG22	1.41	0.83
1:B:287:GLY:HA2	1:L:321:ASP:CG	1.96	0.83
1:K:309:THR:HG22	1:K:336:ILE:HA	1.60	0.83
1:K:286:ILE:HG21	1:K:289:VAL:HG21	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ARG:NH2	1:F:71:GLU:HG3	1.94	0.83
1:H:309:THR:HG22	1:H:336:ILE:HA	1.60	0.83
1:K:31:SER:HA	1:K:329:ASP:HB2	1.61	0.82
1:I:313:TYR:HD1	1:I:332:VAL:HG22	1.40	0.82
1:E:309:THR:HG22	1:E:336:ILE:HA	1.59	0.82
1:H:111:TYR:CZ	1:H:188:VAL:CG2	2.63	0.82
1:I:309:THR:HG22	1:I:336:ILE:HA	1.61	0.82
1:C:31:SER:HA	1:C:329:ASP:HB2	1.62	0.82
1:G:279:LYS:HE3	1:G:281:LYS:HZ2	1.45	0.82
1:H:313:TYR:HD1	1:H:332:VAL:HG22	1.39	0.82
1:L:309:THR:HG22	1:L:336:ILE:HA	1.61	0.82
1:G:31:SER:HA	1:G:329:ASP:HB2	1.62	0.81
1:I:286:ILE:HG21	1:I:289:VAL:HG21	1.59	0.81
1:J:286:ILE:HG21	1:J:289:VAL:HG21	1.61	0.81
1:D:321:ASP:CG	1:G:287:GLY:CA	2.48	0.81
1:H:31:SER:HA	1:H:329:ASP:HB2	1.61	0.81
1:H:321:ASP:CG	1:L:287:GLY:HA2	1.99	0.81
1:E:31:SER:HA	1:E:329:ASP:HB2	1.61	0.81
1:B:286:ILE:HG21	1:B:289:VAL:HG21	1.61	0.81
1:C:286:ILE:HG21	1:C:289:VAL:HG21	1.61	0.81
1:J:31:SER:HA	1:J:329:ASP:HB2	1.63	0.81
1:B:313:TYR:HD1	1:B:332:VAL:HG22	1.40	0.81
1:C:287:GLY:HA3	1:G:321:ASP:OD1	1.79	0.81
1:I:27:ASN:ND2	1:I:29:GLU:HB2	1.96	0.81
1:D:31:SER:HA	1:D:329:ASP:HB2	1.63	0.81
1:G:286:ILE:HG21	1:G:289:VAL:HG21	1.63	0.81
1:I:287:GLY:HA3	1:K:321:ASP:CG	2.01	0.81
1:A:286:ILE:HG21	1:A:289:VAL:HG21	1.63	0.80
1:B:71:GLU:HG3	1:C:100:ARG:NH2	1.96	0.80
1:H:286:ILE:HG21	1:H:289:VAL:HG21	1.61	0.80
1:B:31:SER:HA	1:B:329:ASP:HB2	1.63	0.80
1:G:111:TYR:CZ	1:G:188:VAL:CG2	2.64	0.80
1:J:279:LYS:HE3	1:J:281:LYS:HZ2	1.43	0.80
1:L:111:TYR:CZ	1:L:188:VAL:CG2	2.64	0.80
1:I:111:TYR:CZ	1:I:188:VAL:CG2	2.65	0.80
1:J:71:GLU:HG3	1:K:100:ARG:NH2	1.96	0.80
1:C:279:LYS:HE3	1:C:281:LYS:HZ2	1.46	0.80
1:F:31:SER:HA	1:F:329:ASP:HB2	1.63	0.80
1:K:111:TYR:CZ	1:K:188:VAL:CG2	2.65	0.80
1:C:111:TYR:CZ	1:C:188:VAL:CG2	2.64	0.80
1:L:31:SER:HA	1:L:329:ASP:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HA	1:A:329:ASP:HB2	1.63	0.79
1:L:313:TYR:HD1	1:L:332:VAL:HG22	1.39	0.79
1:D:286:ILE:HG21	1:D:289:VAL:HG21	1.62	0.79
1:E:111:TYR:CZ	1:E:188:VAL:CG2	2.66	0.79
1:B:111:TYR:CZ	1:B:188:VAL:CG2	2.67	0.78
1:A:111:TYR:CZ	1:A:188:VAL:CG2	2.65	0.78
1:I:31:SER:HA	1:I:329:ASP:HB2	1.63	0.78
1:J:111:TYR:CZ	1:J:188:VAL:CG2	2.66	0.78
1:B:287:GLY:HA3	1:L:321:ASP:CG	2.01	0.78
1:E:287:GLY:HA3	1:I:321:ASP:CG	2.03	0.78
1:E:321:ASP:OD1	1:K:287:GLY:HA3	1.81	0.78
1:F:111:TYR:CZ	1:F:188:VAL:CG2	2.66	0.78
1:D:321:ASP:CG	1:G:287:GLY:HA2	2.03	0.78
1:D:313:TYR:HD1	1:D:332:VAL:HG22	1.44	0.78
1:A:279:LYS:HE3	1:A:281:LYS:HZ2	1.48	0.77
1:D:279:LYS:HE3	1:D:281:LYS:HZ2	1.47	0.77
1:H:321:ASP:CG	1:L:287:GLY:HA3	2.05	0.77
1:D:111:TYR:CZ	1:D:188:VAL:CG2	2.68	0.77
1:E:287:GLY:HA2	1:I:321:ASP:CG	2.00	0.76
1:C:321:ASP:CG	1:D:287:GLY:CA	2.53	0.76
1:G:160:LYS:HD3	1:G:162:GLU:OE2	1.86	0.76
1:H:160:LYS:HD3	1:H:162:GLU:OE2	1.86	0.76
1:H:279:LYS:HE3	1:H:281:LYS:NZ	2.01	0.76
1:H:313:TYR:CD1	1:H:332:VAL:CG2	2.69	0.75
1:I:313:TYR:CD1	1:I:332:VAL:CG2	2.70	0.75
1:C:160:LYS:HD3	1:C:162:GLU:OE2	1.86	0.75
1:K:313:TYR:CD1	1:K:332:VAL:CG2	2.70	0.75
1:D:160:LYS:HD3	1:D:162:GLU:OE2	1.86	0.75
1:A:321:ASP:CG	1:J:287:GLY:HA3	2.07	0.75
1:G:279:LYS:HE3	1:G:281:LYS:NZ	2.02	0.75
1:J:313:TYR:CD1	1:J:332:VAL:CG2	2.70	0.75
1:L:160:LYS:HD3	1:L:162:GLU:OE2	1.86	0.74
1:J:160:LYS:HD3	1:J:162:GLU:OE2	1.87	0.74
1:K:160:LYS:HD3	1:K:162:GLU:OE2	1.87	0.74
1:E:71:GLU:HG3	1:F:100:ARG:NH2	2.03	0.74
1:L:313:TYR:CD1	1:L:332:VAL:CG2	2.69	0.74
1:E:160:LYS:HD3	1:E:162:GLU:OE2	1.88	0.74
1:E:313:TYR:CD1	1:E:332:VAL:CG2	2.71	0.74
1:A:160:LYS:HD3	1:A:162:GLU:OE2	1.87	0.74
1:A:279:LYS:HE3	1:A:281:LYS:NZ	2.02	0.74
1:A:287:GLY:HA2	1:F:321:ASP:CG	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:TYR:CD1	1:C:332:VAL:CG2	2.70	0.73
1:L:286:ILE:HG21	1:L:289:VAL:CG2	2.18	0.73
1:A:287:GLY:CA	1:F:321:ASP:CG	2.56	0.73
1:B:160:LYS:HD3	1:B:162:GLU:OE2	1.87	0.73
1:F:160:LYS:HD3	1:F:162:GLU:OE2	1.88	0.73
1:C:279:LYS:HE3	1:C:281:LYS:NZ	2.03	0.73
1:D:279:LYS:HE3	1:D:281:LYS:NZ	2.04	0.73
1:I:286:ILE:CG2	1:I:289:VAL:CG2	2.67	0.73
1:K:279:LYS:HE3	1:K:281:LYS:NZ	2.03	0.73
1:F:286:ILE:HD12	1:F:286:ILE:N	2.02	0.73
1:I:279:LYS:HE3	1:I:281:LYS:NZ	2.04	0.73
1:L:279:LYS:HE3	1:L:281:LYS:NZ	2.02	0.73
1:A:313:TYR:CD1	1:A:332:VAL:CG2	2.71	0.73
1:E:286:ILE:N	1:E:286:ILE:HD12	2.03	0.73
1:J:100:ARG:NH2	1:L:71:GLU:HG3	2.04	0.73
1:E:279:LYS:HE3	1:E:281:LYS:NZ	2.03	0.73
1:B:313:TYR:CD1	1:B:332:VAL:CG2	2.71	0.72
1:H:286:ILE:HD12	1:H:286:ILE:N	2.04	0.72
1:H:71:GLU:HG3	1:I:100:ARG:NH2	2.04	0.72
1:J:279:LYS:HE3	1:J:281:LYS:NZ	2.02	0.72
1:L:286:ILE:CG2	1:L:289:VAL:CG2	2.66	0.72
1:K:286:ILE:HG21	1:K:289:VAL:CG2	2.19	0.72
1:B:279:LYS:HE3	1:B:281:LYS:NZ	2.04	0.72
1:K:286:ILE:CG2	1:K:289:VAL:CG2	2.68	0.72
1:I:286:ILE:HD12	1:I:286:ILE:N	2.05	0.72
1:A:100:ARG:NH2	1:C:71:GLU:HG3	2.05	0.72
1:D:321:ASP:CG	1:G:287:GLY:HA3	2.10	0.72
1:J:286:ILE:N	1:J:286:ILE:HD12	2.05	0.72
1:D:313:TYR:CD1	1:D:332:VAL:CG2	2.73	0.72
1:I:160:LYS:HD3	1:I:162:GLU:OE2	1.88	0.72
1:I:286:ILE:HG21	1:I:289:VAL:CG2	2.19	0.72
1:G:313:TYR:CD1	1:G:332:VAL:CG2	2.70	0.71
1:F:279:LYS:HE3	1:F:281:LYS:NZ	2.04	0.71
1:A:286:ILE:HD12	1:A:286:ILE:N	2.04	0.71
1:C:111:TYR:OH	1:C:188:VAL:CG2	2.38	0.71
1:F:313:TYR:CD1	1:F:332:VAL:CG2	2.71	0.71
1:L:111:TYR:OH	1:L:188:VAL:CG2	2.39	0.71
1:D:286:ILE:HD12	1:D:286:ILE:N	2.05	0.71
1:K:111:TYR:OH	1:K:188:VAL:CG2	2.39	0.71
1:B:286:ILE:N	1:B:286:ILE:HD12	2.04	0.71
1:F:286:ILE:HG21	1:F:289:VAL:CG2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:286:ILE:N	1:L:286:ILE:HD12	2.05	0.71
1:F:286:ILE:CG2	1:F:289:VAL:CG2	2.69	0.71
1:G:100:ARG:NH2	1:I:71:GLU:HG3	2.06	0.71
1:G:286:ILE:N	1:G:286:ILE:HD12	2.06	0.71
1:K:286:ILE:HD12	1:K:286:ILE:N	2.04	0.71
1:G:51:ILE:HD13	1:I:303:PHE:HB3	1.73	0.70
1:H:111:TYR:OH	1:H:188:VAL:CG2	2.38	0.70
1:G:111:TYR:OH	1:G:188:VAL:CG2	2.40	0.70
1:H:286:ILE:CG2	1:H:289:VAL:CG2	2.69	0.70
1:C:111:TYR:CZ	1:C:188:VAL:HG21	2.27	0.70
1:A:71:GLU:HG3	1:B:100:ARG:NH2	2.07	0.70
1:A:111:TYR:OH	1:A:188:VAL:CG2	2.39	0.70
1:C:286:ILE:N	1:C:286:ILE:HD12	2.06	0.70
1:E:286:ILE:CG2	1:E:289:VAL:CG2	2.69	0.70
1:H:286:ILE:HG21	1:H:289:VAL:CG2	2.21	0.70
1:F:287:GLY:HA3	1:J:321:ASP:OD1	1.87	0.70
1:C:286:ILE:HG21	1:C:289:VAL:CG2	2.21	0.70
1:J:286:ILE:HG21	1:J:289:VAL:CG2	2.21	0.70
1:E:244:PHE:CZ	1:K:285:GLY:HA3	2.27	0.70
1:D:286:ILE:HG21	1:D:289:VAL:CG2	2.22	0.70
1:B:286:ILE:HG21	1:B:289:VAL:CG2	2.21	0.69
1:C:286:ILE:CG2	1:C:289:VAL:CG2	2.70	0.69
1:C:321:ASP:CG	1:D:287:GLY:HA3	2.13	0.69
1:D:286:ILE:CG2	1:D:289:VAL:CG2	2.70	0.69
1:E:286:ILE:HG21	1:E:289:VAL:CG2	2.21	0.69
1:F:287:GLY:CA	1:J:321:ASP:CG	2.61	0.69
1:B:111:TYR:OH	1:B:188:VAL:CG2	2.41	0.69
1:B:286:ILE:CG2	1:B:289:VAL:CG2	2.70	0.69
1:H:111:TYR:CZ	1:H:188:VAL:HG21	2.26	0.69
1:A:111:TYR:CZ	1:A:188:VAL:HG21	2.28	0.69
1:G:111:TYR:CZ	1:G:188:VAL:HG21	2.27	0.69
1:J:111:TYR:OH	1:J:188:VAL:CG2	2.40	0.69
1:J:286:ILE:CG2	1:J:289:VAL:CG2	2.70	0.69
1:A:286:ILE:CG2	1:A:289:VAL:CG2	2.71	0.69
1:E:111:TYR:CZ	1:E:188:VAL:HG21	2.28	0.68
1:I:111:TYR:CZ	1:I:188:VAL:HG21	2.28	0.68
1:A:286:ILE:HG21	1:A:289:VAL:CG2	2.23	0.68
1:I:111:TYR:OH	1:I:188:VAL:CG2	2.41	0.68
1:B:111:TYR:CZ	1:B:188:VAL:HG21	2.29	0.68
1:H:111:TYR:CZ	1:H:188:VAL:HG23	2.28	0.68
1:E:111:TYR:OH	1:E:188:VAL:CG2	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:ILE:HG21	1:G:289:VAL:CG2	2.22	0.68
1:G:286:ILE:CG2	1:G:289:VAL:CG2	2.71	0.68
1:I:128:PHE:O	1:I:133:VAL:HG11	1.94	0.68
1:F:111:TYR:OH	1:F:188:VAL:CG2	2.42	0.68
1:F:111:TYR:CZ	1:F:188:VAL:HG21	2.28	0.68
1:I:111:TYR:CZ	1:I:188:VAL:HG23	2.29	0.68
1:K:111:TYR:CZ	1:K:188:VAL:HG21	2.28	0.68
1:F:287:GLY:HA3	1:J:321:ASP:CG	2.15	0.67
1:G:47:GLY:HA3	1:I:338:TYR:CZ	2.28	0.67
1:L:111:TYR:CZ	1:L:188:VAL:HG21	2.28	0.67
1:C:174:VAL:HG12	1:C:175:GLY:N	2.10	0.67
1:L:111:TYR:CZ	1:L:188:VAL:HG23	2.29	0.67
1:I:286:ILE:HG22	1:I:289:VAL:HG22	1.75	0.67
1:B:128:PHE:O	1:B:133:VAL:HG11	1.94	0.67
1:G:128:PHE:O	1:G:133:VAL:HG11	1.94	0.67
1:K:128:PHE:O	1:K:133:VAL:HG11	1.94	0.67
1:L:286:ILE:HG22	1:L:289:VAL:HG22	1.76	0.67
1:E:244:PHE:CZ	1:K:285:GLY:CA	2.77	0.67
1:J:128:PHE:O	1:J:133:VAL:HG11	1.95	0.67
1:K:111:TYR:CZ	1:K:188:VAL:HG23	2.29	0.67
1:D:71:GLU:HG3	1:E:100:ARG:NH2	2.10	0.67
1:K:286:ILE:HG22	1:K:289:VAL:HG22	1.77	0.67
1:B:287:GLY:HA3	1:L:321:ASP:OD2	1.94	0.66
1:C:128:PHE:O	1:C:133:VAL:HG11	1.96	0.66
1:C:287:GLY:HA3	1:G:321:ASP:CG	2.15	0.66
1:D:174:VAL:HG12	1:D:175:GLY:N	2.10	0.66
1:D:128:PHE:O	1:D:133:VAL:HG11	1.94	0.66
1:G:71:GLU:HG3	1:H:100:ARG:NH2	2.10	0.66
1:H:262:GLN:OE1	1:H:270:ARG:NH1	2.29	0.66
1:J:111:TYR:CZ	1:J:188:VAL:HG21	2.28	0.66
1:K:174:VAL:HG12	1:K:175:GLY:N	2.11	0.66
1:D:111:TYR:CZ	1:D:188:VAL:HG21	2.31	0.66
1:E:111:TYR:CZ	1:E:188:VAL:HG23	2.31	0.66
1:E:174:VAL:HG12	1:E:175:GLY:N	2.10	0.66
1:E:321:ASP:CG	1:K:287:GLY:HA3	2.16	0.66
1:G:111:TYR:CZ	1:G:188:VAL:HG23	2.29	0.66
1:G:338:TYR:CZ	1:H:47:GLY:HA3	2.31	0.66
1:J:174:VAL:HG12	1:J:175:GLY:N	2.11	0.66
1:C:111:TYR:CZ	1:C:188:VAL:HG23	2.30	0.66
1:D:111:TYR:OH	1:D:188:VAL:CG2	2.43	0.66
1:F:286:ILE:HG22	1:F:289:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:GLN:OE1	1:D:270:ARG:NH1	2.29	0.66
1:E:128:PHE:O	1:E:133:VAL:HG11	1.95	0.66
1:F:128:PHE:O	1:F:133:VAL:HG11	1.95	0.66
1:A:128:PHE:O	1:A:133:VAL:HG11	1.96	0.66
1:B:174:VAL:HG12	1:B:175:GLY:N	2.11	0.66
1:E:205:LEU:HG	1:E:247:THR:HG22	1.78	0.66
1:G:174:VAL:HG12	1:G:175:GLY:N	2.11	0.66
1:L:128:PHE:O	1:L:133:VAL:HG11	1.96	0.65
1:F:286:ILE:HD12	1:F:286:ILE:H	1.62	0.65
1:C:262:GLN:OE1	1:C:270:ARG:NH1	2.30	0.65
1:D:338:TYR:CZ	1:E:47:GLY:HA3	2.31	0.65
1:H:286:ILE:HG22	1:H:289:VAL:HG22	1.78	0.65
1:J:262:GLN:OE1	1:J:270:ARG:NH1	2.28	0.65
1:C:285:GLY:HA3	1:G:244:PHE:CZ	2.32	0.65
1:D:191:TYR:HD1	1:D:214:TRP:HB3	1.62	0.65
1:E:262:GLN:OE1	1:E:270:ARG:NH1	2.30	0.65
1:H:128:PHE:O	1:H:133:VAL:HG11	1.95	0.65
1:B:111:TYR:CZ	1:B:188:VAL:HG23	2.31	0.65
1:B:262:GLN:OE1	1:B:270:ARG:NH1	2.30	0.65
1:C:286:ILE:HG22	1:C:289:VAL:HG22	1.79	0.65
1:J:286:ILE:HG22	1:J:289:VAL:HG22	1.79	0.65
1:A:111:TYR:CZ	1:A:188:VAL:HG23	2.30	0.65
1:B:205:LEU:HG	1:B:247:THR:HG22	1.79	0.65
1:B:286:ILE:HG22	1:B:289:VAL:HG22	1.78	0.65
1:L:265:PHE:HB3	1:L:267:PHE:CE1	2.32	0.65
1:D:286:ILE:HG22	1:D:289:VAL:HG22	1.79	0.64
1:G:191:TYR:HD1	1:G:214:TRP:HB3	1.61	0.64
1:H:205:LEU:HG	1:H:247:THR:HG22	1.79	0.64
1:J:191:TYR:HD1	1:J:214:TRP:HB3	1.62	0.64
1:F:223:ASN:O	1:F:224:ASN:HB2	1.98	0.64
1:F:262:GLN:OE1	1:F:270:ARG:NH1	2.30	0.64
1:J:111:TYR:CZ	1:J:188:VAL:HG23	2.30	0.64
1:K:286:ILE:HD12	1:K:286:ILE:H	1.63	0.64
1:I:287:GLY:HA2	1:K:321:ASP:CG	2.00	0.64
1:A:47:GLY:HA3	1:C:338:TYR:CZ	2.33	0.64
1:E:286:ILE:HG22	1:E:289:VAL:HG22	1.78	0.64
1:F:174:VAL:HG12	1:F:175:GLY:N	2.12	0.64
1:H:265:PHE:HB3	1:H:267:PHE:CE1	2.32	0.64
1:I:191:TYR:HD1	1:I:214:TRP:HB3	1.63	0.64
1:L:262:GLN:OE1	1:L:270:ARG:NH1	2.31	0.64
1:A:262:GLN:OE1	1:A:270:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:TYR:HD1	1:C:214:TRP:HB3	1.62	0.64
1:G:262:GLN:OE1	1:G:270:ARG:NH1	2.30	0.64
1:F:144:PHE:HB2	1:F:151:LEU:HD23	1.79	0.64
1:L:174:VAL:HG12	1:L:175:GLY:N	2.11	0.64
1:L:191:TYR:HD1	1:L:214:TRP:HB3	1.62	0.64
1:L:286:ILE:CG2	1:L:289:VAL:HG22	2.28	0.64
1:A:174:VAL:HG12	1:A:175:GLY:N	2.11	0.64
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.62	0.64
1:D:111:TYR:CZ	1:D:188:VAL:HG23	2.33	0.64
1:H:174:VAL:HG12	1:H:175:GLY:N	2.12	0.64
1:K:262:GLN:OE1	1:K:270:ARG:NH1	2.31	0.64
1:A:286:ILE:HG22	1:A:289:VAL:HG22	1.79	0.64
1:B:144:PHE:HB2	1:B:151:LEU:HD23	1.79	0.64
1:H:144:PHE:HB2	1:H:151:LEU:HD23	1.80	0.64
1:I:174:VAL:HG12	1:I:175:GLY:N	2.12	0.64
1:B:191:TYR:HD1	1:B:214:TRP:HB3	1.63	0.64
1:H:191:TYR:HD1	1:H:214:TRP:HB3	1.62	0.64
1:I:286:ILE:CG2	1:I:289:VAL:HG21	2.28	0.64
1:C:144:PHE:HB2	1:C:151:LEU:HD23	1.81	0.63
1:E:191:TYR:HD1	1:E:214:TRP:HB3	1.62	0.63
1:I:262:GLN:OE1	1:I:270:ARG:NH1	2.31	0.63
1:D:205:LEU:HG	1:D:247:THR:HG22	1.80	0.63
1:F:191:TYR:HD1	1:F:214:TRP:HB3	1.63	0.63
1:E:265:PHE:HB3	1:E:267:PHE:CE1	2.33	0.63
1:F:111:TYR:CZ	1:F:188:VAL:HG23	2.31	0.63
1:G:286:ILE:HG22	1:G:289:VAL:HG22	1.79	0.63
1:K:191:TYR:HD1	1:K:214:TRP:HB3	1.63	0.63
1:B:303:PHE:HB3	1:C:51:ILE:HD13	1.79	0.63
1:K:265:PHE:HB3	1:K:267:PHE:CE1	2.33	0.63
1:G:205:LEU:HG	1:G:247:THR:HG22	1.80	0.63
1:I:165:THR:HG21	1:I:167:ARG:HB3	1.81	0.63
1:I:286:ILE:CG2	1:I:289:VAL:HG22	2.28	0.63
1:A:287:GLY:HA3	1:F:321:ASP:CG	2.19	0.63
1:F:265:PHE:HB3	1:F:267:PHE:CE1	2.33	0.63
1:L:205:LEU:HG	1:L:247:THR:HG22	1.80	0.63
1:A:144:PHE:HB2	1:A:151:LEU:HD23	1.80	0.63
1:G:18:VAL:HG13	1:G:337:VAL:HG22	1.80	0.63
1:G:144:PHE:HB2	1:G:151:LEU:HD23	1.81	0.63
1:J:18:VAL:HG13	1:J:337:VAL:HG22	1.80	0.63
1:K:18:VAL:HG13	1:K:337:VAL:HG22	1.81	0.63
1:K:286:ILE:CG2	1:K:289:VAL:HG22	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:PHE:HB2	1:I:151:LEU:HD23	1.80	0.63
1:J:265:PHE:HB3	1:J:267:PHE:CE1	2.33	0.63
1:K:165:THR:HG21	1:K:167:ARG:HB3	1.81	0.63
1:C:205:LEU:HG	1:C:247:THR:HG22	1.81	0.62
1:D:144:PHE:HB2	1:D:151:LEU:HD23	1.80	0.62
1:J:47:GLY:HA3	1:L:338:TYR:CZ	2.34	0.62
1:C:265:PHE:HB3	1:C:267:PHE:CE1	2.34	0.62
1:A:265:PHE:HB3	1:A:267:PHE:CE1	2.34	0.62
1:D:303:PHE:HB3	1:E:51:ILE:HD13	1.81	0.62
1:A:18:VAL:HG13	1:A:337:VAL:HG22	1.80	0.62
1:I:265:PHE:HB3	1:I:267:PHE:CE1	2.34	0.62
1:L:223:ASN:O	1:L:224:ASN:HB2	1.99	0.62
1:J:144:PHE:HB2	1:J:151:LEU:HD23	1.81	0.62
1:B:18:VAL:HG13	1:B:337:VAL:HG22	1.82	0.62
1:D:51:ILE:HD13	1:F:303:PHE:HB3	1.81	0.62
1:G:265:PHE:HB3	1:G:267:PHE:CE1	2.34	0.62
1:I:223:ASN:O	1:I:224:ASN:HB2	2.00	0.62
1:A:286:ILE:HD12	1:A:286:ILE:H	1.65	0.62
1:B:265:PHE:HB3	1:B:267:PHE:CE1	2.34	0.62
1:B:286:ILE:HD12	1:B:286:ILE:H	1.63	0.62
1:H:296:GLU:OE2	1:H:312:ASP:OD1	2.18	0.62
1:A:205:LEU:HG	1:A:247:THR:HG22	1.81	0.62
1:E:303:PHE:HB3	1:F:51:ILE:HD13	1.80	0.62
1:L:286:ILE:HD12	1:L:286:ILE:H	1.64	0.62
1:B:338:TYR:CZ	1:C:47:GLY:HA3	2.35	0.62
1:E:205:LEU:HG	1:E:247:THR:CG2	2.30	0.62
1:K:144:PHE:HB2	1:K:151:LEU:HD23	1.81	0.62
1:L:18:VAL:HG13	1:L:337:VAL:HG22	1.82	0.62
1:B:205:LEU:HG	1:B:247:THR:CG2	2.30	0.62
1:F:285:GLY:HA3	1:J:244:PHE:CZ	2.35	0.62
1:G:296:GLU:OE2	1:G:312:ASP:OD1	2.18	0.62
1:L:144:PHE:HB2	1:L:151:LEU:HD23	1.80	0.62
1:D:18:VAL:HG13	1:D:337:VAL:HG22	1.81	0.61
1:I:205:LEU:HG	1:I:247:THR:HG22	1.80	0.61
1:K:205:LEU:HG	1:K:247:THR:HG22	1.82	0.61
1:L:165:THR:HG21	1:L:167:ARG:HB3	1.82	0.61
1:D:100:ARG:HH21	1:F:71:GLU:HG3	1.65	0.61
1:E:223:ASN:O	1:E:224:ASN:HB2	2.00	0.61
1:G:286:ILE:HD12	1:G:286:ILE:H	1.64	0.61
1:G:303:PHE:HB3	1:H:51:ILE:HD13	1.82	0.61
1:H:286:ILE:HD12	1:H:286:ILE:H	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ILE:HD12	1:E:286:ILE:H	1.63	0.61
1:D:47:GLY:HA3	1:F:338:TYR:CZ	2.36	0.61
1:D:265:PHE:HB3	1:D:267:PHE:CE1	2.35	0.61
1:F:18:VAL:HG13	1:F:337:VAL:HG22	1.81	0.61
1:G:205:LEU:HG	1:G:247:THR:CG2	2.30	0.61
1:B:165:THR:HG21	1:B:167:ARG:HB3	1.83	0.61
1:B:223:ASN:O	1:B:224:ASN:HB2	2.01	0.61
1:F:205:LEU:HG	1:F:247:THR:HG22	1.82	0.61
1:J:165:THR:HG21	1:J:167:ARG:HB3	1.83	0.61
1:B:71:GLU:HG3	1:C:100:ARG:HH21	1.65	0.61
1:E:287:GLY:HA3	1:I:321:ASP:OD2	2.00	0.61
1:J:296:GLU:OE2	1:J:312:ASP:OD1	2.19	0.61
1:C:18:VAL:HG13	1:C:337:VAL:HG22	1.82	0.61
1:D:205:LEU:HG	1:D:247:THR:CG2	2.31	0.61
1:F:286:ILE:CG2	1:F:289:VAL:HG22	2.30	0.61
1:I:296:GLU:OE2	1:I:312:ASP:OD1	2.19	0.61
1:D:286:ILE:HD12	1:D:286:ILE:H	1.64	0.61
1:H:286:ILE:CG2	1:H:289:VAL:HG22	2.31	0.61
1:L:205:LEU:HG	1:L:247:THR:CG2	2.31	0.61
1:B:286:ILE:CG2	1:B:289:VAL:HG21	2.30	0.61
1:I:286:ILE:HD12	1:I:286:ILE:H	1.64	0.61
1:J:51:ILE:HD13	1:L:303:PHE:HB3	1.82	0.61
1:J:286:ILE:CG2	1:J:289:VAL:HG22	2.31	0.61
1:K:71:GLU:HG3	1:L:100:ARG:HH21	1.64	0.61
1:G:165:THR:HG21	1:G:167:ARG:HB3	1.83	0.61
1:H:18:VAL:HG13	1:H:337:VAL:HG22	1.83	0.61
1:H:165:THR:HG21	1:H:167:ARG:HB3	1.83	0.61
1:E:338:TYR:CZ	1:F:47:GLY:HA3	2.35	0.60
1:H:205:LEU:HG	1:H:247:THR:CG2	2.30	0.60
1:K:223:ASN:O	1:K:224:ASN:HB2	2.01	0.60
1:B:286:ILE:CG2	1:B:289:VAL:HG22	2.31	0.60
1:C:286:ILE:CG2	1:C:289:VAL:HG22	2.31	0.60
1:D:165:THR:HG21	1:D:167:ARG:HB3	1.83	0.60
1:G:286:ILE:CG2	1:G:289:VAL:HG22	2.32	0.60
1:D:286:ILE:CG2	1:D:289:VAL:HG22	2.31	0.60
1:E:144:PHE:HB2	1:E:151:LEU:HD23	1.83	0.60
1:E:286:ILE:CG2	1:E:289:VAL:HG22	2.31	0.60
1:F:296:GLU:OE2	1:F:312:ASP:OD1	2.20	0.60
1:J:205:LEU:HG	1:J:247:THR:HG22	1.82	0.60
1:C:205:LEU:HG	1:C:247:THR:CG2	2.32	0.60
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:LEU:HG	1:I:247:THR:CG2	2.31	0.60
1:A:165:THR:HG21	1:A:167:ARG:HB3	1.84	0.60
1:F:319:ASP:OD2	1:F:321:ASP:HB2	2.02	0.60
1:C:258:LEU:CD1	1:C:276:THR:HG23	2.32	0.60
1:D:286:ILE:CG2	1:D:289:VAL:HG21	2.31	0.60
1:E:258:LEU:CD1	1:E:276:THR:HG23	2.32	0.60
1:F:165:THR:HG21	1:F:167:ARG:HB3	1.83	0.60
1:K:27:ASN:HD22	1:K:29:GLU:HB2	1.67	0.60
1:L:286:ILE:CG2	1:L:289:VAL:HG21	2.28	0.60
1:L:296:GLU:OE2	1:L:312:ASP:OD1	2.20	0.60
1:A:338:TYR:CZ	1:B:47:GLY:HA3	2.37	0.60
1:C:296:GLU:OE2	1:C:312:ASP:OD1	2.19	0.60
1:F:205:LEU:HG	1:F:247:THR:CG2	2.32	0.59
1:J:286:ILE:HD12	1:J:286:ILE:H	1.64	0.59
1:A:205:LEU:HG	1:A:247:THR:CG2	2.32	0.59
1:F:286:ILE:CG2	1:F:289:VAL:HG21	2.29	0.59
1:G:286:ILE:CG2	1:G:289:VAL:HG21	2.32	0.59
1:I:18:VAL:HG13	1:I:337:VAL:HG22	1.82	0.59
1:A:223:ASN:O	1:A:224:ASN:HB2	2.02	0.59
1:A:286:ILE:CG2	1:A:289:VAL:HG22	2.31	0.59
1:J:307:MET:O	1:J:308:SER:HB3	2.02	0.59
1:D:223:ASN:O	1:D:224:ASN:HB2	2.01	0.59
1:K:205:LEU:HG	1:K:247:THR:CG2	2.32	0.59
1:B:258:LEU:CD1	1:B:276:THR:HG23	2.32	0.59
1:H:286:ILE:CG2	1:H:289:VAL:HG21	2.30	0.59
1:E:165:THR:HG21	1:E:167:ARG:HB3	1.84	0.59
1:J:205:LEU:HG	1:J:247:THR:CG2	2.32	0.59
1:B:296:GLU:OE2	1:B:312:ASP:OD1	2.21	0.59
1:C:286:ILE:HD12	1:C:286:ILE:H	1.65	0.59
1:F:258:LEU:CD1	1:F:276:THR:HG23	2.33	0.59
1:C:165:THR:HG21	1:C:167:ARG:HB3	1.84	0.59
1:G:307:MET:O	1:G:308:SER:HB3	2.03	0.59
1:G:319:ASP:OD2	1:G:321:ASP:HB2	2.03	0.59
1:K:258:LEU:CD1	1:K:276:THR:HG23	2.32	0.59
1:K:296:GLU:OE2	1:K:312:ASP:OD1	2.21	0.59
1:H:258:LEU:CD1	1:H:276:THR:HG23	2.33	0.59
1:D:258:LEU:CD1	1:D:276:THR:HG23	2.33	0.59
1:H:223:ASN:O	1:H:224:ASN:HB2	2.02	0.59
1:H:338:TYR:CZ	1:I:47:GLY:HA3	2.38	0.59
1:D:296:GLU:OE2	1:D:312:ASP:OD1	2.20	0.58
1:J:223:ASN:O	1:J:224:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:GLY:CA	1:G:244:PHE:CZ	2.85	0.58
1:F:307:MET:O	1:F:308:SER:HB3	2.02	0.58
1:J:286:ILE:CG2	1:J:289:VAL:HG21	2.31	0.58
1:A:303:PHE:HB3	1:B:51:ILE:HD13	1.85	0.58
1:I:287:GLY:HA3	1:K:321:ASP:OD2	2.03	0.58
1:B:319:ASP:OD2	1:B:321:ASP:HB2	2.02	0.58
1:C:319:ASP:OD2	1:C:321:ASP:HB2	2.04	0.58
1:I:258:LEU:CD1	1:I:276:THR:HG23	2.34	0.58
1:J:319:ASP:OD2	1:J:321:ASP:HB2	2.04	0.58
1:A:307:MET:O	1:A:308:SER:HB3	2.04	0.58
1:A:258:LEU:CD1	1:A:276:THR:HG23	2.32	0.58
1:A:296:GLU:OE2	1:A:312:ASP:OD1	2.21	0.58
1:L:307:MET:O	1:L:308:SER:HB3	2.03	0.58
1:H:45:PHE:O	1:H:45:PHE:CD1	2.57	0.58
1:C:104:VAL:HG22	1:C:156:GLN:OE1	2.04	0.58
1:I:319:ASP:OD2	1:I:321:ASP:HB2	2.02	0.58
1:J:71:GLU:HG3	1:K:100:ARG:HH21	1.69	0.58
1:J:258:LEU:CD1	1:J:276:THR:HG23	2.34	0.58
1:B:244:PHE:CZ	1:H:285:GLY:HA3	2.39	0.58
1:D:104:VAL:HG22	1:D:156:GLN:OE1	2.04	0.57
1:E:296:GLU:OE2	1:E:312:ASP:OD1	2.21	0.57
1:G:223:ASN:O	1:G:224:ASN:HB2	2.03	0.57
1:K:319:ASP:OD2	1:K:321:ASP:HB2	2.04	0.57
1:B:307:MET:O	1:B:308:SER:HB3	2.05	0.57
1:I:45:PHE:O	1:I:45:PHE:CD1	2.57	0.57
1:A:319:ASP:OD2	1:A:321:ASP:HB2	2.05	0.57
1:I:307:MET:O	1:I:308:SER:HB3	2.04	0.57
1:A:105:VAL:HG12	1:A:105:VAL:O	2.03	0.57
1:C:223:ASN:O	1:C:224:ASN:HB2	2.03	0.57
1:B:143:ASN:O	1:B:146:GLY:N	2.38	0.57
1:H:303:PHE:HB3	1:I:51:ILE:HD13	1.86	0.57
1:L:258:LEU:CD1	1:L:276:THR:HG23	2.34	0.57
1:G:105:VAL:HG12	1:G:105:VAL:O	2.04	0.57
1:G:47:GLY:HA3	1:I:338:TYR:CE2	2.40	0.57
1:K:307:MET:O	1:K:308:SER:HB3	2.05	0.57
1:A:45:PHE:CD1	1:A:45:PHE:O	2.58	0.56
1:G:104:VAL:HG22	1:G:156:GLN:OE1	2.04	0.56
1:H:319:ASP:OD2	1:H:321:ASP:HB2	2.05	0.56
1:D:240:ILE:HD13	1:D:251:ALA:HB2	1.87	0.56
1:L:319:ASP:OD2	1:L:321:ASP:HB2	2.04	0.56
1:A:286:ILE:CG2	1:A:289:VAL:HG21	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASP:OD1	1:H:287:GLY:HA3	1.96	0.56
1:H:307:MET:O	1:H:308:SER:HB3	2.05	0.56
1:I:286:ILE:HG22	1:I:289:VAL:CG2	2.34	0.56
1:B:45:PHE:O	1:B:45:PHE:CD1	2.58	0.56
1:C:270:ARG:O	1:C:270:ARG:HG2	2.05	0.56
1:D:307:MET:O	1:D:308:SER:HB3	2.04	0.56
1:E:143:ASN:O	1:E:146:GLY:N	2.38	0.56
1:I:104:VAL:HG22	1:I:156:GLN:OE1	2.05	0.56
1:D:105:VAL:HG12	1:D:105:VAL:O	2.05	0.56
1:D:319:ASP:OD2	1:D:321:ASP:HB2	2.04	0.56
1:E:319:ASP:OD2	1:E:321:ASP:HB2	2.05	0.56
1:B:303:PHE:CB	1:C:51:ILE:HD13	2.36	0.56
1:E:307:MET:O	1:E:308:SER:HB3	2.04	0.56
1:H:111:TYR:CE2	1:H:188:VAL:HG23	2.40	0.56
1:A:143:ASN:O	1:A:146:GLY:N	2.38	0.56
1:B:244:PHE:CZ	1:H:285:GLY:CA	2.89	0.56
1:C:143:ASN:O	1:C:146:GLY:N	2.39	0.56
1:D:143:ASN:O	1:D:146:GLY:N	2.38	0.56
1:E:45:PHE:O	1:E:45:PHE:CD1	2.58	0.56
1:G:45:PHE:O	1:G:45:PHE:CD1	2.59	0.56
1:B:104:VAL:HG22	1:B:156:GLN:OE1	2.06	0.56
1:B:270:ARG:O	1:B:270:ARG:HG2	2.05	0.56
1:F:285:GLY:CA	1:J:244:PHE:CZ	2.89	0.56
1:A:104:VAL:HG22	1:A:156:GLN:OE1	2.06	0.56
1:G:11:VAL:HG21	1:I:340:PHE:HB2	1.88	0.56
1:C:307:MET:O	1:C:308:SER:HB3	2.06	0.56
1:E:286:ILE:CG2	1:E:289:VAL:HG21	2.30	0.56
1:K:105:VAL:HG12	1:K:105:VAL:O	2.05	0.56
1:C:105:VAL:HG12	1:C:105:VAL:O	2.05	0.55
1:I:270:ARG:O	1:I:270:ARG:HG2	2.06	0.55
1:K:286:ILE:CG2	1:K:289:VAL:HG21	2.29	0.55
1:E:104:VAL:HG22	1:E:156:GLN:OE1	2.06	0.55
1:G:258:LEU:CD1	1:G:276:THR:HG23	2.36	0.55
1:J:45:PHE:O	1:J:45:PHE:CD1	2.59	0.55
1:K:165:THR:CG2	1:K:167:ARG:HB3	2.37	0.55
1:A:281:LYS:O	1:A:282:ASP:HB2	2.06	0.55
1:E:270:ARG:O	1:E:270:ARG:HG2	2.06	0.55
1:I:27:ASN:HD22	1:I:29:GLU:CB	2.12	0.55
1:L:45:PHE:O	1:L:45:PHE:CD1	2.59	0.55
1:B:281:LYS:O	1:B:282:ASP:HB2	2.07	0.55
1:F:111:TYR:CE2	1:F:188:VAL:HG23	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:ASP:O	1:H:222:ALA:HB2	2.05	0.55
1:L:143:ASN:HA	1:L:148:VAL:O	2.07	0.55
1:G:51:ILE:HD13	1:I:303:PHE:CB	2.34	0.55
1:I:165:THR:CG2	1:I:167:ARG:HB3	2.37	0.55
1:B:309:THR:HG22	1:B:336:ILE:CA	2.35	0.55
1:I:105:VAL:HG12	1:I:105:VAL:O	2.07	0.55
1:I:221:ASP:O	1:I:222:ALA:HB2	2.07	0.55
1:J:303:PHE:HB3	1:K:51:ILE:HD13	1.89	0.55
1:J:338:TYR:CZ	1:K:47:GLY:HA3	2.42	0.55
1:K:143:ASN:O	1:K:146:GLY:N	2.39	0.55
1:K:281:LYS:O	1:K:282:ASP:HB2	2.07	0.55
1:L:286:ILE:HG22	1:L:289:VAL:CG2	2.34	0.55
1:B:321:ASP:CG	1:H:287:GLY:HA3	2.26	0.55
1:J:105:VAL:HG12	1:J:105:VAL:O	2.06	0.55
1:K:71:GLU:CG	1:L:100:ARG:HH21	2.19	0.55
1:F:143:ASN:O	1:F:146:GLY:N	2.39	0.55
1:F:281:LYS:O	1:F:282:ASP:HB2	2.07	0.55
1:J:111:TYR:CE2	1:J:188:VAL:HG23	2.42	0.55
1:A:221:ASP:O	1:A:222:ALA:HB2	2.06	0.55
1:H:286:ILE:HG22	1:H:289:VAL:CG2	2.36	0.55
1:J:104:VAL:HG22	1:J:156:GLN:OE1	2.07	0.55
1:K:104:VAL:HG22	1:K:156:GLN:OE1	2.06	0.55
1:L:111:TYR:CE2	1:L:188:VAL:HG23	2.41	0.55
1:E:111:TYR:CE2	1:E:188:VAL:HG23	2.42	0.54
1:H:281:LYS:O	1:H:282:ASP:HB2	2.07	0.54
1:I:111:TYR:CE2	1:I:188:VAL:HG23	2.41	0.54
1:I:143:ASN:HA	1:I:148:VAL:O	2.07	0.54
1:K:45:PHE:CD1	1:K:45:PHE:O	2.59	0.54
1:A:111:TYR:CE2	1:A:188:VAL:HG23	2.43	0.54
1:A:321:ASP:OD2	1:J:287:GLY:HA3	2.06	0.54
1:B:321:ASP:CG	1:H:287:GLY:CA	2.72	0.54
1:B:338:TYR:CE2	1:C:47:GLY:HA3	2.43	0.54
1:L:143:ASN:O	1:L:146:GLY:N	2.41	0.54
1:G:111:TYR:CE2	1:G:188:VAL:HG23	2.41	0.54
1:G:143:ASN:HA	1:G:148:VAL:O	2.07	0.54
1:L:221:ASP:O	1:L:222:ALA:HB2	2.07	0.54
1:D:221:ASP:O	1:D:222:ALA:HB2	2.07	0.54
1:F:105:VAL:HG12	1:F:105:VAL:O	2.08	0.54
1:H:143:ASN:O	1:H:146:GLY:N	2.40	0.54
1:I:141:ASN:HB3	1:I:153:PHE:CE1	2.43	0.54
1:C:111:TYR:CE2	1:C:188:VAL:HG23	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ARG:HH21	1:F:71:GLU:CG	2.21	0.54
1:J:281:LYS:O	1:J:282:ASP:HB2	2.08	0.54
1:F:45:PHE:CD1	1:F:45:PHE:O	2.60	0.54
1:F:104:VAL:HG22	1:F:156:GLN:OE1	2.07	0.54
1:F:165:THR:CG2	1:F:167:ARG:HB3	2.38	0.54
1:G:143:ASN:O	1:G:146:GLY:N	2.41	0.54
1:H:104:VAL:HG22	1:H:156:GLN:OE1	2.08	0.54
1:A:240:ILE:HD13	1:A:251:ALA:HB2	1.90	0.54
1:B:143:ASN:HA	1:B:148:VAL:O	2.08	0.54
1:F:221:ASP:O	1:F:222:ALA:HB2	2.07	0.54
1:H:143:ASN:HA	1:H:148:VAL:O	2.08	0.54
1:L:165:THR:CG2	1:L:167:ARG:HB3	2.37	0.54
1:A:51:ILE:HD13	1:C:303:PHE:HB3	1.89	0.53
1:E:281:LYS:O	1:E:282:ASP:HB2	2.07	0.53
1:F:270:ARG:O	1:F:270:ARG:HG2	2.07	0.53
1:K:111:TYR:CE2	1:K:188:VAL:HG23	2.43	0.53
1:K:144:PHE:O	1:K:145:PHE:HB2	2.08	0.53
1:B:105:VAL:HG12	1:B:105:VAL:O	2.08	0.53
1:H:165:THR:CG2	1:H:167:ARG:HB3	2.38	0.53
1:I:143:ASN:O	1:I:146:GLY:N	2.41	0.53
1:K:270:ARG:O	1:K:270:ARG:HG2	2.08	0.53
1:B:111:TYR:CE2	1:B:188:VAL:HG23	2.43	0.53
1:B:221:ASP:O	1:B:222:ALA:HB2	2.07	0.53
1:H:105:VAL:HG12	1:H:105:VAL:O	2.08	0.53
1:B:240:ILE:HD13	1:B:251:ALA:HB2	1.91	0.53
1:C:174:VAL:CG1	1:C:175:GLY:N	2.72	0.53
1:D:45:PHE:O	1:D:45:PHE:CD1	2.61	0.53
1:G:144:PHE:O	1:G:145:PHE:HB2	2.09	0.53
1:K:221:ASP:O	1:K:222:ALA:HB2	2.07	0.53
1:D:165:THR:CG2	1:D:167:ARG:HB3	2.39	0.53
1:C:281:LYS:O	1:C:282:ASP:HB2	2.08	0.53
1:F:286:ILE:H	1:F:286:ILE:CD1	2.22	0.53
1:G:3:ILE:HD12	1:I:3:ILE:HG21	1.91	0.53
1:G:141:ASN:HB3	1:G:153:PHE:CE1	2.44	0.53
1:G:165:THR:CG2	1:G:167:ARG:HB3	2.38	0.53
1:J:221:ASP:O	1:J:222:ALA:HB2	2.08	0.53
1:A:270:ARG:O	1:A:270:ARG:HG2	2.08	0.53
1:C:221:ASP:O	1:C:222:ALA:HB2	2.08	0.53
1:D:281:LYS:O	1:D:282:ASP:HB2	2.08	0.53
1:E:221:ASP:O	1:E:222:ALA:HB2	2.08	0.53
1:G:221:ASP:O	1:G:222:ALA:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:174:VAL:CG1	1:K:175:GLY:N	2.72	0.53
1:A:144:PHE:O	1:A:145:PHE:HB2	2.09	0.53
1:C:286:ILE:HG22	1:C:289:VAL:CG2	2.37	0.53
1:E:321:ASP:CG	1:K:287:GLY:CA	2.68	0.53
1:F:143:ASN:HA	1:F:148:VAL:O	2.08	0.53
1:K:240:ILE:HD13	1:K:251:ALA:HB2	1.91	0.53
1:L:144:PHE:O	1:L:145:PHE:HB2	2.09	0.53
1:C:45:PHE:O	1:C:45:PHE:CD1	2.62	0.53
1:D:321:ASP:OD2	1:G:287:GLY:HA3	2.09	0.53
1:E:143:ASN:HA	1:E:148:VAL:O	2.09	0.53
1:I:281:LYS:O	1:I:282:ASP:HB2	2.09	0.53
1:J:144:PHE:O	1:J:145:PHE:HB2	2.08	0.53
1:J:222:ALA:O	1:J:223:ASN:HB2	2.09	0.53
1:B:340:PHE:HB2	1:C:11:VAL:HG21	1.91	0.52
1:D:111:TYR:CE2	1:D:188:VAL:HG23	2.44	0.52
1:D:174:VAL:CG1	1:D:175:GLY:N	2.71	0.52
1:E:105:VAL:HG12	1:E:105:VAL:O	2.08	0.52
1:F:286:ILE:HG22	1:F:289:VAL:CG2	2.36	0.52
1:G:222:ALA:O	1:G:223:ASN:HB2	2.09	0.52
1:B:71:GLU:CG	1:C:100:ARG:HH21	2.23	0.52
1:B:165:THR:CG2	1:B:167:ARG:HB3	2.39	0.52
1:C:165:THR:CG2	1:C:167:ARG:HB3	2.39	0.52
1:E:286:ILE:N	1:E:286:ILE:CD1	2.72	0.52
1:G:281:LYS:O	1:G:282:ASP:HB2	2.09	0.52
1:G:338:TYR:CE2	1:H:47:GLY:HA3	2.45	0.52
1:H:270:ARG:O	1:H:270:ARG:HG2	2.08	0.52
1:J:143:ASN:HA	1:J:148:VAL:O	2.09	0.52
1:L:105:VAL:HG12	1:L:105:VAL:O	2.10	0.52
1:L:174:VAL:CG1	1:L:175:GLY:N	2.72	0.52
1:L:270:ARG:HG2	1:L:270:ARG:O	2.09	0.52
1:A:309:THR:HG22	1:A:336:ILE:CA	2.34	0.52
1:E:222:ALA:O	1:E:223:ASN:HB2	2.09	0.52
1:H:144:PHE:O	1:H:145:PHE:HB2	2.08	0.52
1:C:143:ASN:HA	1:C:148:VAL:O	2.08	0.52
1:D:143:ASN:HA	1:D:148:VAL:O	2.09	0.52
1:E:174:VAL:CG1	1:E:175:GLY:N	2.72	0.52
1:H:141:ASN:HB3	1:H:153:PHE:CE1	2.45	0.52
1:I:144:PHE:O	1:I:145:PHE:HB2	2.10	0.52
1:I:264:GLN:OE1	1:I:270:ARG:HB2	2.09	0.52
1:J:165:THR:CG2	1:J:167:ARG:HB3	2.38	0.52
1:J:174:VAL:CG1	1:J:175:GLY:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:281:LYS:O	1:L:282:ASP:HB2	2.09	0.52
1:C:222:ALA:O	1:C:223:ASN:HB2	2.09	0.52
1:C:286:ILE:CG2	1:C:289:VAL:HG21	2.31	0.52
1:D:309:THR:HG22	1:D:336:ILE:CA	2.34	0.52
1:A:143:ASN:HA	1:A:148:VAL:O	2.09	0.52
1:B:174:VAL:CG1	1:B:175:GLY:N	2.73	0.52
1:B:303:PHE:CG	1:C:51:ILE:HD13	2.45	0.52
1:G:309:THR:HG22	1:G:336:ILE:CA	2.35	0.52
1:H:240:ILE:HD13	1:H:251:ALA:HB2	1.92	0.52
1:J:309:THR:HG22	1:J:336:ILE:CA	2.35	0.52
1:K:143:ASN:HA	1:K:148:VAL:O	2.08	0.52
1:L:104:VAL:HG22	1:L:156:GLN:OE1	2.08	0.52
1:D:51:ILE:HD13	1:F:303:PHE:CB	2.39	0.52
1:E:165:THR:CG2	1:E:167:ARG:HB3	2.39	0.52
1:F:258:LEU:HD13	1:F:276:THR:HG23	1.92	0.52
1:C:144:PHE:O	1:C:145:PHE:HB2	2.10	0.52
1:E:286:ILE:H	1:E:286:ILE:CD1	2.23	0.52
1:A:165:THR:CG2	1:A:167:ARG:HB3	2.39	0.52
1:E:303:PHE:CB	1:F:51:ILE:HD13	2.40	0.52
1:F:161:ASN:HB2	1:F:170:ASN:OD1	2.11	0.52
1:F:286:ILE:N	1:F:286:ILE:CD1	2.71	0.52
1:K:154:ALA:O	1:K:176:GLY:HA2	2.10	0.52
1:G:174:VAL:CG1	1:G:175:GLY:N	2.73	0.51
1:A:174:VAL:CG1	1:A:175:GLY:N	2.73	0.51
1:B:141:ASN:HB3	1:B:153:PHE:CE1	2.46	0.51
1:B:154:ALA:O	1:B:176:GLY:HA2	2.11	0.51
1:G:270:ARG:HG2	1:G:270:ARG:O	2.10	0.51
1:I:161:ASN:HB2	1:I:170:ASN:OD1	2.09	0.51
1:I:240:ILE:HD13	1:I:251:ALA:HB2	1.92	0.51
1:I:309:THR:HG22	1:I:336:ILE:CA	2.38	0.51
1:K:286:ILE:H	1:K:286:ILE:CD1	2.23	0.51
1:D:141:ASN:HB3	1:D:153:PHE:CE1	2.45	0.51
1:F:144:PHE:O	1:F:145:PHE:HB2	2.10	0.51
1:H:244:PHE:CZ	1:L:285:GLY:HA3	2.45	0.51
1:J:270:ARG:O	1:J:270:ARG:HG2	2.09	0.51
1:A:141:ASN:HB3	1:A:153:PHE:CE1	2.45	0.51
1:D:270:ARG:O	1:D:270:ARG:HG2	2.08	0.51
1:F:240:ILE:HD13	1:F:251:ALA:HB2	1.92	0.51
1:J:141:ASN:HB3	1:J:153:PHE:CE1	2.45	0.51
1:K:264:GLN:OE1	1:K:270:ARG:HB2	2.10	0.51
1:B:130:VAL:HG13	1:B:213:GLN:CD	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:PHE:CB	1:C:11:VAL:HG21	2.40	0.51
1:C:258:LEU:HD13	1:C:276:THR:HG23	1.93	0.51
1:D:47:GLY:HA3	1:F:338:TYR:CE2	2.45	0.51
1:E:154:ALA:O	1:E:176:GLY:HA2	2.10	0.51
1:F:174:VAL:CG1	1:F:175:GLY:N	2.73	0.51
1:G:204:PRO:HD2	1:G:248:SER:O	2.10	0.51
1:L:141:ASN:HB3	1:L:153:PHE:CE1	2.46	0.51
1:D:144:PHE:O	1:D:145:PHE:HB2	2.10	0.51
1:E:144:PHE:O	1:E:145:PHE:HB2	2.09	0.51
1:H:174:VAL:CG1	1:H:175:GLY:N	2.73	0.51
1:K:141:ASN:HB3	1:K:153:PHE:CE1	2.46	0.51
1:K:204:PRO:HB2	1:K:247:THR:CG2	2.41	0.51
1:A:154:ALA:O	1:A:176:GLY:HA2	2.10	0.51
1:E:286:ILE:HG22	1:E:289:VAL:CG2	2.37	0.51
1:F:154:ALA:O	1:F:176:GLY:HA2	2.11	0.51
1:G:240:ILE:HD13	1:G:251:ALA:HB2	1.92	0.51
1:J:143:ASN:O	1:J:146:GLY:N	2.43	0.51
1:L:165:THR:CG2	1:L:167:ARG:H	2.13	0.51
1:A:258:LEU:HD13	1:A:276:THR:HG23	1.93	0.51
1:B:264:GLN:OE1	1:B:270:ARG:HB2	2.11	0.51
1:D:258:LEU:HD13	1:D:276:THR:HG23	1.92	0.51
1:D:338:TYR:CE2	1:E:47:GLY:HA3	2.46	0.51
1:E:141:ASN:HB3	1:E:153:PHE:CE1	2.46	0.51
1:E:258:LEU:HD13	1:E:276:THR:HG23	1.92	0.51
1:I:174:VAL:CG1	1:I:175:GLY:N	2.73	0.51
1:B:144:PHE:O	1:B:145:PHE:HB2	2.11	0.51
1:G:11:VAL:HG21	1:I:340:PHE:CB	2.41	0.51
1:H:222:ALA:O	1:H:223:ASN:HB2	2.11	0.51
1:J:258:LEU:HD13	1:J:276:THR:HG23	1.93	0.51
1:J:286:ILE:N	1:J:286:ILE:CD1	2.74	0.51
1:L:222:ALA:O	1:L:223:ASN:HB2	2.11	0.51
1:J:240:ILE:HD13	1:J:251:ALA:HB2	1.92	0.50
1:L:136:VAL:CG1	1:L:158:LEU:HD13	2.41	0.50
1:D:222:ALA:O	1:D:223:ASN:HB2	2.11	0.50
1:E:240:ILE:HD13	1:E:251:ALA:HB2	1.91	0.50
1:G:136:VAL:CG1	1:G:158:LEU:HD13	2.42	0.50
1:H:321:ASP:OD2	1:L:287:GLY:HA3	2.11	0.50
1:I:154:ALA:O	1:I:176:GLY:HA2	2.11	0.50
1:J:154:ALA:O	1:J:176:GLY:HA2	2.11	0.50
1:K:130:VAL:HG13	1:K:213:GLN:CD	2.32	0.50
1:C:309:THR:HG22	1:C:336:ILE:CA	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:VAL:CG1	1:H:158:LEU:HD13	2.41	0.50
1:L:154:ALA:O	1:L:176:GLY:HA2	2.11	0.50
1:A:222:ALA:O	1:A:223:ASN:HB2	2.11	0.50
1:D:154:ALA:O	1:D:176:GLY:HA2	2.11	0.50
1:F:309:THR:HG22	1:F:336:ILE:CA	2.36	0.50
1:G:340:PHE:HB2	1:H:11:VAL:HG21	1.93	0.50
1:H:161:ASN:HB2	1:H:170:ASN:OD1	2.11	0.50
1:I:204:PRO:HB2	1:I:247:THR:CG2	2.42	0.50
1:J:286:ILE:HG22	1:J:289:VAL:CG2	2.38	0.50
1:J:286:ILE:H	1:J:286:ILE:CD1	2.25	0.50
1:G:286:ILE:N	1:G:286:ILE:CD1	2.74	0.50
1:H:130:VAL:HG13	1:H:213:GLN:CD	2.32	0.50
1:K:161:ASN:HB2	1:K:170:ASN:OD1	2.12	0.50
1:A:286:ILE:H	1:A:286:ILE:CD1	2.25	0.50
1:B:286:ILE:H	1:B:286:ILE:CD1	2.24	0.50
1:F:130:VAL:HG13	1:F:213:GLN:CD	2.32	0.50
1:G:154:ALA:O	1:G:176:GLY:HA2	2.11	0.50
1:I:258:LEU:HD13	1:I:276:THR:HG23	1.93	0.50
1:J:161:ASN:HB2	1:J:170:ASN:OD1	2.11	0.50
1:B:286:ILE:N	1:B:286:ILE:CD1	2.73	0.50
1:C:321:ASP:OD2	1:D:287:GLY:HA3	2.12	0.50
1:E:130:VAL:HG13	1:E:213:GLN:CD	2.32	0.50
1:I:286:ILE:H	1:I:286:ILE:CD1	2.24	0.50
1:J:294:TYR:CD1	1:J:294:TYR:C	2.85	0.50
1:L:204:PRO:HD2	1:L:248:SER:O	2.11	0.50
1:E:153:PHE:HA	1:E:177:SER:O	2.12	0.50
1:E:204:PRO:HB2	1:E:247:THR:CG2	2.42	0.50
1:G:286:ILE:H	1:G:286:ILE:CD1	2.25	0.50
1:I:136:VAL:CG1	1:I:158:LEU:HD13	2.41	0.50
1:J:71:GLU:CG	1:K:100:ARG:HH21	2.25	0.50
1:L:286:ILE:H	1:L:286:ILE:CD1	2.25	0.50
1:E:161:ASN:HB2	1:E:170:ASN:OD1	2.12	0.50
1:G:105:VAL:HA	1:G:190:ALA:HB1	1.94	0.50
1:G:153:PHE:HA	1:G:177:SER:O	2.12	0.50
1:G:161:ASN:HB2	1:G:170:ASN:OD1	2.11	0.50
1:G:313:TYR:HD1	1:G:332:VAL:CG2	2.18	0.50
1:H:204:PRO:HD2	1:H:248:SER:O	2.12	0.50
1:I:286:ILE:N	1:I:286:ILE:CD1	2.74	0.50
1:C:154:ALA:O	1:C:176:GLY:HA2	2.12	0.49
1:C:204:PRO:HD2	1:C:248:SER:O	2.12	0.49
1:D:11:VAL:HG21	1:F:340:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PRO:HB2	1:D:247:THR:CG2	2.42	0.49
1:H:286:ILE:H	1:H:286:ILE:CD1	2.24	0.49
1:K:294:TYR:CD1	1:K:294:TYR:C	2.85	0.49
1:L:240:ILE:HD13	1:L:251:ALA:HB2	1.92	0.49
1:L:264:GLN:OE1	1:L:270:ARG:HB2	2.12	0.49
1:B:161:ASN:HB2	1:B:170:ASN:OD1	2.11	0.49
1:C:240:ILE:HD13	1:C:251:ALA:HB2	1.94	0.49
1:F:153:PHE:HA	1:F:177:SER:O	2.13	0.49
1:H:154:ALA:O	1:H:176:GLY:HA2	2.11	0.49
1:I:204:PRO:HD2	1:I:248:SER:O	2.12	0.49
1:L:130:VAL:HG13	1:L:213:GLN:CD	2.32	0.49
1:B:303:PHE:HB3	1:C:51:ILE:HG21	1.94	0.49
1:D:286:ILE:HG22	1:D:289:VAL:CG2	2.38	0.49
1:F:141:ASN:HB3	1:F:153:PHE:CE1	2.47	0.49
1:J:153:PHE:HA	1:J:177:SER:O	2.12	0.49
1:K:309:THR:HG22	1:K:336:ILE:CA	2.37	0.49
1:L:309:THR:HG22	1:L:336:ILE:CA	2.37	0.49
1:C:136:VAL:CG1	1:C:158:LEU:HD13	2.42	0.49
1:I:66:GLN:HG3	1:I:78:GLY:HA3	1.94	0.49
1:J:51:ILE:HD13	1:L:303:PHE:CB	2.43	0.49
1:J:136:VAL:CG1	1:J:158:LEU:HD13	2.42	0.49
1:K:222:ALA:O	1:K:223:ASN:HB2	2.12	0.49
1:K:236:ASN:OD1	1:K:252:ASN:HA	2.12	0.49
1:K:286:ILE:N	1:K:286:ILE:CD1	2.73	0.49
1:K:338:TYR:CZ	1:L:47:GLY:HA3	2.48	0.49
1:L:258:LEU:HD13	1:L:276:THR:HG23	1.94	0.49
1:C:236:ASN:OD1	1:C:252:ASN:HA	2.13	0.49
1:E:136:VAL:CG1	1:E:158:LEU:HD13	2.42	0.49
1:K:204:PRO:HD2	1:K:248:SER:O	2.12	0.49
1:A:294:TYR:CD1	1:A:294:TYR:C	2.85	0.49
1:C:141:ASN:HB3	1:C:153:PHE:CE1	2.47	0.49
1:D:340:PHE:HB2	1:E:11:VAL:HG21	1.94	0.49
1:H:66:GLN:HG3	1:H:78:GLY:HA3	1.94	0.49
1:I:267:PHE:H	1:I:267:PHE:HD1	1.61	0.49
1:L:286:ILE:N	1:L:286:ILE:CD1	2.73	0.49
1:A:47:GLY:HA3	1:C:338:TYR:CE2	2.48	0.49
1:B:204:PRO:HB2	1:B:247:THR:CG2	2.43	0.49
1:I:222:ALA:O	1:I:223:ASN:HB2	2.11	0.49
1:K:136:VAL:CG1	1:K:158:LEU:HD13	2.43	0.49
1:L:161:ASN:HB2	1:L:170:ASN:OD1	2.13	0.49
1:B:153:PHE:HA	1:B:177:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:HD13	1:B:276:THR:HG23	1.94	0.49
1:D:161:ASN:HB2	1:D:170:ASN:OD1	2.12	0.49
1:E:244:PHE:HZ	1:K:285:GLY:CA	2.26	0.49
1:H:258:LEU:HD13	1:H:276:THR:HG23	1.94	0.49
1:K:258:LEU:HD13	1:K:276:THR:HG23	1.93	0.49
1:E:71:GLU:HG3	1:F:100:ARG:HH21	1.77	0.49
1:E:264:GLN:OE1	1:E:270:ARG:HB2	2.13	0.49
1:F:31:SER:CA	1:F:329:ASP:HB2	2.40	0.49
1:H:264:GLN:OE1	1:H:270:ARG:HB2	2.12	0.49
1:L:269:LEU:HG	1:L:271:PRO:HD3	1.95	0.49
1:A:286:ILE:HG22	1:A:289:VAL:CG2	2.39	0.49
1:E:236:ASN:OD1	1:E:252:ASN:HA	2.13	0.49
1:G:204:PRO:HB2	1:G:247:THR:CG2	2.43	0.49
1:H:309:THR:HG22	1:H:336:ILE:CA	2.37	0.49
1:J:204:PRO:HB2	1:J:247:THR:CG2	2.43	0.49
1:A:100:ARG:HH21	1:C:71:GLU:HG3	1.76	0.48
1:G:267:PHE:HD1	1:G:267:PHE:H	1.61	0.48
1:I:165:THR:CG2	1:I:167:ARG:H	2.15	0.48
1:A:153:PHE:HA	1:A:177:SER:O	2.12	0.48
1:B:105:VAL:HA	1:B:190:ALA:HB1	1.94	0.48
1:C:204:PRO:HB2	1:C:247:THR:CG2	2.43	0.48
1:C:286:ILE:H	1:C:286:ILE:CD1	2.26	0.48
1:D:286:ILE:H	1:D:286:ILE:CD1	2.25	0.48
1:F:204:PRO:HD2	1:F:248:SER:O	2.13	0.48
1:I:153:PHE:HA	1:I:177:SER:O	2.13	0.48
1:I:236:ASN:OD1	1:I:252:ASN:HA	2.13	0.48
1:K:66:GLN:HG3	1:K:78:GLY:HA3	1.95	0.48
1:A:3:ILE:HD12	1:C:3:ILE:HG21	1.95	0.48
1:A:11:VAL:HG21	1:C:340:PHE:HB2	1.95	0.48
1:H:61:TRP:CZ2	1:H:63:TYR:HB2	2.48	0.48
1:H:236:ASN:OD1	1:H:252:ASN:HA	2.13	0.48
1:I:130:VAL:HG13	1:I:213:GLN:CD	2.34	0.48
1:J:269:LEU:HG	1:J:271:PRO:HD3	1.95	0.48
1:L:294:TYR:C	1:L:294:TYR:CD1	2.86	0.48
1:A:31:SER:CA	1:A:329:ASP:HB2	2.40	0.48
1:A:161:ASN:HB2	1:A:170:ASN:OD1	2.13	0.48
1:A:264:GLN:OE1	1:A:270:ARG:HB2	2.12	0.48
1:C:294:TYR:CD1	1:C:294:TYR:C	2.87	0.48
1:D:61:TRP:CZ2	1:D:63:TYR:HB2	2.48	0.48
1:K:165:THR:CG2	1:K:167:ARG:H	2.14	0.48
1:L:204:PRO:HB2	1:L:247:THR:CG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLN:HG3	1:A:78:GLY:HA3	1.96	0.48
1:A:204:PRO:HB2	1:A:247:THR:CG2	2.43	0.48
1:E:267:PHE:HD1	1:E:267:PHE:H	1.62	0.48
1:F:136:VAL:CG1	1:F:158:LEU:HD13	2.43	0.48
1:E:204:PRO:HB2	1:E:247:THR:HG23	1.95	0.48
1:G:130:VAL:HG13	1:G:213:GLN:CD	2.33	0.48
1:H:31:SER:CA	1:H:329:ASP:HB2	2.39	0.48
1:H:204:PRO:HB2	1:H:247:THR:CG2	2.43	0.48
1:I:61:TRP:CZ2	1:I:63:TYR:HB2	2.48	0.48
1:J:105:VAL:HA	1:J:190:ALA:HB1	1.96	0.48
1:L:153:PHE:HA	1:L:177:SER:O	2.13	0.48
1:L:236:ASN:OD1	1:L:252:ASN:HA	2.14	0.48
1:E:313:TYR:HD1	1:E:332:VAL:CG2	2.19	0.48
1:K:204:PRO:HB2	1:K:247:THR:HG23	1.95	0.48
1:B:136:VAL:CG1	1:B:158:LEU:HD13	2.44	0.48
1:B:222:ALA:O	1:B:223:ASN:HB2	2.12	0.48
1:B:294:TYR:CD1	1:B:294:TYR:C	2.86	0.48
1:C:130:VAL:HG13	1:C:213:GLN:CD	2.33	0.48
1:E:31:SER:CA	1:E:329:ASP:HB2	2.39	0.48
1:F:267:PHE:HD1	1:F:267:PHE:H	1.60	0.48
1:G:66:GLN:HG3	1:G:78:GLY:HA3	1.96	0.48
1:H:269:LEU:HG	1:H:271:PRO:HD3	1.96	0.48
1:I:294:TYR:CD1	1:I:294:TYR:C	2.87	0.48
1:J:130:VAL:HG13	1:J:213:GLN:CD	2.34	0.48
1:D:66:GLN:HG3	1:D:78:GLY:HA3	1.96	0.48
1:D:130:VAL:HG13	1:D:213:GLN:CD	2.34	0.48
1:D:236:ASN:OD1	1:D:252:ASN:HA	2.14	0.48
1:E:294:TYR:CD1	1:E:294:TYR:C	2.86	0.48
1:F:294:TYR:CD1	1:F:294:TYR:C	2.86	0.48
1:J:47:GLY:HA3	1:L:338:TYR:CE2	2.48	0.48
1:L:272:SER:N	1:L:298:GLY:O	2.44	0.48
1:A:236:ASN:OD1	1:A:252:ASN:HA	2.14	0.48
1:C:66:GLN:HG3	1:C:78:GLY:HA3	1.96	0.48
1:C:153:PHE:HA	1:C:177:SER:O	2.14	0.48
1:C:264:GLN:OE1	1:C:270:ARG:HB2	2.14	0.48
1:D:204:PRO:HD2	1:D:248:SER:O	2.13	0.48
1:G:236:ASN:OD1	1:G:252:ASN:HA	2.13	0.48
1:J:165:THR:CG2	1:J:167:ARG:H	2.16	0.48
1:J:204:PRO:HD2	1:J:248:SER:O	2.13	0.48
1:L:267:PHE:HD1	1:L:267:PHE:H	1.60	0.48
1:B:66:GLN:HG3	1:B:78:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:HA	1:D:190:ALA:HB1	1.96	0.47
1:F:264:GLN:OE1	1:F:270:ARG:HB2	2.14	0.47
1:F:269:LEU:HG	1:F:271:PRO:HD3	1.96	0.47
1:F:313:TYR:HD1	1:F:332:VAL:CG2	2.19	0.47
1:G:165:THR:HG22	1:G:166:ALA:N	2.28	0.47
1:D:204:PRO:HB2	1:D:247:THR:HG23	1.96	0.47
1:D:264:GLN:OE1	1:D:270:ARG:HB2	2.13	0.47
1:F:204:PRO:HB2	1:F:247:THR:CG2	2.43	0.47
1:F:222:ALA:O	1:F:223:ASN:HB2	2.13	0.47
1:G:340:PHE:CB	1:H:11:VAL:HG21	2.43	0.47
1:I:105:VAL:HA	1:I:190:ALA:HB1	1.96	0.47
1:J:273:ILE:CD1	1:J:297:VAL:HG22	2.45	0.47
1:K:286:ILE:HG22	1:K:289:VAL:CG2	2.36	0.47
1:A:136:VAL:CG1	1:A:158:LEU:HD13	2.44	0.47
1:B:165:THR:HG22	1:B:166:ALA:N	2.29	0.47
1:B:204:PRO:HB2	1:B:247:THR:HG23	1.96	0.47
1:D:294:TYR:CD1	1:D:294:TYR:C	2.88	0.47
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.49	0.47
1:J:165:THR:HG22	1:J:166:ALA:N	2.29	0.47
1:K:31:SER:CA	1:K:329:ASP:HB2	2.39	0.47
1:L:169:SER:O	1:L:170:ASN:HB3	2.15	0.47
1:A:267:PHE:HD1	1:A:267:PHE:H	1.60	0.47
1:C:31:SER:CA	1:C:329:ASP:HB2	2.39	0.47
1:D:31:SER:CA	1:D:329:ASP:HB2	2.41	0.47
1:D:153:PHE:HA	1:D:177:SER:O	2.13	0.47
1:E:338:TYR:CE2	1:F:47:GLY:HA3	2.49	0.47
1:H:267:PHE:HD1	1:H:267:PHE:H	1.60	0.47
1:B:286:ILE:HG22	1:B:289:VAL:CG2	2.37	0.47
1:C:267:PHE:HD1	1:C:267:PHE:H	1.61	0.47
1:D:165:THR:HG22	1:D:166:ALA:N	2.29	0.47
1:E:61:TRP:CZ2	1:E:63:TYR:HB2	2.50	0.47
1:E:66:GLN:HG3	1:E:78:GLY:HA3	1.96	0.47
1:G:286:ILE:HG22	1:G:289:VAL:CG2	2.38	0.47
1:G:303:PHE:CB	1:H:51:ILE:HD13	2.42	0.47
1:J:144:PHE:O	1:J:144:PHE:CD2	2.68	0.47
1:B:179:SER:HB3	1:B:188:VAL:HG13	1.96	0.47
1:B:236:ASN:OD1	1:B:252:ASN:HA	2.14	0.47
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.49	0.47
1:E:169:SER:O	1:E:170:ASN:HB3	2.15	0.47
1:H:313:TYR:HD1	1:H:332:VAL:CG2	2.17	0.47
1:L:61:TRP:CZ2	1:L:63:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:66:GLN:HG3	1:L:78:GLY:HA3	1.96	0.47
1:A:80:LYS:HD2	1:C:71:GLU:CB	2.28	0.47
1:A:130:VAL:HG13	1:A:213:GLN:CD	2.35	0.47
1:B:31:SER:CA	1:B:329:ASP:HB2	2.41	0.47
1:B:303:PHE:HB3	1:C:51:ILE:CG2	2.44	0.47
1:C:161:ASN:HB2	1:C:170:ASN:OD1	2.13	0.47
1:D:169:SER:O	1:D:170:ASN:HB3	2.14	0.47
1:D:267:PHE:H	1:D:267:PHE:HD1	1.61	0.47
1:E:143:ASN:O	1:E:144:PHE:C	2.53	0.47
1:F:236:ASN:OD1	1:F:252:ASN:HA	2.14	0.47
1:G:144:PHE:O	1:G:144:PHE:CD2	2.68	0.47
1:H:153:PHE:HA	1:H:177:SER:O	2.13	0.47
1:H:258:LEU:N	1:H:258:LEU:HD22	2.30	0.47
1:H:294:TYR:CD1	1:H:294:TYR:C	2.87	0.47
1:J:267:PHE:H	1:J:267:PHE:HD1	1.62	0.47
1:L:165:THR:HG22	1:L:166:ALA:N	2.30	0.47
1:E:244:PHE:CZ	1:K:285:GLY:HA2	2.50	0.47
1:F:169:SER:O	1:F:170:ASN:HB3	2.14	0.47
1:G:264:GLN:OE1	1:G:270:ARG:HB2	2.14	0.47
1:H:105:VAL:HA	1:H:190:ALA:HB1	1.96	0.47
1:K:61:TRP:CZ2	1:K:63:TYR:HB2	2.50	0.47
1:K:105:VAL:HA	1:K:190:ALA:HB1	1.96	0.47
1:C:269:LEU:HG	1:C:271:PRO:HD3	1.97	0.47
1:G:71:GLU:HG3	1:H:100:ARG:HH21	1.80	0.47
1:I:269:LEU:HG	1:I:271:PRO:HD3	1.96	0.47
1:L:31:SER:CA	1:L:329:ASP:HB2	2.39	0.47
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.50	0.47
1:B:165:THR:CG2	1:B:167:ARG:H	2.15	0.47
1:B:204:PRO:HD2	1:B:248:SER:O	2.14	0.47
1:C:286:ILE:N	1:C:286:ILE:CD1	2.75	0.47
1:E:105:VAL:HA	1:E:190:ALA:HB1	1.96	0.47
1:H:286:ILE:N	1:H:286:ILE:CD1	2.73	0.47
1:K:153:PHE:HA	1:K:177:SER:O	2.14	0.47
1:L:204:PRO:HB2	1:L:247:THR:HG23	1.96	0.47
1:A:169:SER:O	1:A:170:ASN:HB3	2.15	0.46
1:B:51:ILE:HB	1:B:55:LEU:HB3	1.98	0.46
1:C:204:PRO:HB2	1:C:247:THR:HG23	1.98	0.46
1:D:11:VAL:HG21	1:F:340:PHE:CB	2.45	0.46
1:E:269:LEU:HG	1:E:271:PRO:HD3	1.96	0.46
1:E:340:PHE:HB2	1:F:11:VAL:HG21	1.97	0.46
1:F:272:SER:N	1:F:298:GLY:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:PRO:HB2	1:G:247:THR:HG23	1.96	0.46
1:G:258:LEU:HD13	1:G:276:THR:HG23	1.96	0.46
1:J:3:ILE:HD12	1:L:3:ILE:HG21	1.97	0.46
1:J:236:ASN:OD1	1:J:252:ASN:HA	2.15	0.46
1:K:303:PHE:HB3	1:L:51:ILE:HD13	1.98	0.46
1:L:313:TYR:HD1	1:L:332:VAL:CG2	2.17	0.46
1:A:273:ILE:CD1	1:A:297:VAL:HG22	2.44	0.46
1:E:165:THR:HG22	1:E:166:ALA:N	2.29	0.46
1:J:11:VAL:HG21	1:L:340:PHE:HB2	1.96	0.46
1:J:264:GLN:OE1	1:J:270:ARG:HB2	2.15	0.46
1:A:165:THR:HG22	1:A:166:ALA:N	2.29	0.46
1:D:303:PHE:CB	1:E:51:ILE:HD13	2.44	0.46
1:G:51:ILE:HD13	1:I:303:PHE:CG	2.50	0.46
1:G:100:ARG:HH21	1:I:71:GLU:HG3	1.76	0.46
1:H:143:ASN:O	1:H:144:PHE:C	2.54	0.46
1:H:204:PRO:HB2	1:H:247:THR:HG23	1.96	0.46
1:K:191:TYR:CD1	1:K:214:TRP:HB3	2.49	0.46
1:K:273:ILE:CD1	1:K:297:VAL:HG22	2.46	0.46
1:A:204:PRO:HD2	1:A:248:SER:O	2.15	0.46
1:D:3:ILE:HG21	1:E:3:ILE:HD12	1.97	0.46
1:D:136:VAL:CG1	1:D:158:LEU:HD13	2.45	0.46
1:D:340:PHE:CB	1:E:11:VAL:HG21	2.46	0.46
1:E:204:PRO:HD2	1:E:248:SER:O	2.15	0.46
1:G:3:ILE:HG21	1:H:3:ILE:HD12	1.98	0.46
1:G:191:TYR:CD1	1:G:214:TRP:HB3	2.48	0.46
1:H:169:SER:O	1:H:170:ASN:HB3	2.15	0.46
1:H:273:ILE:CD1	1:H:297:VAL:HG22	2.45	0.46
1:K:144:PHE:O	1:K:144:PHE:CD2	2.69	0.46
1:K:165:THR:HG22	1:K:166:ALA:N	2.30	0.46
1:B:336:ILE:HG23	1:B:336:ILE:O	2.16	0.46
1:D:51:ILE:HD13	1:F:303:PHE:CG	2.50	0.46
1:D:52:ASN:OD1	1:D:53:SER:N	2.48	0.46
1:E:309:THR:HG22	1:E:336:ILE:CA	2.37	0.46
1:H:340:PHE:HB2	1:I:11:VAL:HG21	1.98	0.46
1:K:169:SER:O	1:K:170:ASN:HB3	2.15	0.46
1:A:11:VAL:HG21	1:C:340:PHE:CB	2.46	0.46
1:E:144:PHE:O	1:E:144:PHE:CD2	2.69	0.46
1:I:204:PRO:HB2	1:I:247:THR:HG23	1.96	0.46
1:J:204:PRO:HB2	1:J:247:THR:HG23	1.97	0.46
1:L:105:VAL:HA	1:L:190:ALA:HB1	1.96	0.46
1:A:105:VAL:HA	1:A:190:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:O	1:A:144:PHE:C	2.54	0.46
1:A:204:PRO:HB2	1:A:247:THR:HG23	1.96	0.46
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.50	0.46
1:B:143:ASN:O	1:B:144:PHE:C	2.53	0.46
1:J:191:TYR:CD1	1:J:214:TRP:HB3	2.49	0.46
1:J:193:ALA:HA	1:J:211:ALA:O	2.16	0.46
1:A:191:TYR:CD1	1:A:214:TRP:HB3	2.48	0.46
1:C:105:VAL:HA	1:C:190:ALA:HB1	1.97	0.46
1:D:3:ILE:HD12	1:F:3:ILE:HG21	1.97	0.46
1:D:286:ILE:N	1:D:286:ILE:CD1	2.74	0.46
1:E:193:ALA:HA	1:E:211:ALA:O	2.16	0.46
1:F:143:ASN:O	1:F:144:PHE:C	2.54	0.46
1:F:204:PRO:HB2	1:F:247:THR:HG23	1.97	0.46
1:G:61:TRP:CZ2	1:G:63:TYR:HB2	2.50	0.46
1:K:193:ALA:HA	1:K:211:ALA:O	2.16	0.46
1:D:143:ASN:O	1:D:144:PHE:C	2.55	0.46
1:F:309:THR:HG22	1:F:336:ILE:HG13	1.98	0.46
1:G:309:THR:HG22	1:G:336:ILE:HG13	1.98	0.46
1:I:51:ILE:HB	1:I:55:LEU:HB3	1.97	0.46
1:I:165:THR:HG22	1:I:166:ALA:N	2.30	0.46
1:J:61:TRP:CZ2	1:J:63:TYR:HB2	2.50	0.46
1:J:100:ARG:HH21	1:L:71:GLU:HG3	1.77	0.46
1:J:169:SER:O	1:J:170:ASN:HB3	2.16	0.46
1:L:286:ILE:HG23	1:L:323:LYS:CB	2.46	0.46
1:I:144:PHE:O	1:I:144:PHE:CD2	2.69	0.46
1:I:179:SER:HB3	1:I:188:VAL:HG13	1.98	0.46
1:I:191:TYR:CD1	1:I:214:TRP:HB3	2.49	0.46
1:L:193:ALA:HA	1:L:211:ALA:O	2.16	0.46
1:B:193:ALA:HA	1:B:211:ALA:O	2.16	0.45
1:B:267:PHE:H	1:B:267:PHE:HD1	1.62	0.45
1:B:287:GLY:CA	1:L:321:ASP:OD2	2.61	0.45
1:C:165:THR:HG22	1:C:166:ALA:N	2.30	0.45
1:G:294:TYR:C	1:G:294:TYR:CD1	2.88	0.45
1:H:71:GLU:HG3	1:I:100:ARG:HH21	1.78	0.45
1:H:163:ARG:HD2	1:H:168:ARG:O	2.16	0.45
1:A:52:ASN:OD1	1:A:53:SER:N	2.50	0.45
1:F:165:THR:HG22	1:F:166:ALA:N	2.31	0.45
1:G:193:ALA:HA	1:G:211:ALA:O	2.17	0.45
1:H:165:THR:HG22	1:H:166:ALA:N	2.30	0.45
1:I:169:SER:O	1:I:170:ASN:HB3	2.16	0.45
1:A:336:ILE:O	1:A:336:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:O	1:B:180:TYR:HA	2.17	0.45
1:E:273:ILE:CD1	1:E:297:VAL:HG22	2.46	0.45
1:F:66:GLN:HG3	1:F:78:GLY:HA3	1.96	0.45
1:H:191:TYR:CD1	1:H:214:TRP:HB3	2.48	0.45
1:A:144:PHE:O	1:A:144:PHE:CD2	2.70	0.45
1:C:143:ASN:O	1:C:144:PHE:C	2.54	0.45
1:C:309:THR:HG22	1:C:336:ILE:HG13	1.98	0.45
1:D:272:SER:N	1:D:298:GLY:O	2.43	0.45
1:G:286:ILE:HG23	1:G:323:LYS:CB	2.47	0.45
1:I:193:ALA:HA	1:I:211:ALA:O	2.16	0.45
1:K:51:ILE:HB	1:K:55:LEU:HB3	1.99	0.45
1:K:71:GLU:CG	1:L:100:ARG:NH2	2.70	0.45
1:A:105:VAL:O	1:A:105:VAL:CG1	2.65	0.45
1:A:269:LEU:HG	1:A:271:PRO:HD3	1.99	0.45
1:B:269:LEU:HG	1:B:271:PRO:HD3	1.98	0.45
1:D:269:LEU:HG	1:D:271:PRO:HD3	1.98	0.45
1:E:258:LEU:N	1:E:258:LEU:HD22	2.32	0.45
1:F:51:ILE:HB	1:F:55:LEU:HB3	1.99	0.45
1:G:273:ILE:CD1	1:G:297:VAL:HG22	2.47	0.45
1:G:309:THR:CG2	1:G:336:ILE:HG13	2.46	0.45
1:H:193:ALA:HA	1:H:211:ALA:O	2.16	0.45
1:H:272:SER:N	1:H:298:GLY:O	2.46	0.45
1:J:52:ASN:OD1	1:J:53:SER:N	2.50	0.45
1:K:179:SER:HB3	1:K:188:VAL:HG13	1.97	0.45
1:D:144:PHE:O	1:D:144:PHE:CD2	2.70	0.45
1:F:105:VAL:HA	1:F:190:ALA:HB1	1.97	0.45
1:J:11:VAL:HG21	1:L:340:PHE:CB	2.47	0.45
1:J:66:GLN:HG3	1:J:78:GLY:HA3	1.98	0.45
1:J:338:TYR:CE2	1:K:47:GLY:HA3	2.52	0.45
1:K:336:ILE:HG23	1:K:336:ILE:O	2.17	0.45
1:B:3:ILE:HG21	1:C:3:ILE:HD12	1.99	0.45
1:B:273:ILE:CD1	1:B:297:VAL:HG22	2.47	0.45
1:F:193:ALA:HA	1:F:211:ALA:O	2.17	0.45
1:G:169:SER:O	1:G:170:ASN:HB3	2.16	0.45
1:L:144:PHE:O	1:L:144:PHE:CD2	2.70	0.45
1:L:309:THR:HG22	1:L:336:ILE:HG13	1.99	0.45
1:D:273:ILE:CD1	1:D:297:VAL:HG22	2.46	0.45
1:D:286:ILE:HG23	1:D:323:LYS:CB	2.47	0.45
1:E:272:SER:N	1:E:298:GLY:O	2.45	0.45
1:I:150:GLY:O	1:I:180:TYR:HA	2.17	0.45
1:I:286:ILE:HG23	1:I:323:LYS:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:ARG:HD2	1:K:168:ARG:O	2.15	0.45
1:B:286:ILE:HG23	1:B:323:LYS:CB	2.47	0.45
1:C:193:ALA:HA	1:C:211:ALA:O	2.17	0.45
1:H:179:SER:HB3	1:H:188:VAL:HG13	1.99	0.45
1:I:143:ASN:O	1:I:144:PHE:C	2.55	0.45
1:J:336:ILE:HG23	1:J:336:ILE:O	2.17	0.45
1:K:269:LEU:HG	1:K:271:PRO:HD3	1.97	0.45
1:L:179:SER:HB3	1:L:188:VAL:HG13	1.97	0.45
1:L:273:ILE:CD1	1:L:297:VAL:HG22	2.46	0.45
1:B:169:SER:O	1:B:170:ASN:HB3	2.16	0.45
1:B:191:TYR:CD1	1:B:214:TRP:HB3	2.49	0.45
1:C:163:ARG:HD2	1:C:168:ARG:O	2.17	0.45
1:E:229:ALA:CB	1:E:259:LEU:HD23	2.47	0.45
1:G:258:LEU:N	1:G:258:LEU:HD22	2.32	0.45
1:I:273:ILE:CD1	1:I:297:VAL:HG22	2.47	0.45
1:J:179:SER:HB3	1:J:188:VAL:HG13	1.98	0.45
1:K:143:ASN:O	1:K:144:PHE:C	2.56	0.45
1:L:258:LEU:N	1:L:258:LEU:HD22	2.32	0.45
1:A:258:LEU:N	1:A:258:LEU:HD22	2.32	0.44
1:C:51:ILE:HB	1:C:55:LEU:HB3	1.99	0.44
1:C:165:THR:CG2	1:C:167:ARG:H	2.16	0.44
1:D:51:ILE:HB	1:D:55:LEU:HB3	1.99	0.44
1:F:336:ILE:O	1:F:336:ILE:HG23	2.17	0.44
1:G:272:SER:N	1:G:298:GLY:O	2.44	0.44
1:A:286:ILE:HG23	1:A:323:LYS:CB	2.47	0.44
1:C:258:LEU:N	1:C:258:LEU:HD22	2.33	0.44
1:C:287:GLY:CA	1:G:321:ASP:CG	2.67	0.44
1:E:3:ILE:HG21	1:F:3:ILE:HD12	1.99	0.44
1:E:309:THR:HG22	1:E:336:ILE:HG13	1.98	0.44
1:E:336:ILE:HG23	1:E:336:ILE:O	2.16	0.44
1:G:51:ILE:HB	1:G:55:LEU:HB3	1.99	0.44
1:K:272:SER:N	1:K:298:GLY:O	2.45	0.44
1:A:309:THR:CG2	1:A:336:ILE:HG13	2.48	0.44
1:H:51:ILE:HB	1:H:55:LEU:HB3	1.99	0.44
1:H:338:TYR:CE2	1:I:47:GLY:HA3	2.52	0.44
1:I:229:ALA:CB	1:I:259:LEU:HD23	2.47	0.44
1:J:90:TYR:CD2	1:J:93:VAL:HG21	2.52	0.44
1:A:51:ILE:HB	1:A:55:LEU:HB3	1.98	0.44
1:A:165:THR:CG2	1:A:167:ARG:H	2.15	0.44
1:A:229:ALA:CB	1:A:259:LEU:HD23	2.47	0.44
1:E:309:THR:CG2	1:E:336:ILE:HG13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:ILE:HG23	1:F:323:LYS:CB	2.48	0.44
1:H:3:ILE:HG21	1:I:3:ILE:HD12	1.99	0.44
1:H:286:ILE:HG23	1:H:323:LYS:CB	2.47	0.44
1:H:303:PHE:CB	1:I:51:ILE:HD13	2.48	0.44
1:J:303:PHE:CB	1:K:51:ILE:HD13	2.47	0.44
1:K:258:LEU:HD22	1:K:258:LEU:N	2.32	0.44
1:L:143:ASN:O	1:L:144:PHE:C	2.56	0.44
1:A:193:ALA:HA	1:A:211:ALA:O	2.17	0.44
1:I:163:ARG:HD2	1:I:168:ARG:O	2.18	0.44
1:I:309:THR:HG22	1:I:336:ILE:HG13	1.98	0.44
1:L:51:ILE:HB	1:L:55:LEU:HB3	1.99	0.44
1:B:144:PHE:O	1:B:144:PHE:CD2	2.70	0.44
1:B:283:VAL:O	1:B:284:GLU:C	2.56	0.44
1:C:309:THR:CG2	1:C:336:ILE:HG13	2.47	0.44
1:D:51:ILE:HG21	1:F:303:PHE:HB3	2.00	0.44
1:D:71:GLU:HG3	1:E:100:ARG:HH21	1.81	0.44
1:F:309:THR:CG2	1:F:336:ILE:HG13	2.47	0.44
1:G:235:ARG:HA	1:G:235:ARG:HD3	1.79	0.44
1:J:51:ILE:HB	1:J:55:LEU:HB3	2.00	0.44
1:J:54:ASP:HB3	1:J:91:ALA:HB2	2.00	0.44
1:J:309:THR:CG2	1:J:336:ILE:HG13	2.48	0.44
1:L:336:ILE:HG23	1:L:336:ILE:O	2.17	0.44
1:E:71:GLU:CG	1:F:100:ARG:HH21	2.31	0.44
1:E:90:TYR:CD2	1:E:93:VAL:HG21	2.53	0.44
1:F:144:PHE:O	1:F:144:PHE:CD2	2.71	0.44
1:I:235:ARG:HA	1:I:235:ARG:HD3	1.80	0.44
1:K:286:ILE:HG23	1:K:323:LYS:CB	2.48	0.44
1:C:105:VAL:O	1:C:105:VAL:CG1	2.66	0.44
1:C:191:TYR:CD1	1:C:214:TRP:HB3	2.48	0.44
1:D:336:ILE:HG23	1:D:336:ILE:O	2.17	0.44
1:E:286:ILE:HG23	1:E:323:LYS:CB	2.47	0.44
1:G:105:VAL:O	1:G:105:VAL:CG1	2.66	0.44
1:G:269:LEU:HG	1:G:271:PRO:HD3	1.99	0.44
1:I:31:SER:CA	1:I:329:ASP:HB2	2.40	0.44
1:I:336:ILE:HG23	1:I:336:ILE:O	2.17	0.44
1:K:309:THR:HG22	1:K:336:ILE:HG13	2.00	0.44
1:B:229:ALA:CB	1:B:259:LEU:HD23	2.48	0.44
1:C:179:SER:HB3	1:C:188:VAL:HG13	1.99	0.44
1:E:52:ASN:OD1	1:E:53:SER:N	2.51	0.44
1:I:313:TYR:HD1	1:I:332:VAL:CG2	2.17	0.44
1:J:143:ASN:O	1:J:144:PHE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:272:SER:N	1:J:298:GLY:O	2.46	0.44
1:L:273:ILE:HD13	1:L:273:ILE:HA	1.86	0.44
1:C:229:ALA:CB	1:C:259:LEU:HD23	2.47	0.43
1:E:51:ILE:HB	1:E:55:LEU:HB3	1.99	0.43
1:G:336:ILE:HG23	1:G:336:ILE:O	2.17	0.43
1:H:235:ARG:HA	1:H:235:ARG:HD3	1.80	0.43
1:J:286:ILE:HG23	1:J:323:LYS:CB	2.48	0.43
1:K:283:VAL:O	1:K:284:GLU:C	2.56	0.43
1:A:272:SER:N	1:A:298:GLY:O	2.46	0.43
1:A:286:ILE:N	1:A:286:ILE:CD1	2.73	0.43
1:B:52:ASN:OD1	1:B:53:SER:N	2.50	0.43
1:B:272:SER:N	1:B:298:GLY:O	2.44	0.43
1:C:272:SER:N	1:C:298:GLY:O	2.44	0.43
1:C:336:ILE:HG23	1:C:336:ILE:O	2.17	0.43
1:G:229:ALA:CB	1:G:259:LEU:HD23	2.48	0.43
1:G:303:PHE:CG	1:H:51:ILE:HD13	2.53	0.43
1:H:150:GLY:O	1:H:180:TYR:HA	2.19	0.43
1:A:309:THR:HG22	1:A:336:ILE:HG13	2.00	0.43
1:B:258:LEU:N	1:B:258:LEU:HD22	2.33	0.43
1:D:71:GLU:CB	1:E:80:LYS:HD2	2.26	0.43
1:E:286:ILE:HG23	1:E:323:LYS:HB3	2.00	0.43
1:J:309:THR:HG22	1:J:336:ILE:HG13	1.99	0.43
1:A:303:PHE:CB	1:B:51:ILE:HD13	2.48	0.43
1:H:144:PHE:O	1:H:144:PHE:CD2	2.71	0.43
1:D:163:ARG:HD2	1:D:168:ARG:O	2.19	0.43
1:E:303:PHE:CG	1:F:51:ILE:HD13	2.54	0.43
1:A:111:TYR:OH	1:A:188:VAL:HG23	2.18	0.43
1:C:144:PHE:O	1:C:144:PHE:CD2	2.72	0.43
1:C:169:SER:O	1:C:170:ASN:HB3	2.18	0.43
1:D:105:VAL:O	1:D:105:VAL:CG1	2.66	0.43
1:D:150:GLY:O	1:D:180:TYR:HA	2.19	0.43
1:F:283:VAL:O	1:F:284:GLU:C	2.56	0.43
1:G:90:TYR:CD2	1:G:93:VAL:HG21	2.54	0.43
1:G:179:SER:HB3	1:G:188:VAL:HG13	2.00	0.43
1:H:309:THR:HG22	1:H:336:ILE:HG13	2.00	0.43
1:K:229:ALA:CB	1:K:259:LEU:HD23	2.48	0.43
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.90	0.43
1:A:338:TYR:CE2	1:B:47:GLY:HA3	2.52	0.43
1:A:340:PHE:HB2	1:B:11:VAL:HG21	2.00	0.43
1:C:286:ILE:HG23	1:C:323:LYS:CB	2.48	0.43
1:D:179:SER:HB3	1:D:188:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ALA:HA	1:D:211:ALA:O	2.18	0.43
1:D:229:ALA:CB	1:D:259:LEU:HD23	2.48	0.43
1:D:309:THR:HG22	1:D:336:ILE:HG13	2.00	0.43
1:E:163:ARG:HD2	1:E:168:ARG:O	2.19	0.43
1:F:52:ASN:OD1	1:F:53:SER:N	2.51	0.43
1:F:165:THR:CG2	1:F:167:ARG:H	2.16	0.43
1:F:273:ILE:CD1	1:F:297:VAL:HG22	2.49	0.43
1:G:143:ASN:O	1:G:144:PHE:C	2.57	0.43
1:H:229:ALA:CB	1:H:259:LEU:HD23	2.49	0.43
1:I:286:ILE:HG23	1:I:323:LYS:HB3	2.01	0.43
1:B:115:LEU:HD21	1:B:274:ALA:HB2	2.01	0.43
1:C:285:GLY:CA	1:G:244:PHE:HZ	2.31	0.43
1:E:340:PHE:CB	1:F:11:VAL:HG21	2.49	0.43
1:G:12:ASP:O	1:G:45:PHE:HA	2.18	0.43
1:H:336:ILE:HG23	1:H:336:ILE:O	2.19	0.43
1:K:309:THR:CG2	1:K:336:ILE:HG13	2.49	0.43
1:L:54:ASP:HB3	1:L:91:ALA:HB2	2.01	0.43
1:L:309:THR:CG2	1:L:336:ILE:HG13	2.49	0.43
1:B:235:ARG:NH2	1:B:253:LYS:HZ3	2.17	0.43
1:C:235:ARG:HA	1:C:235:ARG:HD3	1.80	0.43
1:D:309:THR:CG2	1:D:336:ILE:HG13	2.48	0.43
1:F:235:ARG:HA	1:F:235:ARG:HD3	1.80	0.43
1:G:51:ILE:HG21	1:I:303:PHE:HB3	2.01	0.43
1:L:150:GLY:O	1:L:180:TYR:HA	2.19	0.43
1:B:286:ILE:HG23	1:B:323:LYS:HB3	2.00	0.43
1:B:309:THR:CG2	1:B:336:ILE:HG13	2.49	0.43
1:B:313:TYR:HD1	1:B:332:VAL:CG2	2.19	0.43
1:C:273:ILE:CD1	1:C:297:VAL:HG22	2.49	0.43
1:E:235:ARG:NH2	1:E:253:LYS:HZ3	2.17	0.43
1:F:229:ALA:CB	1:F:259:LEU:HD23	2.48	0.43
1:G:31:SER:CA	1:G:329:ASP:HB2	2.39	0.43
1:G:286:ILE:HG23	1:G:323:LYS:HB3	2.01	0.43
1:H:244:PHE:CZ	1:L:285:GLY:CA	3.02	0.43
1:I:12:ASP:O	1:I:45:PHE:HA	2.19	0.43
1:I:45:PHE:CD1	1:I:45:PHE:C	2.92	0.43
1:K:267:PHE:HD1	1:K:267:PHE:H	1.62	0.43
1:L:229:ALA:CB	1:L:259:LEU:HD23	2.49	0.43
1:F:179:SER:HB3	1:F:188:VAL:HG13	2.01	0.42
1:G:165:THR:CG2	1:G:167:ARG:H	2.16	0.42
1:H:340:PHE:CB	1:I:11:VAL:HG21	2.49	0.42
1:I:272:SER:N	1:I:298:GLY:O	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:ALA:CB	1:J:259:LEU:HD23	2.48	0.42
1:J:283:VAL:O	1:J:284:GLU:C	2.57	0.42
1:K:286:ILE:HG23	1:K:323:LYS:HB3	2.01	0.42
1:L:52:ASN:OD1	1:L:53:SER:N	2.52	0.42
1:L:283:VAL:O	1:L:284:GLU:C	2.57	0.42
1:A:71:GLU:HG3	1:B:100:ARG:HH21	1.80	0.42
1:C:54:ASP:HB3	1:C:91:ALA:HB2	2.01	0.42
1:C:235:ARG:NH2	1:C:253:LYS:HZ3	2.16	0.42
1:D:100:ARG:NH2	1:F:71:GLU:CG	2.73	0.42
1:G:150:GLY:O	1:G:180:TYR:HA	2.19	0.42
1:J:286:ILE:HG23	1:J:323:LYS:HB3	2.01	0.42
1:J:313:TYR:HD1	1:J:332:VAL:CG2	2.17	0.42
1:L:90:TYR:CD2	1:L:93:VAL:HG21	2.54	0.42
1:B:287:GLY:N	1:L:321:ASP:OD1	2.45	0.42
1:E:235:ARG:NE	1:E:253:LYS:HG2	2.34	0.42
1:H:283:VAL:O	1:H:284:GLU:C	2.57	0.42
1:L:265:PHE:CB	1:L:267:PHE:CE1	3.02	0.42
1:A:150:GLY:O	1:A:180:TYR:HA	2.19	0.42
1:B:309:THR:HG22	1:B:336:ILE:HG13	2.00	0.42
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.89	0.42
1:D:283:VAL:O	1:D:284:GLU:C	2.57	0.42
1:H:235:ARG:NE	1:H:253:LYS:HG2	2.33	0.42
1:K:90:TYR:CD2	1:K:93:VAL:HG21	2.54	0.42
1:K:179:SER:HB2	1:K:188:VAL:HG22	2.02	0.42
1:L:12:ASP:O	1:L:45:PHE:HA	2.19	0.42
1:A:283:VAL:O	1:A:284:GLU:C	2.58	0.42
1:E:150:GLY:O	1:E:180:TYR:HA	2.19	0.42
1:E:179:SER:HB3	1:E:188:VAL:HG13	2.01	0.42
1:H:235:ARG:NH2	1:H:253:LYS:HZ3	2.17	0.42
1:I:258:LEU:N	1:I:258:LEU:HD22	2.34	0.42
1:L:136:VAL:CG1	1:L:158:LEU:CD1	2.98	0.42
1:A:179:SER:HB3	1:A:188:VAL:HG13	2.01	0.42
1:H:90:TYR:CD2	1:H:93:VAL:HG21	2.54	0.42
1:I:285:GLY:HA3	1:K:244:PHE:CZ	2.54	0.42
1:I:309:THR:CG2	1:I:336:ILE:HG13	2.49	0.42
1:B:12:ASP:O	1:B:45:PHE:HA	2.20	0.42
1:C:52:ASN:OD1	1:C:53:SER:N	2.53	0.42
1:D:258:LEU:HD22	1:D:258:LEU:N	2.35	0.42
1:D:273:ILE:HD13	1:D:273:ILE:HA	1.86	0.42
1:E:303:PHE:HB3	1:F:51:ILE:HG21	2.01	0.42
1:F:258:LEU:N	1:F:258:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:309:THR:CG2	1:H:336:ILE:HG13	2.50	0.42
1:L:231:TYR:HD1	1:L:257:VAL:HG22	1.85	0.42
1:L:286:ILE:HG23	1:L:323:LYS:HB3	2.00	0.42
1:E:283:VAL:O	1:E:284:GLU:C	2.58	0.42
1:F:54:ASP:HB3	1:F:91:ALA:HB2	2.02	0.42
1:G:283:VAL:O	1:G:284:GLU:C	2.57	0.42
1:H:71:GLU:CG	1:I:100:ARG:HH21	2.32	0.42
1:K:54:ASP:HB3	1:K:91:ALA:HB2	2.02	0.42
1:K:235:ARG:NE	1:K:253:LYS:HG2	2.35	0.42
1:A:286:ILE:HG23	1:A:323:LYS:HB3	2.00	0.42
1:D:54:ASP:HB3	1:D:91:ALA:HB2	2.02	0.42
1:F:235:ARG:NE	1:F:253:LYS:HG2	2.35	0.42
1:G:54:ASP:HB3	1:G:91:ALA:HB2	2.02	0.42
1:J:100:ARG:HH21	1:L:71:GLU:CG	2.32	0.42
1:J:303:PHE:CG	1:K:51:ILE:HD13	2.55	0.42
1:K:12:ASP:O	1:K:45:PHE:HA	2.20	0.42
1:A:54:ASP:HB3	1:A:91:ALA:HB2	2.02	0.42
1:B:55:LEU:HD12	1:B:55:LEU:HA	1.91	0.42
1:C:283:VAL:O	1:C:284:GLU:C	2.58	0.42
1:F:150:GLY:O	1:F:180:TYR:HA	2.20	0.42
1:A:90:TYR:CD2	1:A:93:VAL:HG21	2.55	0.41
1:B:179:SER:HB2	1:B:188:VAL:HG22	2.02	0.41
1:F:90:TYR:CD2	1:F:93:VAL:HG21	2.55	0.41
1:H:45:PHE:CD1	1:H:45:PHE:C	2.93	0.41
1:H:52:ASN:OD1	1:H:53:SER:N	2.53	0.41
1:H:265:PHE:CB	1:H:267:PHE:CE1	3.02	0.41
1:H:286:ILE:HG23	1:H:323:LYS:HB3	2.01	0.41
1:K:52:ASN:OD1	1:K:53:SER:N	2.53	0.41
1:K:105:VAL:O	1:K:105:VAL:CG1	2.67	0.41
1:L:191:TYR:CD1	1:L:214:TRP:HB3	2.49	0.41
1:A:163:ARG:HD2	1:A:168:ARG:O	2.20	0.41
1:C:1:ALA:N	1:C:340:PHE:OXT	2.42	0.41
1:D:286:ILE:HG23	1:D:323:LYS:HB3	2.01	0.41
1:G:163:ARG:HD2	1:G:168:ARG:O	2.20	0.41
1:J:105:VAL:O	1:J:105:VAL:CG1	2.67	0.41
1:K:150:GLY:O	1:K:180:TYR:HA	2.19	0.41
1:L:45:PHE:CD1	1:L:45:PHE:C	2.93	0.41
1:B:54:ASP:HB3	1:B:91:ALA:HB2	2.01	0.41
1:C:150:GLY:O	1:C:180:TYR:HA	2.19	0.41
1:E:12:ASP:O	1:E:45:PHE:HA	2.20	0.41
1:G:100:ARG:HH21	1:I:71:GLU:CG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:LEU:HD21	1:G:274:ALA:HB2	2.02	0.41
1:H:12:ASP:O	1:H:45:PHE:HA	2.19	0.41
1:I:180:TYR:CE2	1:I:182:TYR:HB2	2.55	0.41
1:J:309:THR:HG22	1:J:336:ILE:CB	2.51	0.41
1:K:71:GLU:CD	1:L:100:ARG:HH21	2.24	0.41
1:L:223:ASN:O	1:L:224:ASN:CB	2.68	0.41
1:B:163:ARG:HD2	1:B:168:ARG:O	2.20	0.41
1:E:265:PHE:CB	1:E:267:PHE:CE1	3.02	0.41
1:G:203:GLN:HA	1:G:204:PRO:HD3	1.86	0.41
1:J:303:PHE:HB3	1:K:51:ILE:HG21	2.01	0.41
1:L:163:ARG:HD2	1:L:168:ARG:O	2.20	0.41
1:A:309:THR:HG22	1:A:336:ILE:CB	2.50	0.41
1:C:174:VAL:CG1	1:C:175:GLY:H	2.34	0.41
1:C:286:ILE:HG23	1:C:323:LYS:HB3	2.03	0.41
1:D:142:SER:HA	1:D:152:ASN:OD1	2.21	0.41
1:E:54:ASP:HB3	1:E:91:ALA:HB2	2.01	0.41
1:F:253:LYS:HD2	1:F:254:THR:N	2.36	0.41
1:H:104:VAL:HG13	1:H:156:GLN:HB2	2.03	0.41
1:I:235:ARG:NE	1:I:253:LYS:HG2	2.35	0.41
1:K:115:LEU:HD21	1:K:274:ALA:HB2	2.03	0.41
1:F:45:PHE:CD1	1:F:45:PHE:C	2.94	0.41
1:G:1:ALA:N	1:G:340:PHE:OXT	2.41	0.41
1:G:52:ASN:OD1	1:G:53:SER:N	2.53	0.41
1:H:235:ARG:NH2	1:H:253:LYS:NZ	2.69	0.41
1:I:52:ASN:OD1	1:I:53:SER:N	2.53	0.41
1:I:90:TYR:CD2	1:I:93:VAL:HG21	2.55	0.41
1:A:45:PHE:CD1	1:A:45:PHE:C	2.93	0.41
1:A:235:ARG:HA	1:A:235:ARG:HD3	1.80	0.41
1:A:244:PHE:CZ	1:J:285:GLY:HA3	2.55	0.41
1:G:104:VAL:HG13	1:G:156:GLN:HB2	2.03	0.41
1:G:235:ARG:NE	1:G:253:LYS:HG2	2.36	0.41
1:A:100:ARG:HH21	1:C:71:GLU:CG	2.32	0.41
1:A:179:SER:HB2	1:A:188:VAL:HG22	2.03	0.41
1:B:235:ARG:NE	1:B:253:LYS:HG2	2.35	0.41
1:D:51:ILE:CG2	1:F:303:PHE:HB3	2.50	0.41
1:D:253:LYS:HD2	1:D:254:THR:N	2.36	0.41
1:F:105:VAL:O	1:F:105:VAL:CG1	2.69	0.41
1:I:115:LEU:HD13	1:I:296:GLU:HG3	2.03	0.41
1:J:1:ALA:N	1:J:340:PHE:OXT	2.42	0.41
1:J:31:SER:CA	1:J:329:ASP:HB2	2.40	0.41
1:J:51:ILE:HG21	1:L:303:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:258:LEU:N	1:J:258:LEU:HD22	2.36	0.41
1:J:340:PHE:HB2	1:K:11:VAL:HG21	2.03	0.41
1:L:235:ARG:NE	1:L:253:LYS:HG2	2.35	0.41
1:A:235:ARG:NE	1:A:253:LYS:HG2	2.36	0.41
1:B:45:PHE:CD1	1:B:45:PHE:C	2.94	0.41
1:B:90:TYR:CD2	1:B:93:VAL:HG21	2.55	0.41
1:B:115:LEU:HD13	1:B:296:GLU:HG3	2.02	0.41
1:B:309:THR:HG22	1:B:336:ILE:CB	2.51	0.41
1:D:1:ALA:N	1:D:340:PHE:OXT	2.44	0.41
1:D:55:LEU:HD12	1:D:55:LEU:HA	1.90	0.41
1:D:174:VAL:HG12	1:D:175:GLY:H	1.84	0.41
1:D:174:VAL:CG1	1:D:175:GLY:H	2.33	0.41
1:E:45:PHE:CD1	1:E:45:PHE:C	2.93	0.41
1:F:286:ILE:HG23	1:F:323:LYS:HB3	2.02	0.41
1:G:143:ASN:CA	1:G:148:VAL:O	2.69	0.41
1:H:24:SER:H	1:H:35:ASN:ND2	2.19	0.41
1:I:115:LEU:HD21	1:I:274:ALA:HB2	2.02	0.41
1:I:136:VAL:CG1	1:I:158:LEU:CD1	2.99	0.41
1:J:45:PHE:CD1	1:J:45:PHE:C	2.94	0.41
1:J:150:GLY:O	1:J:180:TYR:HA	2.20	0.41
1:K:45:PHE:CD1	1:K:45:PHE:C	2.94	0.41
1:K:313:TYR:HD1	1:K:332:VAL:CG2	2.18	0.41
1:L:309:THR:HG22	1:L:336:ILE:CB	2.51	0.41
1:E:124:TYR:O	1:E:131:GLY:HA3	2.21	0.41
1:E:174:VAL:CG1	1:E:175:GLY:H	2.35	0.41
1:F:163:ARG:HD2	1:F:168:ARG:O	2.21	0.41
1:H:54:ASP:HB3	1:H:91:ALA:HB2	2.02	0.41
1:I:54:ASP:HB3	1:I:91:ALA:HB2	2.02	0.41
1:J:163:ARG:HD2	1:J:168:ARG:O	2.21	0.41
1:L:64:ASN:O	1:L:79:ASN:HA	2.21	0.41
1:L:115:LEU:HD21	1:L:274:ALA:HB2	2.03	0.41
1:A:253:LYS:HD2	1:A:254:THR:N	2.36	0.40
1:F:231:TYR:HD1	1:F:257:VAL:HG22	1.86	0.40
1:G:71:GLU:CB	1:H:80:LYS:HD2	2.25	0.40
1:I:105:VAL:O	1:I:105:VAL:CG1	2.68	0.40
1:I:124:TYR:O	1:I:131:GLY:HA3	2.21	0.40
1:B:105:VAL:O	1:B:105:VAL:CG1	2.68	0.40
1:D:111:TYR:OH	1:D:188:VAL:HG23	2.21	0.40
1:E:203:GLN:HA	1:E:204:PRO:HD3	1.86	0.40
1:I:265:PHE:CB	1:I:267:PHE:CE1	3.04	0.40
1:G:45:PHE:CD1	1:G:45:PHE:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:PHE:CB	1:G:267:PHE:CE1	3.04	0.40
1:H:136:VAL:CG1	1:H:158:LEU:CD1	2.99	0.40
1:I:231:TYR:HD1	1:I:257:VAL:HG22	1.86	0.40
1:I:283:VAL:O	1:I:284:GLU:C	2.60	0.40
1:J:180:TYR:CE2	1:J:182:TYR:HB2	2.56	0.40
1:A:115:LEU:N	1:A:115:LEU:HD23	2.36	0.40
1:A:340:PHE:CB	1:B:11:VAL:HG21	2.52	0.40
1:D:12:ASP:O	1:D:45:PHE:HA	2.22	0.40
1:D:115:LEU:HD21	1:D:274:ALA:HB2	2.04	0.40
1:F:64:ASN:O	1:F:79:ASN:HA	2.22	0.40
1:G:136:VAL:CG1	1:G:158:LEU:CD1	3.00	0.40
1:J:51:ILE:HD13	1:L:303:PHE:CG	2.56	0.40
1:K:206:GLY:H	1:K:284:GLU:CD	2.25	0.40
1:K:265:PHE:CB	1:K:267:PHE:CE1	3.03	0.40
1:K:309:THR:HG22	1:K:336:ILE:CB	2.51	0.40
1:A:3:ILE:HG21	1:B:3:ILE:HD12	2.03	0.40
1:A:12:ASP:O	1:A:45:PHE:HA	2.21	0.40
1:B:180:TYR:CE2	1:B:182:TYR:HB2	2.56	0.40
1:C:12:ASP:O	1:C:45:PHE:HA	2.21	0.40
1:C:309:THR:HG22	1:C:336:ILE:CB	2.52	0.40
1:D:235:ARG:HD3	1:D:235:ARG:HA	1.79	0.40
1:F:12:ASP:O	1:F:45:PHE:HA	2.20	0.40
1:F:191:TYR:CD1	1:F:214:TRP:HB3	2.49	0.40
1:F:206:GLY:H	1:F:284:GLU:CD	2.24	0.40
1:G:309:THR:HG22	1:G:336:ILE:CB	2.51	0.40
1:J:340:PHE:CB	1:K:11:VAL:HG21	2.52	0.40
1:K:111:TYR:OH	1:K:188:VAL:HG23	2.17	0.40
1:L:115:LEU:HD13	1:L:296:GLU:HG3	2.03	0.40
1:L:126:ASP:HA	1:L:133:VAL:HG12	2.04	0.40
1:L:143:ASN:CA	1:L:148:VAL:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	41	74
1	B	338/340 (99%)	312 (92%)	25 (7%)	1 (0%)	41	74
1	C	338/340 (99%)	311 (92%)	25 (7%)	2 (1%)	25	62
1	D	338/340 (99%)	312 (92%)	25 (7%)	1 (0%)	41	74
1	E	338/340 (99%)	312 (92%)	25 (7%)	1 (0%)	41	74
1	F	338/340 (99%)	311 (92%)	25 (7%)	2 (1%)	25	62
1	G	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	41	74
1	H	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	41	74
1	I	338/340 (99%)	311 (92%)	25 (7%)	2 (1%)	25	62
1	J	338/340 (99%)	310 (92%)	27 (8%)	1 (0%)	41	74
1	K	338/340 (99%)	313 (93%)	24 (7%)	1 (0%)	41	74
1	L	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	41	74
All	All	4056/4080 (99%)	3736 (92%)	305 (8%)	15 (0%)	34	70

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	ALA
1	I	222	ALA
1	L	222	ALA
1	A	222	ALA
1	B	222	ALA
1	C	222	ALA
1	E	222	ALA
1	F	222	ALA
1	G	222	ALA
1	H	222	ALA
1	J	222	ALA
1	K	222	ALA
1	C	284	GLU
1	F	284	GLU
1	I	284	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	B	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	C	263/263 (100%)	257 (98%)	6 (2%)	50	72
1	D	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	E	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	F	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	G	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	H	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	I	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	J	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	K	263/263 (100%)	258 (98%)	5 (2%)	57	76
1	L	263/263 (100%)	258 (98%)	5 (2%)	57	76
All	All	3156/3156 (100%)	3095 (98%)	61 (2%)	57	76

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	170	ASN
1	A	218	LEU
1	A	253	LYS
1	A	279	LYS
1	B	104	VAL
1	B	170	ASN
1	B	218	LEU
1	B	253	LYS
1	B	279	LYS
1	C	27	ASN
1	C	104	VAL
1	C	170	ASN
1	C	218	LEU

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Mol	Chain	Res	Type
1	C	253	LYS
1	C	279	LYS
1	D	104	VAL
1	D	170	ASN
1	D	218	LEU
1	D	253	LYS
1	D	279	LYS
1	E	104	VAL
1	E	170	ASN
1	E	218	LEU
1	E	253	LYS
1	E	279	LYS
1	F	104	VAL
1	F	170	ASN
1	F	218	LEU
1	F	253	LYS
1	F	279	LYS
1	G	104	VAL
1	G	170	ASN
1	G	218	LEU
1	G	253	LYS
1	G	279	LYS
1	H	104	VAL
1	H	170	ASN
1	H	218	LEU
1	H	253	LYS
1	H	279	LYS
1	I	104	VAL
1	I	170	ASN
1	I	218	LEU
1	I	253	LYS
1	I	279	LYS
1	J	104	VAL
1	J	170	ASN
1	J	218	LEU
1	J	253	LYS
1	J	279	LYS
1	K	104	VAL
1	K	170	ASN
1	K	218	LEU
1	K	253	LYS
1	K	279	LYS

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Mol	Chain	Res	Type
1	L	104	VAL
1	L	170	ASN
1	L	218	LEU
1	L	253	LYS
1	L	279	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	60	GLN
1	A	223	ASN
1	A	255	GLN
1	B	35	ASN
1	B	60	GLN
1	B	223	ASN
1	B	255	GLN
1	C	35	ASN
1	C	60	GLN
1	C	223	ASN
1	C	255	GLN
1	D	35	ASN
1	D	60	GLN
1	D	223	ASN
1	D	255	GLN
1	E	35	ASN
1	E	60	GLN
1	E	223	ASN
1	E	255	GLN
1	F	35	ASN
1	F	60	GLN
1	F	223	ASN
1	F	255	GLN
1	G	35	ASN
1	G	60	GLN
1	G	223	ASN
1	G	255	GLN
1	H	35	ASN
1	H	60	GLN
1	H	223	ASN
1	H	255	GLN
1	I	27	ASN

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Mol	Chain	Res	Type
1	I	35	ASN
1	I	60	GLN
1	I	223	ASN
1	I	255	GLN
1	J	35	ASN
1	J	60	GLN
1	J	223	ASN
1	J	255	GLN
1	K	27	ASN
1	K	35	ASN
1	K	60	GLN
1	K	223	ASN
1	K	255	GLN
1	L	35	ASN
1	L	60	GLN
1	L	223	ASN
1	L	255	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	339/340 (99%)	0.23	12 (3%)	44	36	76, 78, 80, 81	0
1	B	340/340 (100%)	0.18	3 (0%)	84	79	76, 78, 80, 82	0
1	C	340/340 (100%)	0.24	6 (1%)	68	61	76, 78, 80, 81	0
1	D	339/340 (99%)	0.26	4 (1%)	79	72	76, 78, 80, 81	0
1	E	340/340 (100%)	0.23	5 (1%)	73	66	76, 78, 80, 81	0
1	F	340/340 (100%)	0.21	4 (1%)	79	72	76, 78, 80, 82	0
1	G	339/340 (99%)	0.36	17 (5%)	28	25	76, 78, 80, 81	0
1	H	340/340 (100%)	0.42	17 (5%)	28	25	76, 78, 80, 82	0
1	I	340/340 (100%)	0.46	23 (6%)	17	13	76, 78, 80, 82	0
1	J	339/340 (99%)	0.34	12 (3%)	44	36	76, 78, 80, 81	0
1	K	340/340 (100%)	0.28	13 (3%)	40	33	76, 78, 80, 82	0
1	L	340/340 (100%)	0.45	25 (7%)	14	11	76, 78, 80, 82	0
All	All	4076/4080 (99%)	0.31	141 (3%)	44	36	76, 78, 80, 82	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	229	ALA	4.5
1	H	1	ALA	3.7
1	L	218	LEU	3.5
1	A	230	ASN	3.5
1	L	230	ASN	3.4
1	L	288	ASP	3.4
1	G	7	ASP	3.3
1	L	253	LYS	3.3
1	I	216	THR	3.3
1	L	319	ASP	3.2
1	H	94	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	8	GLY	3.1
1	K	243	LYS	3.1
1	J	256	ASP	3.0
1	I	59	GLY	3.0
1	C	92	ASP	3.0
1	L	93	VAL	3.0
1	E	275	TYR	2.9
1	J	340	PHE	2.9
1	J	248	SER	2.9
1	I	250	PHE	2.9
1	K	1	ALA	2.8
1	H	229	ALA	2.8
1	K	317	GLN	2.8
1	H	321	ASP	2.8
1	H	2	GLU	2.8
1	A	277	LYS	2.7
1	H	320	SER	2.7
1	J	243	LYS	2.7
1	G	242	ASN	2.7
1	I	249	GLY	2.7
1	A	94	GLY	2.7
1	L	186	GLY	2.6
1	G	321	ASP	2.6
1	F	220	TYR	2.6
1	L	287	GLY	2.6
1	K	244	PHE	2.6
1	K	93	VAL	2.6
1	D	180	TYR	2.6
1	L	54	ASP	2.6
1	I	220	TYR	2.6
1	L	56	THR	2.6
1	C	279	LYS	2.5
1	L	290	ASP	2.5
1	A	229	ALA	2.5
1	H	244	PHE	2.5
1	I	89	LYS	2.5
1	E	243	LYS	2.5
1	A	276	THR	2.5
1	G	149	ASP	2.5
1	I	306	ASN	2.4
1	B	288	ASP	2.4
1	I	230	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	248	SER	2.4
1	J	217	GLY	2.4
1	I	286	ILE	2.4
1	A	216	THR	2.4
1	L	180	TYR	2.4
1	K	323	LYS	2.4
1	G	10	LYS	2.4
1	A	92	ASP	2.4
1	H	10	LYS	2.4
1	G	1	ALA	2.4
1	E	290	ASP	2.4
1	L	89	LYS	2.4
1	I	47	GLY	2.4
1	I	8	GLY	2.4
1	K	303	PHE	2.4
1	L	286	ILE	2.3
1	H	216	THR	2.3
1	J	288	ASP	2.3
1	I	10	LYS	2.3
1	L	282	ASP	2.3
1	K	188	VAL	2.3
1	B	290	ASP	2.3
1	H	271	PRO	2.3
1	I	262	GLN	2.3
1	I	218	LEU	2.3
1	I	187	ILE	2.3
1	H	183	GLU	2.3
1	L	92	ASP	2.3
1	A	144	PHE	2.3
1	A	275	TYR	2.3
1	G	109	LEU	2.2
1	I	1	ALA	2.2
1	H	218	LEU	2.2
1	G	140	ARG	2.2
1	F	221	ASP	2.2
1	I	49	THR	2.2
1	B	280	ALA	2.2
1	K	187	ILE	2.2
1	G	223	ASN	2.2
1	K	268	GLY	2.2
1	K	301	TYR	2.2
1	F	222	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	256	ASP	2.2
1	H	298	GLY	2.2
1	D	215	ALA	2.2
1	H	53	SER	2.2
1	J	250	PHE	2.2
1	I	48	GLU	2.2
1	K	286	ILE	2.2
1	J	290	ASP	2.2
1	L	280	ALA	2.2
1	L	324	LEU	2.2
1	I	290	ASP	2.2
1	J	186	GLY	2.2
1	C	320	SER	2.2
1	H	59	GLY	2.2
1	C	276	THR	2.2
1	E	250	PHE	2.2
1	A	93	VAL	2.1
1	J	230	ASN	2.1
1	G	287	GLY	2.1
1	G	186	GLY	2.1
1	K	304	ASN	2.1
1	J	181	GLU	2.1
1	L	321	ASP	2.1
1	A	108	ALA	2.1
1	G	107	ASP	2.1
1	J	242	ASN	2.1
1	G	225	ILE	2.1
1	L	187	ILE	2.1
1	G	241	THR	2.1
1	G	44	GLY	2.1
1	G	243	LYS	2.1
1	L	217	GLY	2.1
1	F	274	ALA	2.1
1	L	233	GLU	2.1
1	I	217	GLY	2.1
1	L	57	GLY	2.1
1	I	340	PHE	2.1
1	C	299	ALA	2.0
1	D	108	ALA	2.0
1	H	220	TYR	2.0
1	A	232	GLY	2.0
1	D	218	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	236	ASN	2.0
1	I	188	VAL	2.0
1	C	54	ASP	2.0
1	G	248	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.